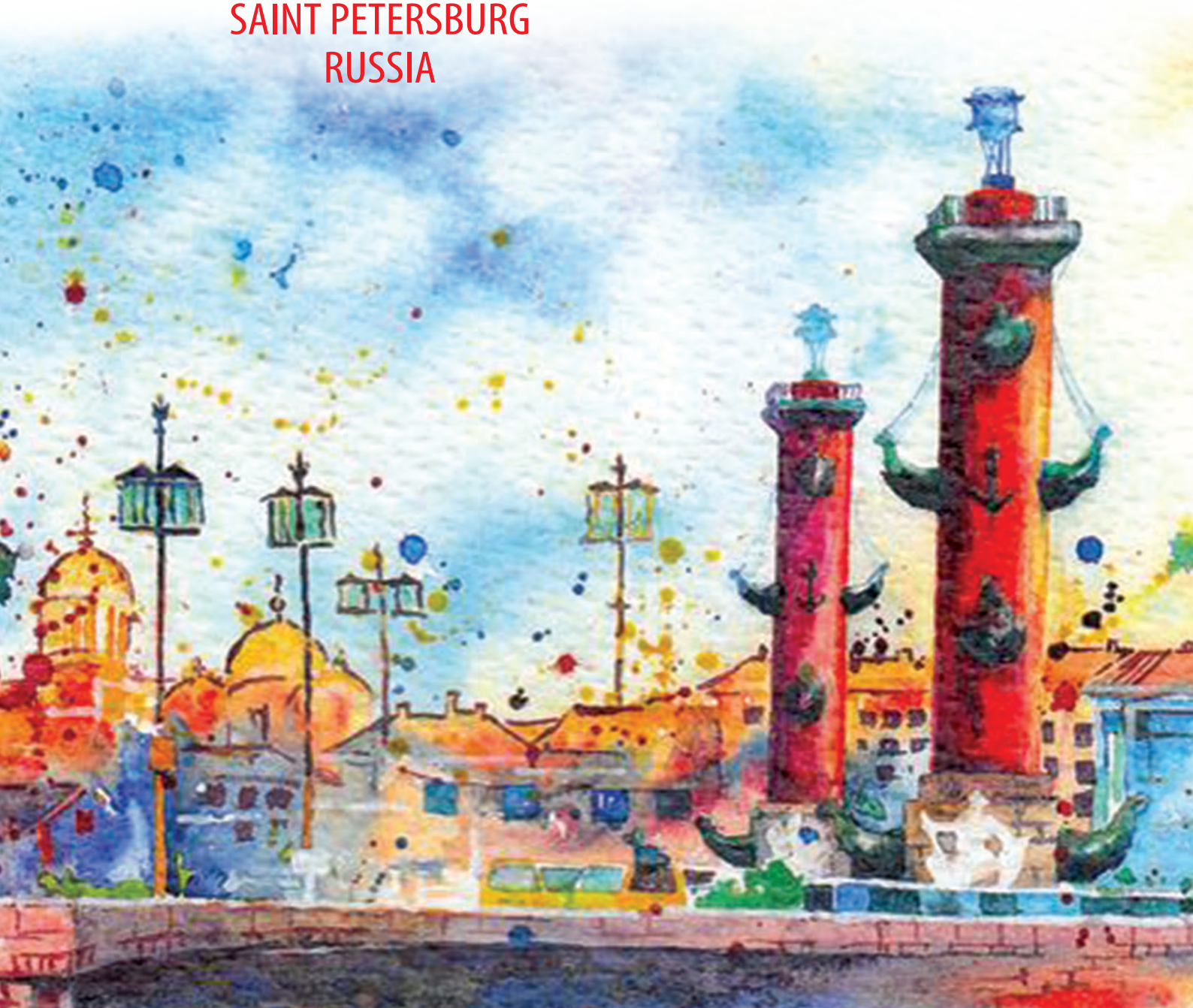
ABSTRACTS ECNS 2019

VII EUROPEAN CONFERENCE ON NEUTRON SCATTERING
June 30-July 5
St. Petersburg
RUSSIA
ECNS 2019

EUROPEAN CONFERENCE
ON
NEUTRON SCATTERING

JUNE 30-JULY 5, 2019

SAINT PETERSBURG
RUSSIA



CONTENTS

Monday, July 1st

VII European Conference on Neutron Scattering 2019 **Saint-Petersburg Hall, first floor** Chair: **Albert Furrer**				
09:00 – 09:45	Plenary lecture: **Ferenc Mezei** (ESS, Sweden) "Facets of neutron economy"			
09:45 – 10:30	Plenary lecture: **Giulia Festa** (CENTRO FERMI, Italy) "Neutrons for cultural heritage"			
	Neutron sources and facilities **Saint-Petersburg Hall, first floor** Chair: **Thomas Gutberlet**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Lucile Mangin-Thro**	**Functional Materials** **Pavlovsk Hall, ground floor** Chair: **Peter Mueller-Buschbaum**	**Engineering Applications** **Kronshtadt Hall, ground floor** Chair: **Ralph Gilles**
11:30 – 12:00	Invited talk **Valery Shvetsov** (JINR, Russia) "Pulsed Fast Reactor IBR-2 after Modernization"	Invited talk **Shibabrata Nandi** (JCNS (FZJ), Germany) "Superconductivity and magnetism in Fe pnictides"	Invited talk **Anatoly Balagurov** (JINR, Russia) "Cluster-like structure of Fe-based alloys with enhanced magnetostriction"	Invited talk **Gizo Bokuchava** (JINR, Russia) "Residual stress measurements using correlation RTOF (Fourier) diffractometry at long-pulse neutron source"
12:00 – 12:15	Invited talk **Robert McGreevy** (ISIS, UK) "ISIS - from TS1 to TS2 to ISIS-II"	Invited talk **Alistair Cameron** (TU Dresden, Germany) "Rotation of the magnetic vortex lattice in the noncentrosymmetric	Invited talk **Francoise Damay** (LLB, France) "$Fe_{3-x}Mn_xBO_5$: an extraordinarily rich magnetic phase diagram"	**Stefano Deledda** (Institute for Energy Technology, Norway) "Neutron Imaging study of Strontium Chloride Ammine system for Heat Storage"

12:15 – 12:30		superconductor Ru_7B_3"		**Christopher Garvey** (Malma University, Sweden) "1D Imaging of Flocculating and Sedimenting Particles"
12:30 – 12:45	**Stefan Mattauch** (JCNS (FZJ),Germany) "Latest developments of neutron scattering instruments of the JCNS at MLZ"	**Alexandre Ivanov** (ILL, France) "Anisotropy of magnetic excitations in iron-based superconductors"	**Katarzyna Rećko** (University of Białystok, Poland) "Magnetism of surface modified and gallium doped magnetite particles"	**Ranggi Sahmura Ramadhan** (Coventry University, UK) "High-resolution residual strain mapping by energy-dispersive neutron imaging"
12:45 – 13:00	**Winfried Petry** (MLZ - TUM, Germany) "High-density uranium fuel for high performance research reactors"	**Alexander Backs** (MLZ - TUM, Germany) "A multiscale approach to the formation of vortex lattice domains in the intermediate mixed state of the type-II/1 superconductor niobium"	**Mogens Christensen (**Aarhus University, Denmark) "Structure and Texture of Nanosized Magnetic Hexaferrites"	**Premysl Beran** (ESS ERIC, Sweden) "In-situ neutron diffraction study of Ni-addition influence on phase transformations in Co-Re-Cr high-temperature alloys"
13:00 – 13:15	**Tianfu Li** (China Institute of Atomic Energy, China) "Neutron Facilities at China Advanced Research Reactor"	**Mehmet Ramazanoglu** (Istanbul Technical University, Turkey, Brockhouse Institute for Materials Research, Canada) "Magnetic Excitations in The Cubic Superconductor CrRu"	**Jose Maria Porro (**BCM, Spain) "Powder and single crystal neutron diffraction in ferromagnetic shape memory alloys: structure vs magnetism"	**Cristian Dragolici** (IFIN-HH, Romania) "Cement-based materials for the conditioning of low and intermediate level radioactive waste: neutron scattering studies"

13:15 – 13:30	**Jamie Schulz** (Australian Centre for Neutron Scattering, Australian Nuclear Science & Technology Organisation, Australia) "Current status of OPAL, the Australian Research Reactor"	**Vladimir Dmitrienko** (Institute of Crystallography, FSRC, Crystallography and Photonics, RAS, Russia) "The Hidden Order in URu_2Si_2: Neutron scattering as a probe of intra-atomic anti-toroidal vortices"	**Uliana Koneva** (Immanuel Kant Baltic Federal University, Russia) "GISAS studies of the shape, size and layout of silicon nanowhiskers"	**Joana Rebelo Kornmeier** (MLZ - TUM, Germany) "Non-destructive neutron surface and high spatial resolved residual stress analysis"
	Special 25th anniversary ENSA session **Saint-Petersburg Hall, first floor**			
14:45 – 14:55	Welcome by **Christiane Alba-Simonesco**, ENSA Chair			
14:55 – 15:10	**Peter Gehring**, NSSA Vice-President, Overview of the NSSA activity			
15:10 – 15:25	**Brendan J. Kennedy**, AONSA President, Overview of the AONSA activity			
15:25 – 15:40	**Andrew Venter**, NESCA, South Africa, Vision of the Neutron Scattering in Africa			
15:40 – 16:25	**2019 Walter Hälg Prize** of the ENSA: awarding ceremony **Lecture** by the 2019 Walter Hälg Prize Winner			
16:25 – 16:55	**Neutron Instrumentation and Innovation Award** of the ENSA: awarding ceremony **Lecture** by the 2019 NI&I Award Winner			

17:55 – 17:20	**Medal of the Russian Neutron Scattering Society** for “Outstanding Achievements in the field of Neutron Scattering”: awarding ceremony **Lecture** by the 2019 RNSS Medal Winner
17:20 – 17:25	**Peter Müller-Buschbaum,** Heinz Maier-Leibnitz Zentrum (MLZ): platinum sponsor of ECNS 2019
17:25 – 17:30	**Michael Schneider,** Swissneutronics (platinum sponsor of ECNS 2019) “20 Years of Swiss Quality for Excellence in Neutron Science“

Tuesday, July 2nd

VII European Conference on Neutron Scattering 2019 **Saint-Petersburg Hall, first floor** Chair: **Laszlo Rosta**				
09:00 – 09:45	Plenary lecture: **Tatiana Guidi** (ISIS, UK) "Neutron scattering techniques for molecular magnetism"			
09:45 – 10:30	Plenary lecture: **Boris Toperverg** (NRC "Kurchatov Institute – PNPI", Russia) "Advances and perspectives of 3D neutron reflectometry in nanomagnetism, soft matter and life sciences"			
	Neutron Instrumentation **Saint-Petersburg Hall, first floor** Chair: **Ken Andersen**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Grégory Chaboussant**	**Soft Matter** **Pavlovsk Hall, ground floor** Chair: **Margarita Kruteva**	**Thin Films and Interfaces** **Kronshtadt Hall, ground floor** Chair: **Maximilian Wolff**
11:30 – 12:00	Invited talk **Sergey Kichanov** (JINR, Dubna, Russia) "Neutron imaging at long-pulse sources: opportunities, results and perspectives"	Invited talk **Beatrice Grenier** (ILL, France) "Tomonaga-Luttinger liquid spin dynamics in the quasi-one dimensional Ising-like antiferromagnet $BaCo_2V_2O_8$"	Invited talk **Anne-Caroline Génix** (Université Montpellier, France) "Structure of adsorbed layers and of chains in polymer nanocomposites"	Invited talk **Nina-Juliane Steinke** (ISIS Neutron and Muon Source, UK) "Magnetic order in topological insulator thin films: transition metal and rare earth doping"

12:00 – 12:30	Invited talk **Francesco Piscitelli** (ESS, Sweden) "Detector developments in BrightnESS: beyond the limits of the current detector technologies for neutron scattering science"	**Petronella Pascale Deen** (ESS, Sweden) "Towards and understanding of the magnetocaloric effect"	**Jaques Jestin** (LLB, France) "SANS/USANS tunable multiscale nanoparticle ordering by polymer crystallization"	Invited talk **Yuri Nikitenko** (JINR, Dubna, Russia) "Reflectometry with registration of secondary radiation at total neutron reflection"
		Stephane Raymond (Université Grenoble Alpes, France) "Spin Fluctuations Drive the Inverse Magnetocaloric Effect in Mn_5Si_3"	**Karyn Wilde** (Australian Nuclear Science & Technology Organisation, Australia) "New Horizons for Molecular Deuteration: Diversity in Molecules and Applications"	
12:30 – 12:45	**Laurence Noirez** (LLB, France) "Using Light to see Neutrons: a new 2D detector with high resolution"	**Henrik Jacobsen** (Oxford University, UK) "Strong quantum fluctuations co-existing with magnetic order in a pyrochlore iridate"	**Andrea Orecchini** (University degli Studi di Perugia, Italy) "Low-temperature Dynamical Transition in Concentrated Microgels"	**Aljosa Hafner** (Universite Libre de Bruxelles, Belgium, ILL, France) "Instabilities of buried polymer layers studied by specular and off-specular neutron reflectometry"
12:45 – 13:00	**Julien Marchal** (ILL, France) "Development of a large cylindrical Trench-MWPC detector for XTremeD neutron diffraction instrument"	**Astrid Schneidewind** (JCNS/MLZ, Germany) "Spin-wave dispersions in the antiferromagnetic phase AF1 of $MnWO_4$ based on the polar atomistic model in P2"	**Maria Aranzazu Arbe** (Centro de Física De Materiales CSIC-UPV/EHU, Spain) "Melts of Single-Chain Polymeric Nano-Particles: Exploring the Impact of Intra-Molecular Cross-Linking by Neutron Scattering, Dielectric Spectroscopy and Rheology"	**Lucas Kreuzer** (TUM - MLZ, Germany) "Phase transition kinetics in a doubly thermo-responsive block copolymer thin film followed with in-situ neutron reflectometry"

13:00 – 13:15	**Sebastian Jaksch** (JCNS (FZJ), Germany) "SoNDe high-flux neutron detector"	**Markos Skoulatos** (MLZ and Physics Department, TUM, Germany) "Putative spin-nematic phase in $BaCdVO(PO_4)_2$"	**Kell Mortensen** (NBI, University of Copenhagen, Denmark) "SANS studies of star-polymers and star-polymer gels exposed to stretch"	**Alessandra Luchini** (Niels Bohr Institute, University of Copenhagen, Denmark) "The role of phosphatidylserine lipids in tuning membrane protein domain location in supported membranes"
13:15 – 13:30	**Bruno Guerard** (ILL, France) "New prospects in ^3He detector techniques"	**Arsen Goukassov** (LLB, France) " Local susceptibility of frustrated pyrochlores. Polarized Neutrons and Point Charge model."	**Daria Noferini** (JCNS at MLZ) "Disentangling polymer network and hydration water dynamics in pHEMA physical and chemical hydrogels"	**Thomas Saerbeck** (ILL, France) "Artificially Designed Magnetic Domain Patterns Investigated by Neutron Scattering"
15:00 – 16:00	Exhibition (**Ground floor lobby, center**) **Poster Session 1** (**Ground floor lobby**) ***1. Neutron Instrumentation, Optics, Sample Environment, Detectors and Software;*** ***2. Neutron Sources and Facilities;*** ***3. Fundamental Science***		**Pavlovsk Hall, ground floor** **Peter Willendrup** (Technical University of Denmark, Denmark) "An online demo of the e-neutrons.org learning platform"	

	Neutron Instrumentation **Saint-Petersburg Hall, first floor** Chair: **Alexander Ioffe**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Arsen Goukassov**	**Functional Material** **Pavlovsk Hall, ground floor** Chair: **Francoise Damay**	**Disordered Systems and Liquids** **Kronshtadt Hall, ground floor** Chair: **Wim G. Bouwman**
16:00 – 16:30	Invited talk **Peter Konik** (NRC KI – PNPI, Russia) "Neutron guide system of the reactor PIK"	Invited talk **Quentin Faure** (University Grenoble Alpes, France) "Topological quantum phase transition in the Ising-like antiferromagnetic spin chain $BaCo_2V_2O_8$"	Invited talk **Karin Schmalzl** (JCNS (FZJ),Germany) "Insights into the magnetocaloric effect in $MnFe_4Si_3$ gained with inelastic neutron scattering"	Invited talk **Aleksander Matic** (Chalmers University of Technology, Sweden) "Structured liquids"
16:30 – 16:45	**Mark Johnson** (ILL, France) "ILL Modernisation Programme: Endurance. The ambitious renewal of the H15 cold neutron guide and instrumentation"	**Irina Safiulina** (ILL, France) "Magnetic excitations of a new potential spin liquid"	**Alexandra Franz** (Helmholtz-Zentrum Berlin, Germany) "$FAPbBr_3$ - about the influence of deuteration: A temperature dependent neutron diffraction study"	**Laszlo Almasy** (Southwest University of Science and Technology, China) "Molecular aggregation in binary mixtures of cyclic amines with water: Thermodynamic, SANS and theoretical studies"
16:45 – 17:00	**Nikolay Pleshanov** (NRC KI - PNPI, Russia) "Mirror flippers: experiments and possible applications"	**Artem Korshunov** (NRC KI - PNPI, Russia) "Short-range and long-range ordering on the quasi-2D honeycomb layered $Na_2Ni_2TeO_6$"	**Fanni Juranyi** (Paul Scherrer Institut, Switzerland) "Water captured in the polysaccharide network of chia mucilage"	**Sandrine Lyonnard** (SyMMES, CEA-CNRS-UGA, France) "Ion dynamics in nanostructured ionic liquid crystals by QENS"

17:30 – 17:45	**Felix J Villacorta** (Consorcio ESS-Bilbao, Spain) "Neutron guide design optimization of MIRACLES, the time-of-flight / backscattering spectrometer at the European Spallation Source"	**Alexander Tsirlin** (University of Augsburg, Germany) "Breaking and re-arrangement of valence bonds in the triangular spin liquid $YbMgGaO_4$"	**Peter Mueller-Buschbaum** (TUM – MLZ, Germany) "Next generation solar cells studied with GISANS"	**Olexander Tomchuk** (JINR, Russia) "About the size cut-off effect on small-angle scattering from stochastic mass fractals"
17:45 – 18:00	**Pierre Courtois** (ILL, France) "Recent achievements in Neutron Optics at the ILL"	**Marc Seifert** (MLZ, TUM, Germany) "Neutron Depolarization Measurements of Quantum Critical Ferromagnets"	**Monica-Elisabeta Lacatusu** (Technical University of Denmark, Denmark) "Neutron imaging study of degradation in commercial Li-ion batteries"	**Anne Stunault** (ILL, France) "D3 at the ILL: structural studies of hydrogenous liquid and amorphous systems using polarised neutrons"
18:00 – 18:15	**Alexandre Petoukhov** (ILL, France) "Project of advanced solid-state polarizer for PF1B"	**Heiko Trepka** (MPI for Solid State Research, Germany) "Critical scattering in classical and quantum critical systems"	**P. Klaus Pranzas** (Helmholtz-Zentrum Geesthacht, Germany) "Characterisation of hydrogen storage materials with neutron imaging and scattering techniques"	**Reiner Zorn** (Juelich Centre for Neutron Science, Germany) "Cooperativity Length in a Glass-Forming Liquid Determined by a Combination of Neutron Spin Echo Spectroscopy and Calorimetric Methods"
18:15 – 18:30	**Vladislav Syromyatnikov** (NRC KI – PNPI, Russia) "New neutron supermirror polarizer"	**Stanislav Nikitin** (Max Planck Institute for Chemical Physics of Solids, Germany) "Pressure-induced evolution of magnetic excitations in CeCoSi"	**Maths Karlsson** (Chalmers University of Technology, Sweden) "Local structure and dynamics of metal hydride-reduced $BaTiO_3$ samples investigated with inelastic and quasielastic neutron scattering"	**SoHyun Park** (Ludwig-Maximilians-Universität München, Germany) "Proton dynamic behaviour in hydrogen bond networks in oxyhydroxides"

18:30 – 18:45	**Thierry Bigault** (ILL, France) "Mass production of neutron polarizing supermirrors for the WASP instrument at the ILL"	Invited talk **Lucile Mangin-Thro** (ILL, France) "High-Tc superconductors and frustrated magnets on the D7 instrument at the ILL"	Invited talk **Michail Avdeev** (JINR, Russia) "Nanoscale structure of electrochemical interfaces for lithium power sources by neutron scattering"	**Igor Gapon** (JINR, Russia) "Impact of the external magnetic and electric fields on behavior of ferrofluids at interfaces: neutron reflectometry data"
18:45 – 19:00	**Sergey Klimko** (LLB, France) "Development and first test on large angle RF-flipper"			**Artur Glavic** (Aarhus University, Denmark) "Structure and Slow Dynamics in Spontelectric Methyl-Formate"

Wednesday, July 3rd

VII European Conference on Neutron Scattering 2019 **Saint-Petersburg Hall, first floor** Chair: **Andreas Schreyer**				
09:00 – 09:45	Plenary lecture: **Katia Pappas** (TU Delft, Netherland) "Novel spiral and skyrmionic states"			
09:45 – 10:30	Plenary lecture: **Richard A. Campbell** (University of Manchester, UK) "Oppositely Charged Polyelectrolyte/Surfactant Mixtures at the Air/Water Interface: Dominance of Non-equilibrium Effects"			
	Neutron Instrumentation **Peterhof Hall, ground floor** Chair: **Stefan Mattauch**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Astrid Schneidewind**	**Soft Matter** **Pavlovsk Hall, ground floor** Chair: **Kell Mortensen**	**Neutron sources and facilities** **Kronshtadt Hall, ground floor** Chair: **Ferenc Mezei**
11:30 – 12:00	Invited talk **Earl Babcock** (JCNS& MLZ, Germany) "Ultra Wide angle 3He polarization analysis for neutron spectroscopy, PASTIS on NEAT"	Invited talk **Albert Furrer** (Swiss Neutronics AG and PSI, Switzerland) "High-Tc Ferromagnetic Semiconductors: Fake or Fact?"	Invited talk **Martin Dulle** (JCNS (FZJ), Germany) "Quasicrystals from block copolymer micelles"	Invited talk **Ken Andersen** (ESS ERIC, Sweden) "Towards the full instrument suite of the European Spallation Source"
12:00 – 12:15	**Goran Nilsen** (ISIS Neutron and Muon Facility, UK) "Uniaxial polarization analysis on the LET time-of-flight spectrometer: first results"	**Denis Salamatin** (JINR, VIHPP, Russia) "Study of high-pressure cubic phase of $RGe_{2.85}$ (R = Tb, Dy) by neutron diffraction"	**Andrew J. Jackson** (ESS, Sweden) "Self-assembly in deep eutectic solvents: from surfactant aggregation to protein folding"	**Helen Walker** (ISIS, UK) "Recent instrument developments in the Excitations Group at ISIS"

12:15 – 12:30	**Holly McPhillips** (ISIS Neutron and Muon Source, UK) "Development of hyperpolarized helium-3 spin-filters for polarised neutron experiments at the ISIS neutron and muon source"	**Stanislav Podchezertsev** (ILL, France) "Magnetic ordering features of the $Co_{5-x}Zn_xTeO_8$ spinel-type series"	**Maximilian Wolff** (Uppsala University, Sweden) "Solid-liquid interfaces: New insights and future opportunities"	**Ken Andersen and Luca Zanini** (ESS ERIC, Sweden) "Neutronic Design of the Bunker Shielding for the European Spallation Source"
12:30 – 12:45	**Avishek Maity** (Institute of physical chemistry, University of Goettingen, Germany) "Novel type polarization analysis using multi-analyzer setup @ PUMA, FRM II"	**Henry Fischer** (ILL, France) "Magnetic frustration in $SrLn_2O_4$ compounds studied by magnetic PDF-analysis"	**Nico Carl** (ILL, France) "Controlling self-assembly with light"	**Konstantin Pavlov** (NRC KI - PNPI) "Simulations of neutron scattering instruments at a compact source"
12:45 – 13:00	**Takuya Okudaira** (J-PARC Japan Atomic Energy Agency, Japan) "Polarized pulsed neutrons using a ^{3}He spin filter with an in-site SEOP method"	**Werner Schweika** (ESS, Sweden) "Chiral spin liquid ground state in a highly frustrated extended kagome system"	**Vyacheslav Molchanov** (MSU, Russia) "Self-assembled soft network of hybrid chains"	**Jorg Voigt** (JCNS, FZJ GmbH, Germany) "Compact Spectrometers for Compact Neutron Sources"
13:00 – 13:15	**Valery Nesvizhevsky** (ILL, France) "Fluorinated nanodiamonds as unique neutron reflector"	**Manila Songvilay** (University of Edinburgh, SPA, UK) "Anharmonic magnon excitations in non-collinear and charge-ordered RbFe2+Fe3+F6"	**Philipp Gutfreund** (ILL, France) "Microscopic structure and dynamics of entangled polymers under shear flow - What neutrons can see"	Invited talk **Thomas Gutberlet** (JCNS, Jülich, Germany) "Making ESS a success - A Landscape of European accelerator based neutron sources"

<table>
<tr><td>13:15 – 13:30</td><td>Kirill Zhernenkov (JCNS, FZJ, MLZ, Germany) MARIA - The high-intensity polarized neutron reflectometer of JCNS</td><td>Ketty Beauvois (CEA, INAC/MEM-MDN, France) “Emergence of a dimer physics in the Cairo frustrated pentagonal magnet $Bi_2Fe_4O_9$”</td><td>Ruslan Smyslov (NRC KI – PNPI, Russia) “Nanocomposites based on Kamagataeibacter xylinus cellulose: Neutron studies”</td><td></td></tr>
<tr><td rowspan="6">15:00 – 16:00</td><td colspan="2" rowspan="6">Exhibition (Ground floor lobby, center)
Poster Session 2 (Ground floor lobby, left side)
1. Soft Condensed Matter
2. Disordered systems & Liquids
3. Life Sciences
4. Cultural Heritage and Archaeometry</td><td colspan="2">Special session “Instrumental program and international cooperation around reactor PIK”
Kronstadt Hall, ground floor</td></tr>
<tr><td colspan="2">V.Voronin (PNPI NRC KI) Russian national state program: recent progress</td></tr>
<tr><td colspan="2">V. Tarnavich (PNPI NRC KI) Instrument base of reactor PIK: perspectives</td></tr>
<tr><td colspan="2">M. Muller, A.Ioffe, W.Petry (MLZ: HZG, FZJ, TUM) Instrumental plans of German partners</td></tr>
<tr><td colspan="2">S. Mattauch (JCNS/FZJ) Potential contribution to PIK from CREMLIN+</td></tr>
<tr><td colspan="2">S.Grigoriev (PNPI NRC KI) PIK neutron facility as international interdisciplinary laboratory</td></tr>
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	Neutron Instrumentation **Peterhof Hall, ground floor** Chair: **Markus Strobl**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Werner Schweika**	**Soft Matter** **Pavlovsk Hall, ground floor** Chair: **Anne-Caroline Génix**	**Solid State Chemistry** **Kronshtadt Hall, ground floor** Chair: **Anatoly Balagurov**
16:00 – 16:30	Invited talk **Margarita Russina** (HZB, Germany) "Implementation of polarized neutron spectroscopy on TOF spectrometer NEAT at Helmholtz Zentrum Berlin"	Invited talk **Marisa Medarde Barragan** (PSI, Switzerland) "Stabilizing magnetic spirals in layered perovskites far beyond room temperature"	Invited talk **Artem Feoktystov** (JCNS, MLZ, Germany) "Magnetic nanoparticles: from self-assembly to drug targeting"	Invited talk **Sergey Ya. Istomin** (MSU, Russia) "Tuning the high-temperature thermal expansion properties of perovskite-related Co-containing oxides"
16:30 – 16:45	**Alexandre Bertin** (Institute of Solid State Physics, TU Dresden, Germany) "Bambus: a new inelastic neutron multiplexed analyzer for Panda at MLZ"	**Igor Zobkalo** (NRC KI – PNPI, Russia) "Control of magnetic chirality in $Nd_{1-x}TbxMn_2O_5$ by external electric field"	**Margarita Kruteva** (JCNS/FZJ, Germany) "Synthetic platform for the encapsulation of nanocrystals with covalently bound polymer shells"	Invited talk **Anatoliy Senyshyn** (MLZ, Germany) "Lithium diffusion pathways in modern solid state Li conductors"
16:45 – 17:00	**Stephane Rols** (ILL, France) "PANTHER: the new thermal time of flight spectrometer at the ILL"	**Tim Tejsner** (ILL, France) "Anomalous lattice dynamics in $La_{(2-x)}Sr_{(x)}CuO_{(4+y)}$: The role of static and mobile dopants"	**Volker Koerstgens** (TUM, Germany) "Hybrid solar cells with laser-ablated titania: morphology investigation of the active layer with TOF-GISANS"	

17:30 – 17:45	**Bernhard Frick** (ILL, France) "IN16B - a most versatile high flux neutron backscattering spectrometer"	**Niels Bech Christensen** (TUD, Denmark) "Magnetic and magnetoelectric phases of $LiNiPO_4$ up to 55T"	**Tom Arnold** (University of Birmingham, UK) "Adsorption and interactions of polymer stabilised lipid nanodiscs with air-liquid and solid-liquid interfaces"	**Brendan Kennedy** (University of Sydney, Australia) "Magneto-Structural Relationships in 4d and 5d Oxides"
17:45 – 18:00	**Jakob Lass** (University of Copenhagen, Denmark) "CAMEA - A novel neutron spectrometer for extreme environment investigations"	**J. Alberto Rodrigues Velamazan** (ILL, France) "Effect of chemical substitution on the magneto-electric coupling of the $(ND_4)_2[FeCl_5(D_2O)]$ hybrid multiferroic"	**Hideki Seto** (CROSS Neutron Science and Technology Center, Japan) "Dynamical behaviour of hydration water between lipid bilayers"	**Holger Kohlmann** (Leipzig University, Germany) "In situ investigation of hydrogenation reactions by neutron powder diffraction"
18:00 – 18:15	**Matteo Zanetti** (CNR, Italia, ISIS Facility, UK) "Crystal Analysers for Indirect-Geometry Broadband Neutron Spectrometers: Adding Reality to Idealised Design"	**Navid Qureshi** (ILL, France) "Proof of the elusive high-temperature incommensurate phase in CuO by spherical neutron polarimetry"	**Wim G. Bouwman** (Faculty of Applied Sciences, Delft University of Technology, Netherlands) "Rational design of food processing methods with aid of neutron scattering"	**Andrea Piovano** (ILL, France) "Understanding the microscopic origin of oxygen diffusion in ion conductors with complex structure"

18:15 – 18:30	**Marcus Appel** (ILL, France) "The BATS option for inverted TOF-Backscattering on IN16B: Design, performance and on going upgrades with variable focusing optics"	**Alexei Belik** (National Institute for Materials Science, Japan) "Unusual Spin Structures in Quadruple and Simple Exotic Perovskites"	**Eleonore Mason** (University of Bath, UK) "Localisation of Membrane Components in Lipid Cubic Phases"	**Felix Fernandez-Alonso** (ISIS, University College London, UK) "Recent Advances in Molecular Spectroscopy at the ISIS Pulsed Neutron & Muon Source"
18:30 – 18:45	**Jeroen Plomp** (Delft University of Technology, Netherlands) "LARMOR a TOF instrument with many modes"	**Petr Cermak** (Charles University, Czech Republic) "Neutrons as a key method for accessing magnetoelastic effects"	**Loreto Misuraca** (ILL, France) "Protomembranes at the origin of life"	**Egor Vezhlev** (JCNS & MLZ) "Neutron Depth profiling at a focused neutron beam: a method of choice to study Li-ion transport in solid state batteries"
18:45 – 19:00	**Victor Bodnarchuk** (JINR, Russia) "Background suppression in neutron scattering experiments at the pulsed IBR-2 reactor by set of choppers"	**Claire V. Colin** (Institut Neel, CNRS, University Grenoble-Alpes, France) "Magnetic structure and magnetic excitations in the multiferroic pyroxene $SrMnGe_2O_6$"	**Kevin Pounot** (ILL, France) "Protein dynamics and diffusion followed during aggregates formation by time-resolved quasi-elastic neutron scattering"	**Palmerina Gonzalez-Izquierdo** (ILL, France) "Magneto-structural correlations, thermal evolution, ionic conductivity and catalytical activity for the pet glycolysis of the (trimim)$[FeCl_4]$ halometallate compound"

Thursday, July 4th

VII European Conference on Neutron Scattering 2019 **Saint-Petersburg Hall, first floor** Chair: **Jiri Kulda**				
09:00 – 09:45	Plenary lecture: **Anne Martel** (ILL, France) "SANS and biology: peptides, proteins in solutions and complexes"			
09:45 – 10:30	Plenary lecture: **Denis Kozlenko** (JINR, Russia) "Neutron scattering under high pressure: towards half-Megabar pressure scale"			
	Neutron Instrumentation **Saint-Petersburg Hall, first floor** Chair: **Vyacheslav Em**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Jonathan White**	**Life Sciences** **Pavlovsk Hall, ground floor** Chair: **Jorg Pieper**	**Planetary Sciences and Extreme Conditions** **Kronstadt Hall, ground floor** Chair: **Denis Kozlenko**
11:30 – 12:00	Invited talk **Robert Bewley** (ISIS, UK) "FARO: A new type of neutron spectrometer with Flux And Resolution Optimised"	Invited talk **Evgeny Kravtsov** (IPM, Russia) "Magnetism of rare-earth/transition metal multilayers"	Invited talk **Andreas Stadler** (JCNS (FZJ), Jülich, Germany) Structure and Dynamics of Intrinsically Disordered and Unfolded Proteins: Insights Gained by Neutron Scattering	Invited talk **Fabienne Duc** (LNCMI, France) Neutron Diffraction in High Magnetic Fields: Application to the heavy fermions systems $U(Ru_{1-x}Rh_x)_2Si_2$
12:00 – 12:30	Invited talk **Gordon J. Kearley**, (Uni.Coll. Dublin, Ireland) "Quasi elastic neutron scattering - could there be another way?"	**Igor Golosovsky** (NRC KI - PNPI, Russia) "Complex magnetic order in the Nd(Tb)Fe3(BO3)4 multiferroic revealed by the single crystal neutron diffraction"	**Martin Schmiele** (University of Copenhagen, Denmark) "Nanostructured lipid carriers for fish oil - A small angle neutron scattering study"	**Alexandre Ivanov** (ILL, France) "High-pressure cells for inelastic neutron scattering studies of proton dynamics in materials"

		Damaris Tartarotti Maimone (PSI, Switzerland) “Evidence for new mechanism of antiferromagnetic domain selection driven by spin-orbit coupling”	**Robert W. Corkery** (Royal Institute of Technology, Sweden, Australian National University, Australia) “Photosynthetic membranes in live cells and organelles studied using SANS”	**Christian Scheffzük** (Institute of Applied Geosciences KIT, Germany, JINR, Dubna, Russia) “Triaxial in situ deformation experiments with pore pressure on a sandstone sample using neutron time-of-flight diffraction at the EPSILON diffractometer”
12:30 – 12:45	**Olaf Holderer** (JCNS (FZJ), Germany) “The new high-resolution neutron spin echo spectrometer J-NSE “PHOENIX” at MLZ”	**Mikael Twengstrum** (Royal Institute of Technology, Sweden) “Zone center physics in magnetic diffuse neutron scattering”	**Marija Dubackic** (Lund University, Sweden) “Small angle neutron scattering study of protein-lipid co-assembly”	**John Loveday** (ESS, Sweden) “High-pressure neutron diffraction: state-of-the-art at the SNS and near future opportunities at the ESS”
12:45 – 13:00	**Peter Falus** (ILL, France) “WASP, the Widest Angle SPin echo spectrometer”	**Yurii Kibalin** (LLB, France) “Rietveld method for polarized neutron powder diffraction”	**Emilie Mahieu** (Institute of Structural Biology, France) “Observing a cellular protein unfolding and degradation machine at work: a time-resolved small-angle neutron scattering study”	**Tatiana I. Ivankina** (JINR, Russia) “To the problem of granite monuments desintegration: structural, texture, ultrasonic and permeability measurements”
13:00 – 13:15	**Markus Strobl** (PSI, Switzerland) “Mapping Small Angle Scattering with Image Resolution in Dark-Field Contrast Imaging”	**Tobias Neuwirth** (MLZ, TUM, Germany) "Embossing induced internal stress in electrical steel sheets”	**Renata Unnep** (Wigner Research Centre for Physics, Hungary) “Low-pH and desiccating induced reorganizations of thylakoid membranes - as revealed by small-angle neutron scattering”	**Valery Shvetsov** (JINR, Russia) “Determination of the planetary soil composition by means of neutron and gamma Detectors”

13:15 – 13:30	**Pavel Trtik** (Paul Scherrer Institut, Switzerland) "Neutron Microtomography"	**Thomas Saerbeck** (ILL, France) "Using polarized neutron reflectometry to study the layer integrity of annealed MgO/CoFeB magnetic tunnel junctions with W diffusion barriers"	**Francois Boue** (INRA-UMR, France) "Monitoring food structure during digestion using small-angle scattering and imaging techniques"	
14:30– 15:00	**Special session "Education and Training for Neutron Scattering" Kronstadt Hall, ground floor**			
	Greetings from officials of Saint-Petersburg State University			
15:00 – 16:00	Exhibition (**Ground floor lobby, center**) **Poster Session 3** (**Ground floor lobby, left side**) 1. ***Magnetism, multiferroics, skyrmions, superconductivity*** 2. ***Solid State Chemistry*** 3. ***Planetary Sciences and Extreme Conditions*** 4. ***Functional Materials*** 5. ***Engineering Applications*** 6. ***Thin Films and Interfaces***			**Beatrice Grenier** (ILL, Grenoble) "HERCULES schools: intensive training in neutrons and synchrotron radiation"
				Adél Len (BNC, Hungary) "20 Years of Hands-on Training on Neutron Techniques at the Budapest Neutron Centre"
				Linda Udby (Niels Bohr Institute, Denmark) "E-learning neutron scattering"
				Sergey Grigoriev (NRC KI - PNPI, Russia) "Master program on neutron scattering at Saint-Petersburg State University"
				Elena Abrosimova (JCNS, Germany) "German-Russian Roadmap: educational aspects"

	Neutron Instrumentation **Saint-Petersburg Hall, first floor** Chair: **Bob Cubitt**	**Magnetism and Superconductivity** **Gatchina Hall, ground floor** Chair: **Vladimir Dmitrienko**	**Life Sciences** **Pavlovsk Hall, ground floor** Chair: **Anne Martel**	**Fundamental Science** **Kronstadt Hall, ground floor** Chair: **Valery Nesvizhevsky**
16:00 – 16:30	Invited talk **Vyacheslav Em** (NRC KI, Russia) "New instruments for materials engineering STRESS and DRAKON at reactor IR-8: performance and first results"	Invited talk **Evgeny Altynbayev** (NRC KI - PNPI, Russia) "Skyrmion lattice in Fe-doped MnGe compounds"	Invited talk **Elizabeth Kelley** (NIST, USA) "Insights into lipid membrane dynamics from neutron scattering"	Invited talk Anatolii Serebrov (NRC KI - PNPI, Russia) "Research program of fundamental interactions at PIK reactor"
16:30 – 16:45	**Michael Heere** (IAM-ESS, KIT, MLZ, TU Munchen, Germany) "New developments in the fast neutron powder diffraction instrument ErwiN at MLZ"	**Victor Ukleev** (LNS PSI, Switzerland) "Complementary study of magnetic frustration in $Co_7Zn_7Mn_6$ chiral magnet by muons, neutrons and X-rays"	**Dubackic Peters** (University Grenoble Alpes LiPhy, ILL, France) "Pressure effects on the protein dynamical transition"	Invited talk **Bastian Märkisch** (TUM, Germany) "No Dark Side to Neutron Decay"
16:45 – 17:00	**Xavier Fabreges** (LLB, France) "MAGiC: a polarized diffractometer at ESS"	**Marta Crisanti** (ILL, France) "The power of small angle neutron scattering for the study of skyrmionic systems"	**Ralf Biehl** (JCNS FZJ, Germany) "Protein Domain Motions as seen by Neutron Spinecho Spectroscopy"	

17:00 – 17:15	**Evgeny Lukin** (JINR, Russia) "DN-6 diffractometer for studies of microsamples at ultrahigh pressures"	**Denis Mettus** (TU Munchen, Germany) "Kinetic small-angle neutron scattering of skyrmion lattice order in chiral magnets"	**Sebastian Jaksch** (JCNS & HMLZ, Germany) "In-plane dynamics of phospholipid membranes"	**Egor Lychagin** (JINR, Russia) "A powerful UCN source at an external beam of thermal neutrons at the PIK reactor"
17:15 – 17:30	**Thomas Keller** (Max Planck Institute for Solid State Research, Germany) "Neutron Larmor Diffraction on samples in magnetic field"	**Tobias Weber, Paul Steffens** (ILL, France) "Polarization analysis of the skyrmion dynamics in MnSi"	**Stephan Longeville** (LLB, France) "Compression of flexible chain due to macromolecular and its biological implications"	**Vladimir Hutanu** (RWTH Aachen University, JCNS & MLZ, Germany) "Measuring T-odd effects in the neutron induced fission of ^{235}U using thermal and hot polarized neutrons on the beamline POLI at MLZ"
17:30 – 17:45	**Ravil Sadykov** (INR RAS, Russia) "Nonmagneic high pressure piston-cylinder type clamp cells for neutron scattering"	**Jonathan White** (PSI, Switzerland) "Multiple-q noncollinear magnetism in the itinerant hexagonal magnet $Y_3Co_8Sn_4$"	**Maria Grazia Ortore** (DLES - Università Politecnica delle Marche, Italia) "Amyloid OI-peptides interaction with model membranes: when dynamics matters"	**Rene Sedmik** (TU Wien / Atominstitut, Austria) "Ramsey Gravity Resonance Spectrosopy with Ultracold Neutrons"

17:45 – 18:00	**Andrew Sazonov** (DMSC ESS, Denmark) "Visualization and Processing of Single-Crystal Diffraction Data Measured with a Point Detector using Davinci Software"	**Isabelle Mirebeau** (LLB, University Paris-Saclay, CEA, France) "Spin textures induced by quenched disorder in a reentrant spin glass: vortices versus frustrated skyrmions"	**Livia Balacescu** (IA, RWTH Aachen, Germany) "Nanosecond dynamics of biopolymers: a comparative neutron spin echo study on folding intermediates of apo-myoglobin"	**German Kulin** (JINR, Russia) "On observation of the Goos-Hanchen shift of a neutron beam"
18:00 – 18:30	Invited talk **Vladimir Luzin** (ANSTO, Australia) "Neutron Diffraction Stress Analysis Down Under: 10 Year Experience in Industrial and Scientific Applications"	Invited talk **Nicolas Martin** (LLB, France) "Liquid crystalline structures and elasticity in a cubic chiral helimagnet"	**Antonio Benedetto** (School of Physics, University College Dublin, Ireland) "High-resolution neutron scattering data reveal the decoupling of proteins and water at the dynamical transition"	Invited talk **Alexander Frank** (JINR, Russia) "Neutron wave in matter - open questions"

Friday, July 5th

VII European Conference on Neutron Scattering 2019 **Saint-Petersburg Hall, first floor** Chair: **Katia Pappas**				
09:00 – 09:45	Plenary lecture: **Valentin Gordeliy** (Université Grenoble Alpes, France) "Structure and mechanisms of membrane proteins and their importance for medicine"			
09:45 – 10:30	Plenary lecture: **Ralph Gilles** (MLZ – TUM, Germany) "How neutrons support technical developments in the field of gas turbines and batteries"			
	Neutron Instrumentation **Saint-Petersburg Hall, first floor** Chair: **Winfried Petry**	**Cultural Heritage and Archaeometry** **Gatchina Hall, ground floor** Chair: **Ina Reiche**	**Life Sciences** **Pavlovsk Hall, ground floor** Chair: **Elizabeth Kelley**	**Fundamental Science** **Kronstadt Hall, ground floor** Chair: **Egor Lychagin**
11:30 – 12:00	Invited talk **Robert Cubitt** (ILL, France) "Neutron Optics And Instrumentation"	Invited talk **Francesco Grazzi** (IFAC, Italy) "Ancient arms and armour production technologies revealed through neutron imaging and neutron diffraction"	Invited talk **Michail Kiselev** (JINR, Russia) "Neutron scattering application for the characterization of the lipid structure of mammalian stratum corneum and drug delivery systems based on the soybean phospholipids"	Invited talk **Victor Ezhov** (NRC KI - PNPI, Russia) "Neutron lifetime measuring experiments with UCN magnetic storage"
12:00 – 12:15	**Jakob Voldum Ahlburg** (Aarhus University, Denmark) "Fast heating - Sample Environments for High Brightness Sources"	Invited talk **Ekaterina Yatsishina** (NRC KI, Russia) "Study of the Gilding Technology of the "Idol" from the 10th Century Mound	**Ekaterina Iashina** (NRC KI – PNPI, Russia) "Logarithmic fractal structure of the large-scale chromatin organization in the interphase HeLa nuclei"	**Vladimir Voronin** (NRC KI - PNPI, Russia) "Crystal-diffraction gain of the Stern-Gerlach effect"

12:15 – 12:30	**Marek Bartkowiak** (Paul Scherrer Institut, Switzerland) "Non-magnetic goniometer for dilution refrigerators"	"Chernaya Mogila" ("Black Grave")"	**Sophie Combet** (LLB, Universite Paris-Saclay, Frence) "Membrane interaction of off-pathway prion oligomers and lipid-induced on-pathway intermediates during prion conversion: a clue for neurotoxicity"	**Valery Nesvizhevsky** (ILL, France) "A new approach to search for free neutron-antineutron oscillations based on coherent neutron and antineutron reflections"
12:30 – 12:45	**Jonathan Taylor** (ESS ERIC, Sweden) "Scientific software developments at the European Spallation Source"	**Antonella Scherillo** (STFC – ISIS, UK) "Neutron diffraction for archaeometry: results obtained on ancient Sardianian bronzes using the Italian Neutron Experimental Station INES"	**Nicolas Coquelle** (ILL, France) "Structural characterization of rsEGFP2 on-state intermediates using neutron diffraction and time-resolved serial femtosecond crystallography experiments reveal its fluorescent state"	**Dmitrii Shapiro** (NRC KI - PNPI, Russia) "Search for new internucleon short-range interaction in neutron scattering"
12:45 – 13:00	**Tatsuro Oda** (Kyoto University, Japan) "Neutron Resonance Spin-Echo Spectrometers at BL06 VIN ROSE at J-PARC MLF"	**Anna Fedrigo** (ISIS, STFC, UK) "Imaging investigation of Chinese bimetallic sword fragment from 2nd-1st century BCE"	**Dmitry Lebedev** (NRC KI - PNPI, Russia) "Insights into genetic information storage, repair and translation provided by neutron scattering, synchrotron radiation and molecular dynamics"	**Maxim Zakharov** (JINR, Russia) "Interaction of ultracold neutrons with a neutron interference filter oscillating in space"

13:00 – 13:15	**Livia Balacescu** (JCNS (FZJ), Germany) "Characterization of Soft-Matter and Biological Systems by Simultaneous Small-Angle Neutron Scattering and in situ Light Scattering and Absorption Complementary Techniques (DLS, UV-Vis, FTIR) at the SANS Diffractometer KWS-2 of JCNS"	**Laura Arcidiacono** (Universita degli studi di Roma Tor Vergata, Italia) "Neutron tomography reveals lead cores in Late Bronze Age palstaves at ISIS Pulsed Neutron and Muon Source"	**Lindsay McGregor** (ILL, France) "Identifying the correct protonation states of reactive intermediates in urate oxidase catalysis"	**Stephan Sponar** (Atominstitut, TU-Wien, Austria) "Weak Measurements and Which-Way Measurements studied in Neutron Optics"
13:15 – 13:30	**Andre Heinemann** (GEMS&MLZ, Germany) "New Features and upgrades of the Small-Angle Neutron Scattering Instrument SANS-1 at MLZ"	**Claudia Mondelli (**ILL, France) "The effects of manufacturing processes on historical ceramic morphology studied by Small Angle Neutron Scattering"	**Jorg Pieper** (University of Tartu, Estonia) "Neutron Scattering Experiments of Photoactive Proteins under Illumination"	**Sergey Kozhevnikov** (JINR, Russia) "On ray and wave optics description in neutron planar waveguides"

Facets of Neutron Economy

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Economy represents, in various contexts and various meanings of the word, key aspects of neutron research since its beginnings around 1950. By now neutron beams used in neutron scattering experiments have exclusively been obtained by knocking out fast neutrons from nuclei at the first place, which implies considerable energy density and costs. The number of fast neutrons initially created in a neutron source did not advance by more than a factor of 6 since 1958 – the start of the Chalk River reactor – until today. The maximum was achieved at HIFR at Oak Ridge in 1966. The tremendous progress in performance of neutron scattering instruments has been achieved by better economy of use of the neutrons produced in a neutron source facility, making sure that a higher, but still vanishingly small fraction of these neutrons reaches the samples to be studied. Another facet of economy is the industrial and other retail use of neutron scattering analysis, which has great traditions. but remained at a modest level. The many orders of magnitude gains in the efficiency in the use of produced neutrons make now neutron sources of modest costs deliver experimental sensitivities that required much more expensive neutron sources in the past. By the logics of economy, the retail market for neutron services with strongly diminished costs has a great chance to grow rapidly in the foreseeable future. Neutrons also are the main commodity in nuclear energy generation, a large sector of the economy. The issue of nuclear waste in fission energy production is fundamentally related to the insufficient number of available neutrons for incinerating through fission the long-lived heavy radioactive species in the nuclear waste. Complementing fission neutrons by spallation neutrons produced without fission could readily change the balance and make nuclear energy production largely waste free, including the elimination of the waste already actually accumulated in significant quantities.by now.

Neutrons for Cultural Heritage

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In modern investigation of Cultural Heritage, frontier advances are opened up by the synergistic use of physical and chemical characterization of the artefacts, creating the meeting point of science, conservation and archaeology. State of art technologies available for neutron-based methods are currently being applied to study of object of historical and cultural interest in several neutron beam facilities throughout the world. Thanks to the neutron interaction with matter, these techniques are non-invasive and non-destructive, ideal to provide us precious structural information, about the artefacts under study such as their composition, presence of alteration, inclusions, structure of the bulk, manufacturing techniques and presence of those elements which give us an overall fingerprint of the object's characteristics.

Neutron scattering techniques for molecular magnetism

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Molecular nanomagnets (MNMs) are clusters made of a finite number of magnetic ions coupled by a strong exchange interaction within the clusters and with a negligible magnetic interaction between adjacent clusters in the crystal lattice. They are promising systems for technological applications in the fields of high-density magnetic memory devices, quantum information processing and spintronics. They are also model systems to study the fundaments of quantum mechanics as they display quantum mechanics effects at the macroscopic level. The advances in the chemical engineering of these molecules have allowed the synthesis of tailor-made systems displaying several interesting quantum phenomena and to improve their properties to bring them closer to technological applications. Neutron scattering techniques have been intensively and successfully used to study the microscopic properties of molecular magnets and have enabled to reveal the signatures of their quantum behaviour.

I will show how advanced neutron scattering experiments have been pivotal for the understanding of the magnetic properties and quantum behaviour of a selection of molecular magnets model systems. The new generation of neutron instruments equipped with position sensitive detectors together with the availability of large single crystals has allowed us to reveal the microscopic details of prototypical MNMs unambiguously characterising their spin Hamiltonian [1,2], to reveal finite size effects on the magnetic properties of linear antiferromagnetic chains [3] and the entanglement between complex spin systems [4].

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Advances and perspectives of 3D neutron reflectometry in nanomagnetism, soft matter and life sciences

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Since last decades Neutron Reflectometry (NR) has become a routine tool widely applied to address fundamental and applied problems in various fields of condensed matter physics, chemistry, material and life sciences, whenever flat interfaces play an essential role. This refers to basic properties of free liquid and solid surfaces, formation and stability of interfaces between different states of mater and different materials, as well as to structure of thin films and heterostructures composed of layers in which boundary conditions substantially affect their characteristics via proximity effects. Active invasion of NR method into new areas of researches and related expansion of the NR user community occurs not only due to the generally growing interest to interfacial and proxy phenomena, but also because of increased accessibility of modern NR facilities, improved on-site experimental environment and availability of easy-to-use software routines for data reduction and modelling. The latter is especially true if only specular reflectivity (SR) is analysed delivering 1D scattering length density (SLD) depth profile, Nb(z), almost totally satisfying a vast majority of the user community. In principle, a reduction of dimensionality applies when laterally homogeneous media are separated by ideally flat interfaces. Then in-plane projections of the incident neutron wave vector are conserved and only specular reflection from and refraction into media can be observed. The reflection, $R(q_z)$, and refraction, $T(q_z)$, coefficients depend on the solely normal to the surface component q_z of the 3D wave vector transfer. Both coefficients can be readily computed with arbitrary precision for any 1D SLD profile via optical algorithms employed in numerous versions of software.

However, capabilities of NR are not restricted to probing only 1D SLD profile when off-specular scattering (OSS) is recorded along with SR. The latter is often observed as real surfaces and interfaces are never ideally flat, while interaction potential generally depends on in-plane coordinates, e.g. due, for instance, to the atomic structure, lateral density or content fluctuations, etc. Regretfully, up to date OSS has not yet entered the custom neutron toolbox, although its potentials were convincingly demonstrated [1-3] in a number of experiments. The same concerns the unique ability of OSS to probe out-of-plane arrangement of laterally periodic structures, opening up perspectives to establishing *shallow incidence neutron crystallography* (SINC) which can deliver 3D information on planar 1D, or 2D arrays of nano-, or micro-elements with complex intrinsic structure. High sensitivity of OSS to long range in-plane structures is achieved at low angles of incidence and scattering when one of the in-plane principle axes of the coherence ellipsoid is dramatically elongated crossing a number of scattering atoms in the SR plane. Then almost all of them scatter neutron wave in-phase into two main directions: specular reflection and/or refraction justifying optical approximation in which real scattering potential is substituted by its mean value averaged over the coherence range. However, neutron waves primarily distorted in optical potential may also be partially scattered in off-specular directions by deviations of real potential from its optical approximation. This happens whenever in-plane dimensions of deviations are smaller than the coherence length. In the particular case of laterally periodic arrays OSS is coherently enhanced when the in-plane component of the wave vector transfer matches Bragg conditions. General principles of SINC of planar 1D and 2D nano- and microarrays will be illustrated by examples demonstrating current and tentative applications of the method in various areas of research.

References

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[2] B.P. Toperverg, Physics of Metals and Metallography, 2015, Vol. 116, No. 13, p. 1337
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Novel spiral and skyrmionic states

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The lack of inversion symmetry in the crystal lattice of magnetic materials gives rise to complex noncollinear spin orders through the Dzyaloshinskii-Moriya interaction, resulting in new physical phenomena, such as emergent electromagnetism.

So far, studies of the archetype chiral magnets, the cubic chiral magnets, have revealed a universal magnetic phase diagram composed of helical spiral, conical spiral, and the skyrmion lattice phase. The latter appears in a narrow region of the phase diagram, the so-called A-phase, just below the magnetic ordering temperature.

Recent SANS and magnetization measurements on the Mott insulator Cu_2OSeO_3, however, indicate remarkable deviations from this universal behavior. Just below the critical field at which the conical spiral state disappears, the spiral wave vector rotates away from the magnetic field direction and a new multidomain state sets-in. This new phase occurs where it is least expected, at low temperatures, where thermal spin fluctuations are suppressed, and at magnetic fields strong enough to align all spirals along their direction [1]. This instability of the conical spiral state, which can be considered as a re-entrance into the helical state, is sensitive to the direction of the magnetic field and occurs only when the field is applied along the [001] easy crystallographic axis. This tilted spiral state originates from the interplay of competing anisotropies, which are generic to chiral magnets, and may stabilize novel skyrmionics states in a wide range of magnetic fields and temperatures, beyond the A-phase [2,3].

Indeed, SANS experiments show that, depending on the magnetic history, extremely robust skyrmionic states can be produced in large areas of the magnetic phase diagram, from the lowest temperatures up to the A-phase [4, 5]. Nascent and disappearing spiral states near critical lines catalyze topological charge changing processes, leading to the formation and destruction of skyrmionic states at low temperatures, which are thermodynamically stable or metastable depending on the orientation and strength of the magnetic field. The metastable low temperature skyrmions are surprisingly resilient to high magnetic fields: the memory of skyrmion states persists in the field polarized state, even when the skyrmion lattice signal has disappeared [5]. These findings highlight the paramount role of magnetic anisotropies in stabilizing skyrmionic states and open up new routes for manipulating these quasi-particles towards energy-efficient spintronics applications.

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Oppositely Charged Polyelectrolyte/Surfactant Mixtures at the Air/Water Interface: Dominance of Non-equilibrium Effects

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Oppositely charged polyelectrolyte/surfactant mixtures control the properties of many of the products we use in our everyday lives like cleaning materials, cosmetics and even some of the foods we eat. While work has been carried out to understand the properties of these systems under dynamic conditions relevant to processing and applications [1–2], there is a growing awareness that even the static properties are strongly influenced by non-equilibrium effects [3–4]. We have worked over the last decade to relate the interfacial properties of these systems to different non-equilibrium processes in the bulk and at interfaces [e.g. 5–12].

It is described in this talk how non-equilibrium effects not only influence but in fact dominate the interfacial properties of such mixtures. Our work focuses on different strongly interacting systems that represent in its simplest form the problem of how a macromolecule interacts with an amphiphile at a surface. Various bulk and surface-sensitive techniques including neutron reflectometry are applied to the problem. With an initial focus on the surface tension behavior, it is shown that these materials inevitably exist out of equilibrium conditions for a prolonged period, even if steady state properties at the air/water interface can be monitored in the meantime. The situation is further complicated by the formation of liquid crystalline particles that are kinetically-trapped and so can be resistant to chemical change. Their formation depletes the solution yet their presence can enhance the interfacial properties through direct interactions, which can result in their dissociation and the spreading of material by Marangoni flow to form kinetically-trapped films. We are currently exploiting this mechanism specifically to come up with some surprising results, such as the ability to control the formation of extended reservoir structures at a fluid interface. This particular advance was resolved using a new, powerful implementation of neutron reflectometry that can be used to determine interfacial compositions under dynamic conditions on the minute time scale [13].

Our systematic unraveling of this complex problem has not come without controversy [14], as still results from the literature are used to support a traditional equilibrium picture. Our perspective on this issue is outlined in terms of the dominance of non-equilibrium effects in many of the historical bulk and interfacial studies on these systems. In summary, we propose the non-equilibrium framework outlined in this talk as a robust platform on which to improve our understanding of the behavior of complex mixtures both used in industry and present in nature.

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Bio-SANS on membrane protein

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Neutron scattering is an ideal tool to probe the relationship between protein and their lipidic environment. I will show how Neutron reflectometry and small angle scattering can be combined to understand the interaction between an amyloid peptide and a lipid bilayer. I will also show the unique information that SANS can bring to the structural description of the enzymatic cycle of membrane transporters, when associated to adequat analysis tools.

Neutron Scattering Under High Pressure at the Long Pulse Neutron Source: Towards Half-Megabar Pressure Scale

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A discovery of novel physical phenomena in condensed matter under extreme conditions stimulated a great progress in instrumentation and methodological developments in this research area. Comparing to other experimental methods, the application of high pressure is a direct tool for controlled modification of structural, magnetic and other physical properties of materials by means of variation of interatomic distances and angles, tuning relevant interactions in the system.

The intrinsically low intensities of neutron sources, many orders of magnitude less than those of synchrotron ones, made the evolution of high pressure neutron scattering techniques a long-standing story. The realization of neutron scattering studies on the pressure scale of 10 GPa and above has become possible only recently. The relevant experimental methods were developed in a few advanced neutron research centers, including NRC “Kurchatov Institute” (Russia); ISIS RAL (UK); LLB (France), ILL (France), PSI (Switzerland), J-PARC (Japan), ORNL (USA), LANL (USA).

At the IBR-2 high flux long pulse reactor (FLNP JINR, Dubna, Russia), the techniques for neutron diffraction (ND) and inelastic neutron scattering (INS) experiments at high pressures were developed during last two decades. The DN-12 spectrometer combining ND and INS options was developed for studies of materials using sapphire and tungsten carbide anvil cells at high pressures up to 10 GPa [1,2]. Based on a positive experience with the DN-12, recently a new high-brilliance diffractometer DN-6 combining high neutron flux at a sample position and wide aperture of detector system have been developed, providing potential access to much extended pressure scale up to 50 GPa [3]. The present state-of-art level in high pressure neutron scattering at these instruments and recent research topics are overviewed. They include studies of the magnetic structure of the novel binary oxide Fe_4O_5, synthesized at high pressure-high temperature conditions, magnetic structure of the pressure-induced post-perovskite form of magnetite Fe_3O_4 and a search for a magnetic phase transition in Cr_2O_3 at high pressures up to 35 GPa [4-6], as well as studies of pressure-induced magnetic phenomena in complex oxides YMn_2O_5 [7] and $Ca_3Co_2O_6$ [8].

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Structure and mechanisms of membrane proteins and their importance for medicine

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Membrane proteins are key macromolecules of cells. Their biomedical importance makes them ideal pharmaceutical targets that are covered by about 60% of drugs currently on the market.

Functional membrane proteins are essential for life and health. Many their specific defects are associated with various severe diseases. Structure-based rational drug design and drug optimization rely on atomic resolution of three-dimensional structures of the proteins of interest.

However, some families of membrane proteins have so far resisted high-resolution structure analysis, so that their functional mechanisms have not been clarified.

A major bottleneck of research and development related to membrane proteins is a lack of structural information. It is widely accepted that the major challenges towards determining the structure of a membrane protein is their expression and the growth of well diffracting crystals. We solved some of these problems and this has led to breakthrough in the studies of several families of membrane proteins. Here we will report on sensors of *two-component signaling systems* (TCS).

TCS is the most abundant signaling system used by organisms in nature. First component of TCS are membrane sensors which are a major and essential class of transmembrane (TM) receptors, present in all domains of life, such as sensor histidine kinases (HKs), chemoreceptors and sensory rhodopsins. TCS is not present in animals and therefore it is considered as a promising target for drugs against infections. A barrier for the understanding of molecular mechanisms and drug design is a lack of full-length high-resolution structures of this type of proteins. We applied considerable efforts to solve the problem[1-4]. We will discuss current state of the field under discussion and recent results obtained by complementary use of neutron scattering and X-ray crystallography.

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How neutrons facilitate research into gas turbines and batteries from development to engineering applications

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The relentless growth in population and industry has lead to an unprecedented global increase in the demand for energy and mobility. Meeting these requirements necessitates supplying far more energy and transportation, and to do so more efficiently. Despite an abundance of possibilities for generating new types of power – especially in the field of renewable energies – the burning of fossil fuels will play a central role in emerging economies in the coming decades. Consequently, it is crucial that power - generating heat engines be as efficient as possible. Gas turbines for aeroplanes and stationary power engines, together with batteries for electro mobility, are two key technological fields for research.

In the field of high-temperature alloy applications, gas turbines play a significant role in terms of energy conversion. In particular, improvements to Ni-based superalloys, from wrought to cast alloys that have excellent properties in regard to high-temperature strength or corrosion and creep resistance, including high fracture toughness, are a case in point. The main goal of existing Ni-based superalloys is to increase the operating temperature of these alloys in gas turbines [1] to allow engine manufacturers to improve fuel efficiency, thereby achieving reduced CO_2 emissions. Most superalloys consist of so- called γ' precipitates coherently embedded in a g matrix plus additional high-temperature phases. The last few decades have seen the scientific community put great effort into the development of Ni-based alloys for stationary gas turbines with operating temperatures above 650 °C whilst keeping the good processing characteristics of the well-known alloy 718. In addition, new alloy concepts such as the CoRe alloys [2] have been investigated with a view to enhancing the service temperature and optimizing the precipitation stability and size [3].

In order to gain a better understanding of the electrochemistry in batteries, a huge demand has emerged for in-situ and operando characterization methods. Due to the high penetration depth and high sensitivity of neutrons to light elements as lithium, a probe of this nature has become ever more attractive over the last decade. The present contribution gives an overview how neutrons, with their unique properties, contribute to the development of new battery cells. During the charging and discharging of cells, the intercalation of Li in the graphite layers can be observed in-situ with neutron diffraction (ND) as such measurements are able to detect LiC_x phases such as LiC_6 and LiC_{12} during the intercaltion/de-intercalation process [4]. Under fast charging conditions and low temperatures, the appearance of Li plating can influence the cell performance. On larger scales of >50 micrometer neutron imaging (radiography and tomography) enablesa non-destructive view inside the cell and e.g. shows how the distribution of the electrolyte filling, in the cell between the layer stacks in a pouch cell takes place [5]. The use of neutron induced prompt gamma activation analysis (PGAA) is a powerful tool to describe the capacity loss of the cell caused by tiny metal deposits on the graphite anode after the charging/discharging processes [6]. The Neutron Depth Profiling (NDP), GISANS and Neutron Reflectivity (NR) are further methods of studying near surface phenomena such as the Li distribution.

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Pulsed Fast Reactor IBR-2 after Modernization

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Frank Laboratory of Neutron Physics is one of the laboratories of the Joint Institute for Nuclear Research (Dubna, Russia), that investigates the neutron as an elementary particle, and employs the neutron as an instrument to investigate the structure and dynamics of condensed matter, including crystals and nanosystems, functional materials, complex liquids and polymers, rocks, etc.

The IBR-2 reactor operating at FLNP since early 80-th of the last century with its unique technical approach produces one of the most intense neutron fluxes at the moderator surface among the world's reactors: ~10^{16} n/cm^2/s, with a peak power of about 1850 MW in pulse.

In 2007, the reactor reached the service life limit on fuel burn up and fluence on the reactor vessel and was shut down for modernization and replacement of the primary reactor equipment. The main objectives of the modernization were to increase safety, reliability and experimental possibilities of the reactor for the next 25 years of operation. During the modernization period 2007 – 2010 the first of three cryogenic moderators was put into operation. The next one is planned to be commissioned by September 2019 and the last one by the end of 2021.

At the 14 beam ports of the IBR-2 we have 16 instruments for neutron scattering, radioanalytical laboratory for neutron activation analysis and irradiation facility. Among neutron scattering instruments FLNP has seven diffractometers, one SANS instrument, three reflectometers, two inelastic scattering spectrometers and one facility for neutron radiography and tomography. Two beamlines are used for the research in nuclear physics.

Status of the IBR-2 experimental facilities and cryogenic moderators will be presented as well as the plans for instrumentation development.

Keywords: pulsed fast reactor; neutron scattering; condensed matter physics; neutron nuclear physics; neutron activation analysis; instrumentation for neutron experiments;

ISIS - from TS1 to TS2 to ISIS-II

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This presentation will outline the current status of ISIS and future plans including the user programme, instrument/sample environment/software development, the Linac Tank IV and TS1 target/moderator replacements planned for 2020/21, and the developments needed to realise a future 'ISIS-II'.

Latest developments of neutron scattering instruments of the JCNS at MLZ

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During last year's significant efforts in developments and upgrade of our neutron scattering instrumentation have been undertaken at the Jülich Centre for Neutron Science (JCNS), thus allowing to keep it in line with continuously changing scientific request.

The high resolution SANS instrument KWS-3 was fully rebuild allowing now for the usage of a polarized neutron beam together with an analyser and a magnet up to 3T on all sample positions and detectors with even higher resolution then before. In this way KWS-3 got even more versatile and interesting for the users.

The backscattering spectrometer SPHERES has been updated with an elliptic focussing neutron guide to increase the intensity on the sample. To increase the background to signal ratio further we have installed a new background chopper in front of the phase space chopper. Running in the 1:2 mode the signal to background ratio has been increased dramatically.

New super conducting coils for the NSE spectrometer allows for pushing their resolution towards the 1µsec; the position-sensitive detectors together with the newly installed chopper at the diffuse scattering spectrometer DNS allow now for inelastic measurements. Furthermore a new neutron supermirror polarizer increases the flux on the sample significantly and broadens the usable wavelength spectrum.

Successful in-house developments of ^{3}He neutron spin filters employing the on-beam gas polarization provide the basis for the polarization analysis in a wide Q-range as at the neutron reflectometer MARIA and small-angle scattering diffractometers KWS. In the case of MARIA the analyser is running in Argon atmosphere to further reduce the background. This approach is working absolutely successfully, regardless of the possible complications. First successful tests of the new polarization setup for TOPAS on the diffractometer POLI will be shown.

Developments of the PASTIS-like wide-angle ^{3}He analyzers are carried out for the polarization analysis in a large scattering angle. They will allow for simultaneous XYZ and 3-d polarization analysis in the angle up to 140° at time-of-flight spectrometers like DNS and

High-density uranium fuel for high performance research reactors

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Worldwide high-flux fission-based neutron sources have a very compact core fueled typically with highly-enriched uranium (HEU). This is due to the simple fact that high flux of thermal neutrons alone is not the criteria, but flux in a small solid angle and in a small energy window, i.e. brilliance is needed. With respect to international efforts to minimize the civilian use of HEU, considerable R&D effort has been invested in the past 20 years to develop uranium fuel with much higher density than the currently used fuel in order to exchange enrichment against density.

Most high-performance research reactors have an uranium density in their fuel assembly in the order of 1 gU/cm^3. For a reduction of the enrichment from 93 % to an enrichment of 19.75 % (so-called low enriched uranium, LEU) an increase in density by at least a factor of 5 is needed, taking into account the effect of losses in neutron flux due to increased absorption caused by the large amount of ^{238}U.

Internationally, the R&D concentrates on three types of high-density uranium fuels, namely U-8wt.%Mo alloy powder embedded in an Al matrix, monolithic foils of U-10wt.%Mo alloy and U_3Si_2 powder embedded in an Al matrix, reaching maximal densities of 8, 15, and 4.8 gU/cm^3, respectively. The European high-flux research reactors (EUHPRRs) together with the fuel manufacturer Framatome-CERCA have formed the consortium HERACLES for the joint development of these high-density fuels. HERACLES strongly interacts with the National Labs of the US-DoE, which are involved in the conversion of the USHPRRs.

We will discuss the swelling behavior of each of those variants, the challenge of an industrial manufacturing of high-density fuels and steps needed for the licensing process.

Neutron Facilities at China Advanced Research Reactor

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The China Advanced Research Reactor (CARR) is a high-flux and multipurpose reactor, located at the campus of China Institute of Atomic Energy in Beijing. This reactor is a tank-in-pool inverse neutron trap type reactor with a power of 60MW. The peak flux in a heavy-water reflector is about 8.0×10^{14}n/cm^2/s. The main applications of the CARR are neutron scattering experiments, radioisotopes production, material irradiation, neutron transmutation doping silicon, neutron activation analysis, etc. The reactor successfully run for ~81 days in 2018.

Up to date, nine neutron instruments have been successfully installed. They are high resolution powder diffractometer(HRPD), high intensity powder diffractometer(HIPD), residual stress diffractometer(RSD), texture diffractometer(TD), single crystal diffractometer(SCD), Bamboo triple axis spectrometer(Bamboo), triple axis spectrometer(TAS), horizontal sample geometry neutron reflectometer(NR) and small angle neutron scattering(SANS). Several other instruments are under developing, including thermal neutron radiography(TNR), cold neutron radiography(CNR), engineering diffractometer(ED), cold neutron triple axis spectrometer(CTAS), multi axis crystal spectrometer(MACS) and neutron activation analysis(NAA) systems. In addition, four more instruments have also been proposed. All the nine installed instruments have successfully got their first neutron results and are now under optimization or operation. These instruments are expected to be available to users soon after CARR comes into service.

Like many other neutron scattering centers, CARR will also be an open user facility. In fact, many research institutes(Institute of Chemistry the China Academy of Sciences, Institute of Physics China Academy of Sciences, Peking University, Central South Univeristy, Renmen University of China and the Juelich Center for Neutron Science of Germany) have already involved as collaborators for the construction of the instruments. More recently, China Institute of Atomic Energy(CIAE) and Helmholtz-Zentrum Berlin (HZB) also set up very fruitful collaboration on neutron scattering. And we are looking forward to more fruitful international collaborations in the future.

Current status of OPAL, the Australian Research Reactor

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The Open Pool Australian Light-water Reactor (OPAL) is a 20 MW pool-type multi-purpose research reactor located south of Sydney. The core is surrounded by a heavy water reflector vessel where all the irradiation facilities are located. OPAL achieved criticality in August 2006 and is effectively being utilised for neutron beam research, production of radioisotopes for medical and research purposes, and for commercial irradiations.

The neutron beam facilities of OPAL consist of neutron beam tubes that penetrate the reflector vessel, a cold neutron source, beam shutters and neutron guides. A suite of neutron beams instruments utilise both the thermal and cold neutron beams for both atomic and molecular structure determination and dynamics measurements, residual stress measurement and neutron imaging. There are 13 instruments available in the user program, with 1 instrument under commissioning. An update will be given on the status of OPAL and its neutron beam facilities, the performance of instruments and user program, and future plans.

Towards the full instrument suite of the European Spallation Source

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The instrument suite at the ESS is taking shape, with first neutrons foreseen for 2022. 15 instruments are under construction, covering SANS, reflectometry, imaging, engineering diffraction, powder and single-crystal diffraction, chopper spectrometers, and crystal-analyser spectrometers. An overview is given of the 15 instruments and a view forward is provided on the path towards the full suite of 22 instruments, and beyond.

Recent instrument developments in the Excitations Group at ISIS

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The excitations group at ISIS is responsible for the direct geometry time of flight spectrometers LET, MAPS, MARI and MERLIN, which perform momentum resolved spectroscopy measurements to study magnetic excitations and phonons. The instruments undergo an optimisation programme of continual development. In this poster, details of some of these recent developments will be presented, including, most notably, the MARI upgrade, as well as information about our software strategy to increase research outputs from the instruments.

The MARI direct geometry time-of-flight spectrometer at the ISIS facility has been upgraded with a new m=3 straight converging guide, and double-disk chopper to allow optimal use of rep-rate multiplication. MARI has had over 25 year's successful use for the study of magnetic excitations and lattice dynamics in ordered and disordered materials and the upgrade will allow it to remain competitive with newer instruments. Commissioning measurements have confirmed gains of up to a factor of 16 at E_i=5 meV, the lowest usable energy on MARI. The flux at high energies was found to be still be nearly doubled from viewing a larger area of the moderator, as expected from the ray-tracing models. Multi-rep operations will use a new double-disk chopper with four slits to allow up to four non-overlapping reps through when the Fermi chopper runs at multiples of 200 Hz. Typical reps of 80, 20 and 9 or 5 meV would allow the overall dispersion or density of states to be mapped, and low energy features such as mode softening or energy gaps to be determined simultaneously. The gains in flux at low energies enables higher chopper speeds to be used to give good energy resolutions at the high energy reps, and excellent resolution for the low energy reps whilst maintaining a usable count rate. The instrument is now in user service.

LET has recently implemented an interchangeable final guide section. This section can either consist of a straight supermirror guide or a supermirror collimator. The collimator consists of an m=4 supermirror top and bottom, leaving the vertical resolution unchanged, and five horizontal channels formed from borofloat walls with a layer of Gd coated with m=1 supermirror. This reduces the horizontal divergence and flux by a factor of two at all wavelengths, giving similar instrument performance to LET before the focussing snout was installed.

The major bottleneck in the productivity of the Excitations Group instruments is a lack of easy-to-use software that can effectively analyse the vast datasets that they collect. Existing packages to visualise and manipulate the data struggle to handle the data, and materials modelling codes are either not implemented for high performance computing (HPC) or their output is not integrated into the analysis framework, and proper account of instrument resolution is rarely performed as it requires parallelisation of the current codes and HPC to be feasible in most cases. PACE (Proper Analysis of Coherent Excitations) is a software project to provide an integrated visualisation, simulation and fitting environment, on massively parallel and distributed computing, which interfaces to experimental data and materials modelling codes. It will deliver parallel computing implementations and integration of proven data analysis packages and modelling codes (Horace, TobyFit, Castep and SpinW) in an integrated framework, on a thirty month timescale beginning in autumn 2018.

Neutronic Design of the Bunker Shielding for the European Spallation Source

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At 5 MW average beam power, the European Spallation Source will be the most powerful spallation source in the world. The 2 GeV proton beam colliding with the tungsten target generates spallation neutrons up to the energy of the incoming beam, and this poses serious shielding challenges. The neutron bunker is a common shielding area that surrounds the ESS monolith (a steel structure around the target), to protect the instrument area from the high dose of ionizing radiation that accompanies the beam extraction system. The instrument area is a supervised zone with access for the experimental users, for this reason radiation dose should be less than 3 μ Sv/h.

In order to perform the neutronic design of the bunker, a comprehensive study of the neutron radiation at the different locations with respect to the proton beam has been performed. This step allowed to define neutron source terms, i.e. the definition of neutrons at the entrance of the beamports, to be used to speed up the MCNP calculations. With such source terms, we have designed the bunker wall and roof. The requirement for the bunker wall design is a dose rate outside the wall lower than 3 μ Sv/h to allow access to the instrument users. The main drive for the bunker roof design were limits of skyshine dose rate at the campus office and site boundaries. Skyshine was calculated with both analytical approach and full MCNP calculation and results were compared. The design required an in-depth analysis of the effect of the high-energy neutron beams with different beamline configurations. The final design was performed for 26 instruments, i.e. beyond ESS full scope, to take into account future upgrades of the facility.

The material choice for the bunker wall and roof is manganese heavy concrete with density of 3.8 g/cm^3. This material shows the best cost effectiveness and is most convenient in terms of operation of the bunker, which requires periodic access, with removal of blocks from the roof, for maintenance of components inside. The comprehensive study of source term, dose rates, activation, and skyshine will be presented.

Simulations of neutron scattering instruments at a compact source

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The world's leading neutron research centers are currently developing a new generation of neutron sources for the needs of condensed matter physics. Compact sources are designed to replace the morally obsolete small- and medium-power reactors and open up the possibilities for creating a neutron scattering laboratories at universities and research institutions. Such a source initially loses several orders of neutron flux to a large accelerator-type source; however, a significant part of these loses can be recouped by increasing the capture aperture and deep instrument optimization, including adaptation of the accelerator, target and moderator parameters to the needs of a particular instrument located at the source.

In this work we formulate a general approach to the conceptual design of a neutron scattering instrument on a compact source, then we design the accelerator and target assembly based on needs of the neutron scattering instruments. Using the examples of three methods - diffraction, spectroscopy and small-angle scattering – we propose the experimental schemes for these method’s implementation. A number of the optical devices was proposed and optimized, their use will allow the most efficient use of the generated neutron flux.

For a powder diffractometer, we propose to use two interchangeable moderators with a thermal and cold neutron spectrum. This will allow this instrument to have two operation modes with an optimal flux at a given resolution, suggesting in the choice of the operating wavelength band and providing high-quality measurements for investigations of both crystalline and magnetic structures.

To implement the neutron spectroscopy method on a compact source, the time-of-flight technique in reverse geometry is proposed. Its use allows one to design a so-called excitation observer in (q,E)-space, which is an effective tool for the analysis of inelastic, quasi-elastic and elastic scattering, and which provides a quick and comprehensive study of the dynamics.

Of the three methods chosen, small-angle neutron scattering is most demanding on the luminosity of the source, since it has the most stringent requirements for the collimation of the beam used. For its implementation we consider the possibility to use the focusing geometry.

In conclusion, we have performed the McStas simulations of neutron scattering instruments based on methods of diffraction, spectroscopy and small-angle scattering at a compact accelerator-driven neutron source.

Compact Spectrometers for Compact Neutron Sources

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Compact neutron sources are optimized for high neutron beam brilliance, not for maximum source strength. Thus they produce also less other radiation than reactor or spallation neutron sources. Thanks to a very efficient coupling into the moderator-target assembly, compact sources can feature a high brilliance comparable to existing medium-to-high flux sources. Instruments at these kind of sources can use phase space volumes that are not accessible at traditional sources due to the minimal distance between the sample and the moderator.

We discuss spectrometer designs that use Bragg optics to shape the initial neutron phase space such, that a narrow region of the dynamical range comes into the focus. In other words, we place a large monochromator at distances ≤ 5 m from the moderator. Using spatial and/or time focusing we explore concepts specialised for large energy loss and for narrow collimated beams. We expect that highly specialised spectrometers will become feasible at low power compact sources, while the performance at the high power compact sources should compare favourably to existing medium flux neutron sources .

Making ESS a success - A Landscape of European accelerator based neutron sources

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With the construction of the high power European Spallation Source (ESS) the European neutron community will have access to the most powerful neutron source worldwide. On the other hand the dwindling of reactor based neutron sources in Europe and the US will lead to reduced access opportunities to neutrons. Training of young scientists and the development of experimental methods will be hampered. An alternative to the classical neutron sources providing scientist with required neutrons, accelerator driven neutron sources present with high brilliance neutron provision. The Jülich Centre for Neutron Science has started a project to develop and design compact accelerator driven high-brilliance neutron sources (HBS) as an efficient and cost effective alternative to current low- and medium-flux reactor and spallation sources. Such compact sources will offer access of science and industry to neutrons as medium-flux, but high-brilliance neutron facilities. HBS will consist of a high current proton accelerator, a compact neutron production and moderator system and an optimized neutron transport system to provide thermal and cold neutrons with high brilliance. The project will allow construction of a scalable neutron source ranging from a university based neutron laboratory to full user facility with open access and service. Embedded within international collaboration with partners from Germany, Europe and Japan the Jülich HBS project will offer flexible solutions to the scientific requirements and establish a new opportunity to exploit neutrons beyond current limitations. We will describe the currents status of the project and its partners, the next steps, milestones and the vision for the future neutron landscape in Europe with the perspective to guarantee the success of the ESS.

E-learning neutron scattering

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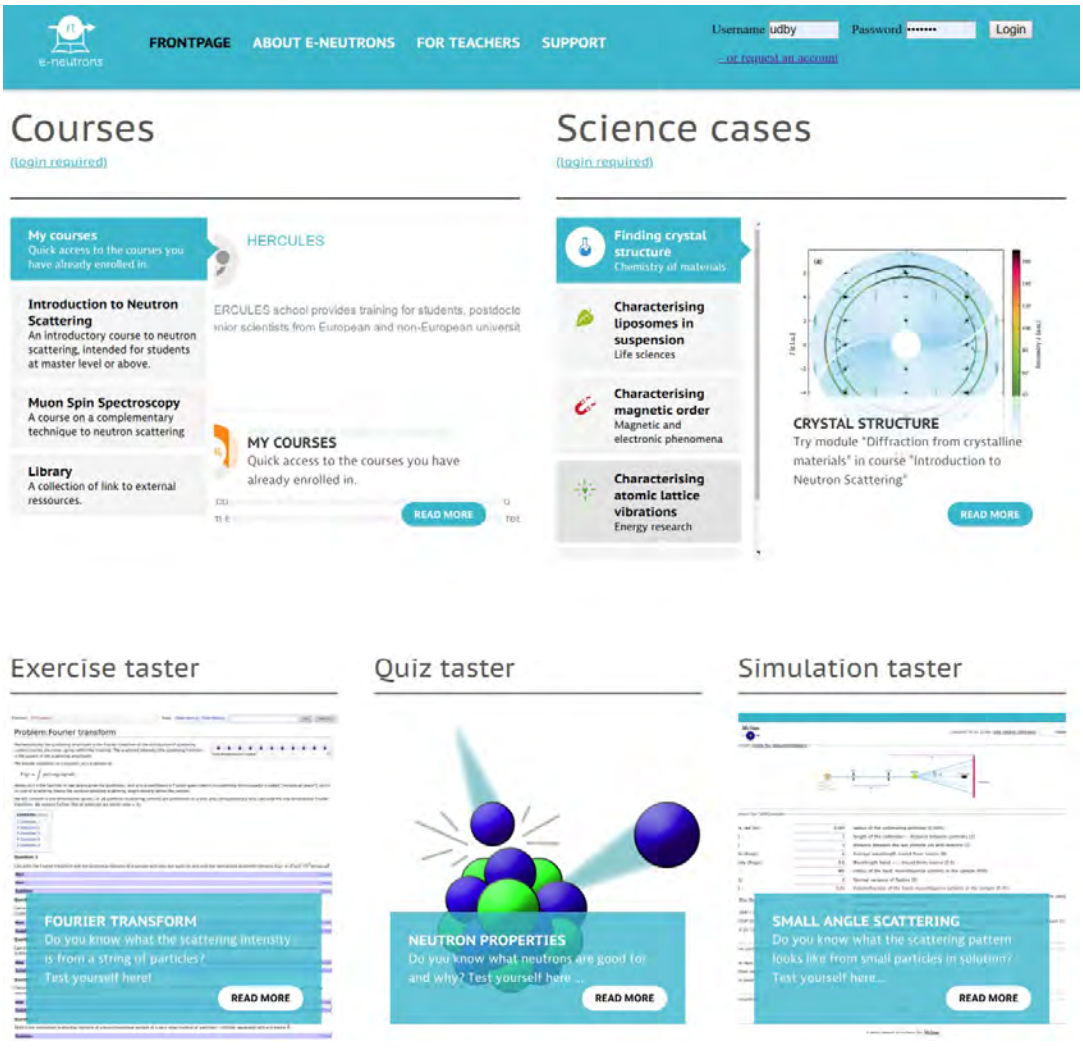
In the modern era of neutron scattering there is an increasing need for digital learning ressources which can be accessed anytime from anywhere. Thus we have created an interactive e-learning platform explicitly for learning neutron scattering theory and experiments www.e-neutrons.org.

Our research has shown that students after completing a training course where a combination of computer-assisted and hands-on training was used, are well equipped to participate in research experiments at large-scale facilities.

The e-neutrons platform is equipped with a learning management system for courses and student administration, an interactive wiki-textbook, a neutron virtual facility learning-game as well as a Monte-Carlo simulation tool for ray-tracing of neutron- and x-ray experiments including data production.

The e-learning platform presently features two courses on neutron scattering and one on muon spin spectroscopy targeted for master- and phd students.

In this talk the freely accessible e-learning platform will be presented and some of the active-learning tools and their advantages will be highligted. Input and ideas for new topics and courses from the audience will be welcomed.



Master program on neutron scattering at Saint-Petersburg State University

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The Neutron and X-ray science has several decades history, which was written in terms of the neutron or synchrotron source generations, which, in turn, are determined by the flux for neutrons and brightness for X-rays. Several tens of the highly technological stations are built around these powerful neutron and X-ray sources for studying structure and dynamics of the hard-, soft-, and live- matter. For effective use of the third generation X-ray sources and high flux neutron sources we are forced to establish the proposal system to distribute the beam time slots among scientific community of the own country and world-wide. The user community counts thousands of scientists with a wide variety of backgrounds in physics, chemistry, biology, and materials science. All of them should be familiar with the basics of Neutron and X-ray science to be able to perform experiments and to treat the data.

The training system around the neutron and x-ray sources is organized via numerous summer and winter schools with the duration from one week to a month. However, it is time to make step further and to establish Master program in "Neutron and X-ray Science" at some of the European Universities willing to really participate in the effective operation of the mega-science facilities such as neutron sources and synchrotrons.

One of the first examples was given by St-Petersburg State University with the master program "Neutron and Synchrotron Physics". The Program is aimed at training the scientists in design, construction and operation of instruments and methods at the high-flux reactor PIK in Petersburg Nuclear Physics Institute of NRC "Kurchatov Institute". The first semester of the program starts with the lectures on "Theory of interaction of neutrons and X-rays with matter", accompanied with the course on "Basics of the neutron and X-ray detection" and one more course on "Sources of neutron and X-ray radiation". The second and third semesters focus on the methods of diffraction, spectroscopy, small-angle scattering and reflectometry to build the basis for the interdisciplinary science developing at the large-scale facilities. The forth semester is devoted to writing the Master's Thesis, which topic is usually at the forefront of modern science.

It is important to note that 7 oral speakers at this conference ECNS2019 (two invited speakers among them) are graduates of the master program "Neutron and Synchrotron Physics" of St-Petersburg State University.

Superconductivity and magnetism in Fe pnictides

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In iron-based high-temperature superconductors, magnetic fluctuations and magneto-elastic effects are believed to be important for the superconducting electron pairing mechanism. To gain insight into the interplay between the different ordering phenomena and the underlying couplings we studied the magnetic order and lattice distortion on AFe$_2$As$_2$ (A = Ca, Sr, Ba, Eu) single crystals by neutron and x-ray diffraction. High-resolution x-ray diffraction and neutron scattering measurements reveal an unusually strong response of the lattice and ordered magnetic moment to superconductivity in Co-doped BaFe$_2$As$_2$. Furthermore, using x-ray resonant magnetic scattering, polarized and unpolarized neutron diffraction techniques, we show that the superconductivity and ferromagnetism coexists in Eu based "122" compounds. Coexistence and competition between magnetism and superconductivity and it's implication to unconventional superconductivity is fundamental to understand the underlying mechanism of superconductivity in Fe pnictides.

Rotation of the magnetic vortex lattice in the noncentrosymmetric superconductor Ru_7B_3

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Superconductivity in a non-centrosymmetric system was first observed in the heavy-fermion compound $CePt_3Si$ [1]. This has led to a great deal of theoretical and experimental interest, due to the novel states predicted for superconductivity in systems with no inversion centre. For these systems, parity is no longer a conserved quantity, and a superconducting state with a superposition of *s*-wave and *p*-wave states is predicted [2]. This results in unusual superconducting properties such as large Pauli limiting fields and 'helical' vortex states [2, 3].

We have performed measurements of the VL using small angle neutron scattering, with magnetic field applied along both the (001) and (100) axes, as well as a selection of angles in-between. We observe, in general, a nearly isotropic hexagonal lattice in all configurations, indicating a reasonably isotropic set of superconducting parameters along all the crystal directions. However, the most striking observation is of a rotation of the VL with respect to the crystal lattice when the applied field is changed while below T_c, leading to an orientation which is dependent on the field history of the superconducting state as opposed to the location within the phase diagram, an example of which is shown in Fig. 1. Furthermore, this behaviour is observed only for fields applied along the **a**-axis, and also exhibits a pronounced hysteresis. This is highly unusual, having not been observed in other superconductors to date, and is neither predicted nor explained by any of the prevailing theories of the vortex lattice. We postulate that this is a result of the broken time-reversal and inversion symmetries of this material, and develop a model in the Ginzburg-Landau formalism which shows how the effect of these couple to the orientation of the vortex lattice.

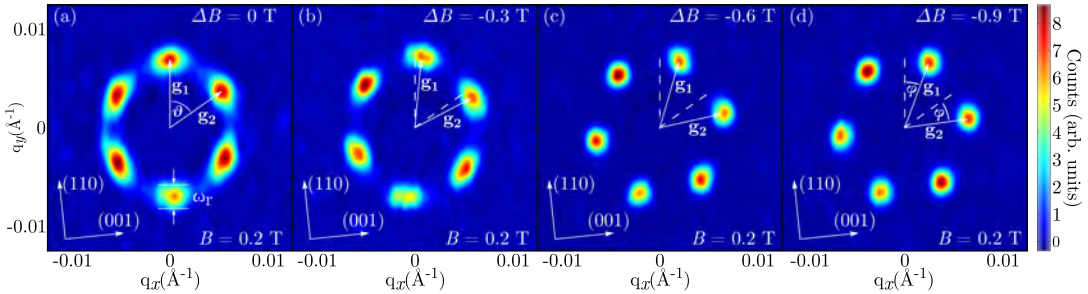

Figure 1: Diffraction patterns from the vortex lattice at 0.2 T, each with different field histories. The field change prior to measurement is indicated in the panel.

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Anisotropy of magnetic excitations in iron-based superconductors

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Magnetic response in unconventional superconductors remains to be attractive subject in attempts to reveal clues to high-temperature superconductivity. A particular attention was given to the phases with oriented electronic arrangements in real space, stripes, linked to the superconducting state. We used inelastic neutron scattering in order to characterize the magnetic excitation spectra in single crystals of different superconductors with orthorhombic distortions of the base tetragonal structure. Such distortions that may create a specific pinning potential for the stripes are observed in different families of copper- and iron-based superconductors. The measurements of the orientation anisotropy in the magnetic spectra should be performed with material samples that contain a singled out orientation of the orthorhombic domains. In the as-grown crystals these elastic domains with different orientation of orthorhombic axes exist in practically equal fractions what makes it impossible to discern the anisotropy. Single domain cuprate samples could be obtained in a special procedure when a single crystal is cooled down to ambient temperature through the higher-temperature tetra-ortho structural transition being subject to a uniaxial mechanical compression. The crystals of the iron-based pnictide superconductors undergo the tetra-ortho structural transitions well below the room temperature so that detwinning procedure has to be performed "*in situ*" in a cryostat. We have used different devices for compressing single crystals including a sample stick designed at ILL that permitted to apply and release uniaxial pressure at low temperature. The measurements of neutron scattering intensity have been performed with a usual single detector set-up and in inclined geometry of the multi-analyser *FlatCone* option. We give examples of the anisotropy of magnetic excitation spectra measured with such detwinned single crystals following recent publications [1,2].

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2. H.Man, R.Zhang, J.T.Park, X.G.Lu, J.Kulda, A.Ivanov, P.C.Dai
Direct observation of spin excitation anisotropy in the paramagnetic orthorhombic state of $BaFe_{2-x}Ni_xAs_2$.- Phys. Rev. B, 2018, vol.97, p.104418(1-7).

A multiscale approach to the formation of vortex lattice domains in the intermediate mixed state of the type-II/1 superconductor niobium

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Besides the well-known Abrikosov vortex lattice (VL), superconductors of the type-II/1 exhibit the intermediate mixed state (IMS), where VL domains and Meissner domains coexist, due to an attractive component of the inter-vortex interaction [1]. Despite ongoing work since its discovery in the early 1970s, the IMS bulk properties remain elusive. Especially the interplay with vortex pinning, due to impurities and surface defects, as well as the sample geometry and connected demagnetization effects, play a crucial role.

We have readdressed the IMS in bulk niobium using a multiscale approach comprised of small angle neuron scattering (SANS), very small angle neutron scattering (VSANS), neutron grating interferometry (NGI) and bulk magnetization measurements (VSM) [2,3]. Investigating the global magnetic state, the local properties of the VL and the morphology of IMS domains we were able to gather a comprehensive data set on the IMS transition in a set of bulk niobium single crystals of varying purity. Focusing on a field cooled protocol we have found that the homogeneous VL in the Shubnikov state (SH) gets rearranged into VL domains of increasing density in the IMS. Surprisingly, the local rearrangement of vortices into domains takes place below the macroscopic freezing transition of the VL. Moreover, the VL properties in the IMS show a universal behavior independent of the sample properties and measurement history, indicating that the IMS is governed by fundamental properties of the superconductor.

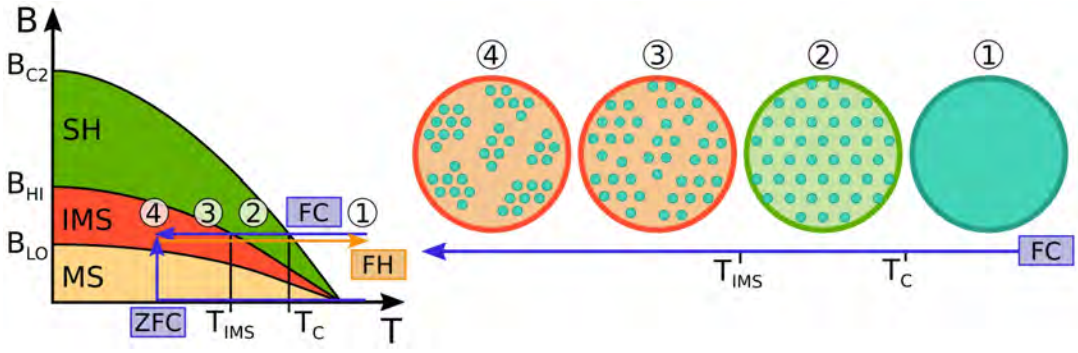

Image 1: Schematic phase diagram of a type-II/1 superconductor, subdivided into the MS (yellow), IMS (red) and SH (green). Arrows depict different measurement protocols: FC, FC/FH and ZFC/FH. For FC measurements, the microscopic magnetic flux redistribution is shown, starting from the normal state (1) with a homogeneous flux distribution, to the regular VL in the SH (2). In the IMS (3, 4) the VL breaks up into small domains containing an increasingly dense VL.

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Magnetic Excitations in The Cubic Superconductor CrRu

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We have studied the spin fluctuations in the normal state of a cubic superconductor of Cr(1-x)Ru(x) alloy for x=~0.2. The electron doping created by Ru ions in Cr(1-x)Ru(x) compound monotonically decreases the antiferromagnetic (AFM) spin wave density (SDW) modulation transition temperature,; TN. As the Ru amount increases through x=~0.1717 %, and the long-range SDW order is completely suppressed and the alloy becomes a superconductor, similar to the unconventional superconductors. The parent material; metallic Cr paramagnetic spin excitations are very energetic and can reach up to several hundreds of meV range. We have conducted our inelastic neutron scattering (INS) experiments with Ru concentration of x=~0.220 % with a superconducting transition temperature of Tc~ 1.6 K. The SDW fluctuations are found to be commensurate with the magnetic propagation vector of QAFM=(100). According to our time of flight (TOF) (for high energy transfer) and triple axis (for low energy transfer) INS studies, we still can see the strong spin fluctuations appearing near the C-QAFM reaching beyond and up to dE~120 meV, like in the metallic Cr parent. These excitations are also found as gapless in the low energy transfer range of dE=2.5 meV to 35 meV range. The parent material; metallic Cr, where paramagnetic spin excitations are very energetic and can reach up to several hundreds of meV range. These excitations are also found to be as gapless in the low energy transfer range of down to energies of dE=2.5 meV. The discussion will be focused on the conventional/unconventional character of the superconductivity in CrRu alloy [1].

[1] : Suppression of antiferromagnetic spin fluctuations in superconducting Cr0.8Ru0.2, **M. Ramazanoglu**, B. G. Ueland, D. K. Pratt, L. W. Harriger, J. W. Lynn, G. Ehlers, G. E. Granroth, S. L. Bud'ko, P. C. Canfield, D. L. Schlagel, A. I. Goldman, T. A. Lograsso, and R. J. McQueeney
Phys. Rev. B 98, 134512 (2018)

The Hidden Order in URu_2Si_2: Neutron scattering as a probe of intra-atomic anti-toroidal vortices

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For more than 30 years, there were tremendous research efforts to understand the mysterious Hidden Order (HO) in the heavy-fermion compound URu_2Si_2 (they are surveyed in [1]). The main problem is that below the HO transition temperature, T_{HO} = 17.5 K, there are practically no obvious physical phenomena associated with the order parameter; the only unequivocal evidence for the order is a rather strong specific heat jump at T_{HO}. We discuss here new approach to the hidden order in URu_2Si_2 and neutron diffraction as an *experimentum crucis* for its verification.

We suppose that there is no spatial symmetry breaking at the HO transition temperature and solely the time-reversal symmetry breaking emerges owing to unusual magnetic ordering [2]. As a result of its high symmetry (*4/mmm*), each uranium atom is a *three-dimensional* magnetic vortex; its intra-atomic magnetization **M**(**r**) is intrinsically noncollinear, so that its dipole, quadrupole, and toroidal magnetic moments vanish, thus making the vortex "hidden". The first nonzero magnetic multipole of the uranium atom is the toroidal quadrupole. In the unit cell, two uranium atoms can have either the same or opposite signs of their vortex magnetization **M**(**r**); this corresponds to either *ferrovortex* or *antiferrovortex* structures with *I4/mmm* or *P$_I$4/mmm* magnetic space groups, respectively.

Our first-principles calculations (DFT with the spin-orbit interaction) show that the vortex magnetic order of URu_2Si_2 is rather strong [2]: the total absolute magnetization |**M**(**r**)| is about 0.9 Bohr magneton per U atom; this value can explain the observed strong specific heat jump at T_{HO}. The vortex structure provides a very unusual form factor of magnetic neutron scattering. The resulting neutron diffraction patterns have been calculated both for *ferrovortex* and *antiferrovortex* structures [2]. The *antiferrovortex* structure has been rejected after comparison with available experimental data. Careful neutron diffraction experiments are needed for revealing the *ferrovortex* structure where magnetic reflections coincide with crystal reflections. We will also discuss other systems with this unusual vortex order.

This work was supported by the Ministry of Science and Higher Education within the State assignment FSRC «Crystallography and Photonics» RAS in part of symmetry considerations and by RFBR Project No.19-52-12029 in part of ab initio simulations.

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Tomonaga-Luttinger liquid spin dynamics in the quasi-one dimensional Ising-like antiferromagnet $BaCo_2V_2O_8$

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$BaCo_2V_2O_8$ is a realization of a spin-1/2 Ising-like quasi-one dimensional antiferromagnet with remarkable static and dynamical behaviors [1]. In zero-field, the excitations of the Néel phase consist in confined two spinon excitations stabilized by weak interchain interactions. They form two interlaced series of long-lived Zeeman ladders with respective transverse and longitudinal character regarding the direction of the magnetic moments (along the chain *c*-axis) [2]. We have explored the influence of an external magnetic field on this spin dynamics by inelastic neutron scattering. A contrasting behavior is observed for a transverse and a longitudinal magnetic field (i.e. perpendicular and parallel to the direction of the moments, respectively). The former case has revealed a very interesting physics as a topological quantum phase transition occurs between two types of solitonic topological objects [3,4].

The present talk is devoted to our results obtained under the application of a longitudinal magnetic field in $BaCo_2V_2O_8$ [5]. We show that the Néel phase excitations keep their transverse or longitudinal character, simply showing a Zeeman splitting up to a critical field of 3.8 T at which the Néel ordering turns into a longitudinal spin density wave (LSDW) [6,7]. This phase has raised a strong interest as it is a unique example of the Tomonaga-Luttinger liquid (TLL) physics experimentally accessible under moderate magnetic field [6,7,8]. The TLL longitudinal fluctuations expected in the purely one dimensional system [9], lacking long range order, are transformed in an LSDW ordering stabilized in $BaCo_2V_2O_8$ through the anisotropy and the weak interchain couplings. The dispersion spectrum in this exotic phase and the magnetic field dependence of the excitations have been investigated by neutron scattering on TASP (PSI, Villigen) and numerical calculations.

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Towards and understanding of the magnetocaloric effect

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The magnetocaloric effect provides great hope for environmentally energy efficient cooling that does not rely on the use of harmful gasses. Fe2P is a compound that has shown great potential for magnetocaloric devices. The magnetic behaviour in Fe2P is characterised by a first order magnetic transition (FOMT) that coexists with and characterises the strong magnetocaloric effect. Neutron diffraction and inelastic scattering, Mossbauer spectroscopy and first principles calculations have been used to determine the structural and magnetic state of Fe2P around the FOMT. The results reveal that ferromagnetic moments in the ordered phase are perturbed at the FOMT such that the moments cant away from the principle directions across a small temperature region. The acoustic phonons modes reveal a temperature dependent non-zero energy gap in the magnetically ordered phase that falls to zero at the FOMT. The interplay between the FOMT and the phonon energy gap indicates hybridisation between magnetic modes strongly affected by spin-orbit coupling and phonon modes leading to magnon-phonon quaisparticles that drives the FOMT and thus the magnetocaloric effect.

Spin Fluctuations Drive the Inverse Magnetocaloric Effect in Mn_5Si_3

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Interest for magnetocaloric materials has been increasing in the last decades in view of applications for room temperature refrigeration. In this context the system $Mn_{5-x}Fe_xSi_3$ has recently been investigated for its moderate magnetocaloric effect (MCE) corresponding to the cooling by adiabatic demagnetization. In that respect, the compounds with a composition around x=4 present, near 300 K, an isothermal entropy change of about -2 J/kgK for a field variation between 0 and 2 T. In contrast to the common direct MCE, the parent compound Mn_5Si_3 exhibits, below 70 K, an inverse MCE, a cooling by adiabatic magnetization, of comparable magnitude, but opposite sign. On cooling from the paramagnetic state, Mn_5Si_3 undergoes two successive antiferromagnetic phase transitions towards AF2 (T_{N2}»100 K) and AF1 (T_{N1}≈66 K) states. AF2 is a collinear phase while AF1 is a non-collinear and non-coplanar magnetic moments phase. In both antiferromagnetic states, magnetic and non-magnetic states of Mn coexist among the different crystallographic sites. The inverse MCE is associated with the transition from AF1 to AF2 under magnetic field.

Inelastic neutron scattering (INS) studies were performed in Mn_5Si_3 in order to get microscopic information on its spin and lattice dynamics and to reveal key ingredients at play in its magneto-thermodynamics properties. By using polarized INS, we have shown that the high temperature antiferromagnetic phase (AF2) is characterized by an unusual magnetic excitation spectrum, where both propagative spin waves and diffuse spin fluctuations coexist. Moreover, we have shown that the cooling by adiabatic magnetization is associated with field induced spin fluctuations. Indeed, when the magnetic field induces the switch from AF1 to AF2, the peculiar magnetic excitation spectrum of AF2 is restored starting from a zero field AF1 phase, where only spin-waves exist. Since spin fluctuations involve more microscopic states than the discrete spin-wave modes, their reappearance increases the magnetic entropy. This peculiar situation leads to the counterintuitive effect of an entropy increase associated with a magnetic field increase, which corresponds to the inverse MCE. We discuss how these properties of functional interest are intricately related to fundamental questions of magnetism: Mn at the verge of magnetic stability due to the competition between bounding and magnetism and geometrical frustration in metallic magnets.

Reference : N. Biniskos et al., Phys. Rev. Lett. 120 (2018) 257205

Strong quantum fluctuations co-existing with magnetic order in a pyrochlore iridate

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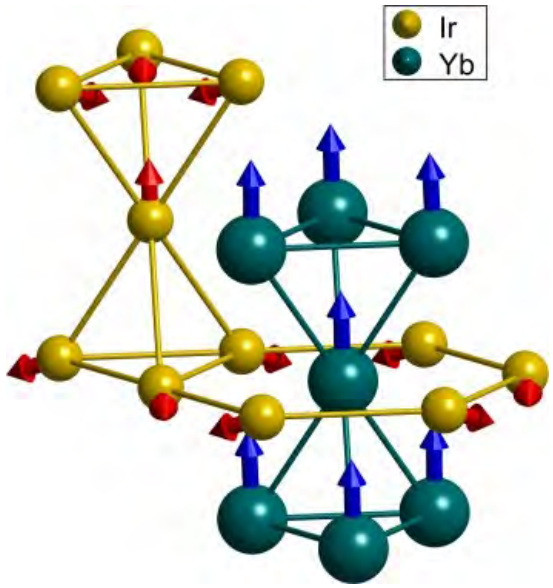
The pyrochlore oxides ($A_2B_2O_7$) consist of corner-sharing tetrahedra which host numerous exotic states of matter such as spin ice found in e.g. $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ [1] and splayed ferromagnetism in close proximity to a spin liquid state in $Yb_2Ti_2O_7$ [2].

The magnetic ground state in these materials can be tuned by external parameters such as pressure [3] and magnetic fields [4]. Local effective magnetic fields can be applied by substituting a magnetic ion on the B sites. For example, in the pyrochlore iridates ($A_2Ir_2O_7$) the Ir moments order in the all-in-all-out structure (AIAO), which creates a molecular field along the local [111] axes on the A site.

Here we present a neutron diffraction study of one of these pyrochlore iridates, $Yb_2Ir_2O_7$. Similarly to $Yb_2Ti_2O_7$ we find the Yb magnetic moments to order ferromagnetically upon cooling below T=1.5 K as shown in the figure. However, even at T=40 mK the ordered Yb moment is only half the value found in $Yb_2Ti_2O_7$ indicating that the presence of the Ir molecular field enhances fluctuations and suppresses order, in contrast to other pyrochlore iridates [5–8]. We interpret the enhanced fluctuations as a consequence of competition between different near degenerate phases.



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Spin-wave dispersions in the antiferromagnetic phase AF1 of $MnWO_4$ based on the polar atomistic model in P2

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Multiferroic properties attract much attention due to their obvious potential of applications in electronic devices, eg. Magnetoelectric sensors and data storages. Several models have been proposed to explain the mechanism of magnetoelectric effects [1]. One key factor could be a noncollinear spin configuration which is in accord with the theory associated with Aharonov-Casher effect or the inverse Dzyaloshinskii-Moriya interaction [2].

MnWO4 is an exemplary prototype of magnetoelectric control and has been intensely investigated for several years [3]. At zero field, three phase transitions are observed: the commensurate AF1 below 8 K, the incommensurate elliptical spiral spin structure AF2 in 8~12.3 K, and the incommensurate collinear sinusoidal spin structure AF3 below 13.5 K[4] . Its space group has been believed to be P2/c until our studies confirmed the true symmetry P2 and the noncollinear spin-canting structure [5]. With this new magnetic model, it is necessary to re-examine the excitation spectra and the exchange couplings as they are sensitive to the spin configurations.

We present spin wave calculations based on the noncollinear magnetic structure [6] and show good agreements with previous experimental spectra [7]. Interestingly, one of the low-lying excitation modes observed in recent neutron scattering study [8] which cannot be described by the collinear model, may be properly described in this work. The resulting consequences for the occurrence of multiferroicity in the phase AF2 are discussed.

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Putative spin-nematic phase in $BaCdVO(PO_4)_2$

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We report neutron scattering and AC magnetic susceptibility measurements of the 2D spin-1/2 frustrated magnet BaCdVO(PO4)2. At temperatures well below TN ≈ 1K, we show that only 34% of the spin moment orders in an up-up-down-down strip structure. Dominant magnetic diffuse scattering and comparison to published μsr measurements indicates that the remaining 66% is fluctuating. This demonstrates the presence of strong frustration, associated with competing ferromagnetic and antiferromagnetic interactions, and points to a subtle ordering mechanism driven by magnon interactions. On applying magnetic field, we find that at T = 0.1K the magnetic order vanishes at 3.78T, whereas magnetic saturation is reached only above 4.5T. We argue that the putative high-field phase is a realisation of the long-sought bond-spin-nematic state.

Local susceptibility of frustrated pyrochlores. Polarized Neutrons and Point Charge model

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Rare earth frustrated pyrochlore magnets are among the materials that exhibit no long range order down to the lowest explored temperatures. To better understand the many complex phenomena observed in the pyrochlores, knowledge of the local interactions present in these materials is necessary. In the pyrochlore lattice, selection between Ising, Heisenberg, or XY types of the anisotropy cannot be based on the analysis of the macroscopic properties because of the presence of four equivalent local anisotropy (<111> -type) axes. Then only an average over the four axes can be measured by classical methods. Polarized neutron diffraction based on the 'local susceptibility approach' allows to determine the local susceptibility tensor on the magnetic site [1]. Its temperature dependence in the paramagnetic phase can be accounted for by the crystal field anisotropy and a molecular field tensor that encompasses exchange and dipolar interactions. It was found that for rare earth pyrochlores an isotropic exchange model is not suitable to explain their magnetic behavior and that, instead, the exchange interaction appear anisotropic to large extent [2,3]. Local susceptibility of rare earth pyrochlores can be calculated using point charge model [].

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Topological quantum phase transition in the Ising-like antiferromagnetic spin chain $BaCo_2V_2O_8$

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Since the seminal ideas of Berezinskii, Kosterlitz and Thouless [1, 2], topological excitations are at the heart of our understanding of a whole novel class of phase transitions. In most of the cases, those transitions are controlled by a single type of topological objects. There are however some situations, still poorly understood, where two dual topological excitations fight to control the phase diagram and the transition. Finding experimental realization of such cases is thus of considerable interest. I will show in this presentation that this situation occurs in $BaCo_2V_2O_8$, a spin-1/2 Ising-like quasi-one dimensional antiferromagnet [3], when subjected to a uniform magnetic field transverse to the Ising axis [4]. In zero-field, the excitations of the Néel phase of this interesting compound consist in confined two-spinon excitations stabilized by weak interchain interactions [5]. The application of a transverse magnetic field along the b direction, because of the non-diagonal anisotropic g-tensor of $BaCo_2V_2O_8$, induces a staggered field along the a-direction [6], that is perpendicular to both the Ising-axis and the uniform field. As a result, a quantum phase transition occurs at about 10 T between two different antiferromagnetic phases: the low-field Néel phase, stabilized by the Ising anisotropy and the weak interchain couplings, and a high field novel phase, stabilized by this induced staggered field, which actually competes with the interchain interaction and the single-ion anisotropy, as determined from single-crystal neutron diffraction [4]. Using inelastic neutron scattering experiments combined with theoretical calculations, a drastic modification of the quantum excitations is evidenced beyond this phase transition: the spinon excitations of the low field phase, each carrying a spin ½ along the Ising axis, give way to their dual topological excitations in the high field phase, solitons carrying a spin 1 along the staggered magnetic field [4]. $BaCo_2V_2O_8$ thus provides a remarkable experimental system in which a novel kind of topological quantum phase transition occurs, which is described through a dual-field double sine-Gordon model in effective field theory.

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Magnetic excitations of a new potential spin liquid

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MSb_2O_6 (M=Co, Ni, Cu, Zn and Mg) usually crystallize in the tetragonal trirutile form [1], $CuSb_2O_6$ slightly distorts into a monoclinic structure due to the Jahn-Teller effect. Recently, MSb_2O_6 has been synthesized in a new structure, the rosiaite ($PbSb_2O_6$) structure, space group P-31m [2]. In this structure, the magnetic cations are arranged in trigonal layers. For M=Co and Ni these layers order antiferromagnetically at low temperatures (11K and 15K respectively), forming spin-frustrated triangles. Neutron diffraction studies confirm the rosiaite-type structure for $CuSb_2O_6$ as well (where the magnetic cations Cu^{2+} carry spin 1/2 [2]).

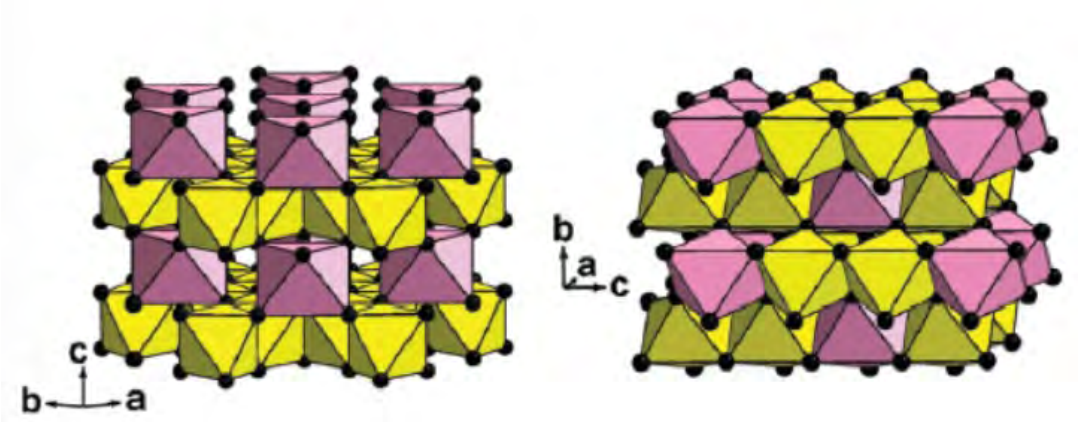

Fig.1. Two crystal structures of $CoSb_2O_6$: new trigonal form (left) and known tetragonal form (right). Yellow octahedra – SbO_6, pink octahedra – CoO_6, black balls – oxygen atoms [2].

The antiferromagnetic (AF) Heisenberg model on the triangular lattice is an example of two-dimensional geometrically frustrated magnets. With only AF nearest-neighbor interaction the ground state of this system is the three-sublattice 120^o structure, which is commensurate to the underlying lattice. With further-neighbor interactions spin liquid or skyrmion phases can be realized [3-5].

In $CuSb_2O_6$, magnetization and susceptibility indicate the presence of sizable antiferromagnetic interactions while magnetic long-range order is absent down to 2K [2]. The isotropy of the Cu^{2+} could imply a quantum (S=1/2) spin liquid scenario.

Recent IN5-data on a powder sample of rosiaite-$CuSb_2O_6$ display indeed spin-liquid like excitations and no long-range order down to 1.6K. The diffuse, steeply rising excitation spectrum is very similar to the dynamic response in 2D quantum spin liquids [6]. A gapless spin-liquid with algebraically decaying correlations is predicted for the triangular J1-J2 Heisenberg antiferromagnet for a range of interactions J2/J1 between about 0.05 and 0.17 [4], sandwiched between the 120-degree Neel state and the collinear striped AF ground state.

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Short-range and long-range ordering on the quasi-2D honeycomb layered $Na_2Ni_2TeO_6$

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The nature of the low-dimensional magnetism has been highly studied for recent years. The ground state and the excited states of such magnetic systems appear more and more exotic as the spin dimension increases and the spin value decreases. Another important question is which mechanisms are responsible for its formation in a particular case.

The current work is devoted to the study of magnetism in the layered $Na_2Ni_2TeO_6$ compound, where the honeycomb ordering of the magnetic Ni^{2+} ions in the high-spin configuration (S = 1) is realized. The magnetic susceptibility and the heat capacity measurements showed the presence of an antiferromagnetic phase transition near T_N = 27 K. Neutron powder diffraction demonstrates the long-range magnetic ordering in the system below T_N and the corresponding additional magnetic reflexes were indexed with the propagation vector k = (1/2 0 0). The following irreducible representations analysis reveals that the most preferred is the “zigzag” magnetic structure [1] with an almost perpendicular to the honeycomb layers magnetic moments direction. This antiferromagnetic ordering is the result of a complex competition of exchange interactions between the nearest and more distant neighbors on the honeycomb net [2]. Moreover, a strong diffuse magnetic scattering was observed on neutron diffraction patterns above T_N. Using XYZ polarization analysis at the DNS instrument (MLZ, Germany), such scattering has been studied [3]. The spin pair correlation function was determined after reverse Monte-Carlo modeling on $Na_2Ni_2TeO_6$ that was realized in SPINVERT program [4]. The results indicate the two-dimensional nature of the magnetic correlations, and the spin arrangement symmetry is found to be similar in both the short-range and long-range ordered magnetic states.

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Breaking and re-arrangement of valence bonds in the triangular spin liquid $YbMgGaO_4$

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Triangular antiferromagnets display complex magnetic excitations that may be distributed over a broad range of energies and momenta forming an excitation continuum. In systems with long-range magnetic order, this continuum appears above spin-wave excitations due to multi-magnon processes. In the absence of long-range order, the continuum extends to zero energy and may have a completely different origin hosting exotic fractionalized (spinon) excitations. Such a scenario has been proposed for $YbMgGaO_4$ [1] that evades the magnetic order and bears all characteristic signatures of a spin-liquid ground state, with spins remaining dynamic down to at least 50 mK.

Here, we probe this scenario experimentally using inelastic neutron scattering on $YbMgGaO_4$ single crystals. We observe the continuum of excitations in the 0-2 meV energy range and interpret them within the valence-bond framework that entails pairs of antiferromagnetically coupled spins distributed over the geometrically frustrated triangular lattice. The continuum consists of two parts. Above 0.2 meV, the excitations are due to the breaking of nearest-neighbor valence bonds [2], whereas below 0.2 meV several processes involving the re-arrangement of valence bonds need to be considered. Such a re-arrangement leads to the propagation of free spins, as expected for spinons. However, structural disorder inherent to $YbMgGaO_4$ renders these excitations strongly localized.

We conclude on several interesting features of the triangular spin liquid in $YbMgGaO_4$. It bears similarities to the resonating-valence-bond (RVB) state of triangular antiferromagnets, as proposed by P.W. Anderson back in 1973 [3], but only the high-energy part of the spectrum reveals excitations that would be expected from such an RVB state. At low energies, free spins become increasingly important and facilitate the re-arrangement of valence bonds, similar to spinon excitations. This mixed ground state combining the valence bonds and free spins, seems to be a consequence of the Mg/Ga structural disorder in the material, and suggests that further unusual valence-bond magnets can be designed using triangular 4*f* oxides with the controlled structural disorder.

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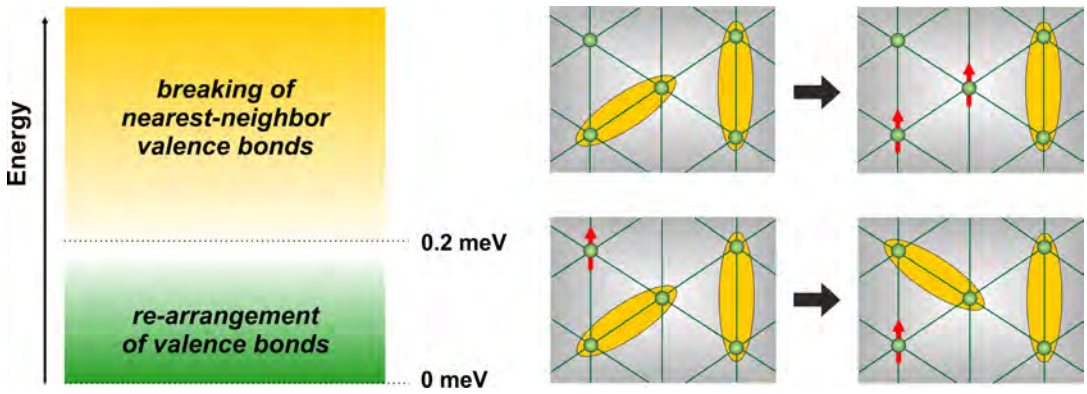

Magnetic excitations in $YbMgGaO_4$ represented by two types of valence-bond processes

Neutron Depolarization Measurements of Quantum Critical Ferromagnets

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In ferromagnetic quantum critical systems it is possible to suppress the Curie temperature to 0 K by changing an external control parameter such as a magnetic field or hydrostatic pressure. Recent theories suggest a generic phase diagram for clean quantum critical ferromagnets featuring a tricritical point where the order of the phase transition changes from 2nd to 1st. This behavior has already been observed e.g. in $ZrZn_2$ and MnSi, and is also discussed for $SrRuO_3$. An exception to this behavior could be the ferromagnetic Kondo lattice CePt as no tricritical point was observed, yet. The neutron depolarization technique offers new insight into ferromagnetic quantum critical systems as it enables us to directly probe ferromagnetism in challenging sample environments, such as magnetic fields, low temperatures, and high pressures. We present two neutron depolarization studies of the compounds $SrRuO_3$ and CePt up to hydrostatic pressures of 17 GPa and 12 GPa, respectively.

Critical scattering in classical and quantum critical systems

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We report on a study of critical scattering in classical and nearly quantum critical antiferromagnets (AFMs). The energy width of the critical scattering was determined by high-resolution neutron spin-echo at TRISP at the MLZ in Munich. The classical systems studied include the s=5/2 AFMs Rb_2MnF_4 and MnF_2 with quasi 2D and 3D spin interactions, respectively. Both compounds are Heisenberg AFMs with a small uniaxial anisotropy resulting from dipolar spin-spin couplings, which leads to a crossover in the critical dynamics close to the Neel-Temperature (T_N). By means of our high-resolution measurement we were able to identify the dynamical critical exponents z for both longitudinal and transverse fluctuations. Thus discrepancies between experiment and theory observed in previous three-axis studies could be resolved. For a study of quantum critical systems, we chose the $CeCu_{(6-x)}Au_{(x)}$ series, which exhibits a quantum critical point at x=0.1 seperating nonmagnetic (x<0.1) and magnetically ordered ground states (x>0.1). First measurements at $CeCu_{5.8}Au_{0.2}$ (T_N=0.22K) show a hitherto unexplained dynamical critical exponent

Pressure-induced evolution of magnetic excitations in CeCoSi

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Ce and Yb-based intermetallic compounds exhibit many exceptional properties, such as unconventional superconductivity, heavy-fermion behavior and mixed-valence states. Usually, a ground state of these systems is defined by a delicate balance between RKKY-interaction and Kondo screening, and it turns out to be rather sensitive to the influence of external tuning parameters, such as pressure, chemical substitution or magnetic field. Here we focus on metallic antiferromagnet CeCoSi, which has an unusual $T - P$ phase diagram. Cerium moments order below T_N = 8.8 K, however, results of resistivity [] and susceptibility measurements [] have shown, that a moderate hydrostatic pressure of $P_{c1} \approx 1.5$ GPa, stabilizes a new pressure-induced-ordered phase with significantly higher transition temperature of $T_C \approx 40$ K. Further pressure increasing induces a quantum phase transition towards a nonmagnetic ground state at $P_{C1} \approx 2.2$ GPa.

Motivated by these observation, we explored magnetic structure and excitation spectra of CeCoSi by means of elastic and inelastic neutron scattering. We found that at ambient pressure cerium moments order in a simple AFM structure with $\boldsymbol{q} = 0$. Using the results of inelastic neutron scattering and specific heat measurements we resolved the Hamiltonian of crystalline electrical field at $P = 0$. Furthermore, we studied low-energy magnon excitations as a function of hydrostatic pressure up to $P \approx 1.5$ GPa using cold INS and discuss a possible origin of the giant enhancement of transition temperature under pressure.

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Insight into high-Tc superconductors and frustrated magnets on the D7 polarized neutron scattering instrument at the ILL

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Polarized neutron scattering is a powerful technique, which allows to distinguish between nuclear and magnetic contributions. The D7 instrument at the Institut Laue-Langevin [1,2] is equipped with permanent polarization analysis, which is useful to separate coherent from incoherent scattering for soft matter but is essentially dedicated to magnetic diffuse scattering, i.e. short-range correlations. Recent work on pyrochlores [3,4] has proven that D7 is particularly strong in the field of frustrated magnetism. Notably, the influence of defects on the nature of the magnetic ground state has been evidenced in $Yb_2Ti_2O_7$ [4]. Furthermore, capability of studying superconductors on D7 is being developed. A mysterious pseudo-gap phase, appearing at temperatures above the superconducting transition in cuprates, is of particular interest [5,6]. Last results on $HgBa_2CuO_{4+d}$ [6] put new constraints on the origin of the observed q=0 magnetism. Through these two examples, we intend to show that D7 plays a crucial role in understanding magnetic properties of strongly correlated systems.

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High-Tc Ferromagnetic Semiconductors: Fake or Fact?

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Traditional semiconductors are based on the control of charge carriers (n- or p-type). Magnetic-ion-doped semiconductors allow in addition the control of the quantum spin state (up or down), which has attracted great interest because of their potential applications in spintronics and blue-light emitting diode (LED) technologies. The main challenge for practical applications is the attainment of a Curie temperature T_C at or preferably above room temperature, whose realization relies on both the large moment of the substituted magnetic ions and carrier-induced ferromagnetic exchange interactions. So far the highest Curie temperatures were obtained for layered $Ga_{1-x}Mn_xAs$, ranging up to T_C=180 K for x>0.1. More recently, the work on diluted magnetic semiconductors has been concentrated on transition-metal-doped ZnO and GaN, for which T_C values above room temperature were predicted [1]. Indeed, several studies reported T_C's above room temperature, but the results have to be considered with caution, since none of these findings has resulted in a device working at room temperature.

Here we discuss how neutron scattering experiments can contribute to resolve the ongoing controversies about high-T_C ferromagnetic semiconductors. The questions to be addressed are fourfold: (i) The solubility of magnetic ions in the host compound is limited, so that the investigated samples are often contaminated by magnetic clusters or other phases which are ferromagnetic in nature. (ii) The doped magnetic ions may be located either at regular lattice positions or at interstitial positions. (iii) What is the valence of the substituted magnetic ions? (iv) The doped magnetic ions inject charge carriers which are expected to generate a sizable ferromagnetic component to the exchange interaction through Zener's kinetic exchange mechanism. Neutron diffraction and neutron spectroscopy are the experimental techniques of choice to shed light on all these issues. This is demonstrated for some semiconductors doped with transition-metal ions, emphasizing on Mn-doped GaN [2]. We conclude from our recent work on polycrystalline samples of $Ga_{1-x}Mn_xN$ [3] that the T_C values reported in the literature to be above room temperature are unsubstantiated.

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Study of high-pressure cubic phase of $RGe_{2.85}$ (R = Tb, Dy) by neutron diffraction

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It was found that in R-Ge family the high pressure cubic phases of $RGe_{2.85}$ compounds exist (where R = Tb, Dy). These metastable compounds have $AuCu_3$ type structure (space group Pm-3m) [1]. By the means of neutron powder diffraction it was shown that at ambient pressure the magnetic moments of Tb and Dy ions in these compounds order in incommensurate antiferromagnetic structure with wave vectors q(Tb) = (0.5, 0, 0.16) in r.l.u. and q(Dy) = (0.5, 0, 0.164) in r.l.u. at T = 10 K and 4 K, respectively. The formation of such unusual magnetic order in this structure was linked with the charge density wave order which exist in these compounds at 145 and 80 K, respectively [2, 3, 4]. In $TbGe_{2.85}$ compound with the application of external pressure the CDW transition temperature decreases with the rate of $dT_{CDW}/dP \approx -48$ K/GPa and the CDW transition disappears above pressure P > 2.6 GPa. The AFM transition temperature is approximately constant in the pressure range P = 0-5 GPa [3]. Above P > 2.6 GPa the second magnetic commensurate phase exist with the wave vector (1/2, 0, 0). The similar behaviour of CDW was observed for $DyGe_{2.85}$ compound where $dT_{CDW}/dP = -65$ K/GPa and CDW transition disappears above P > 1.2 GPa. The Neel temperature for this compound T_N = 20 K and it is approximately pressure independent in the range P = 0-3 GPa. It should be noted that the same commensurate antiferromagnetic structure was observed for RSn_3 compounds with the $AuCu_3$ structure.

By the means of Time differential perturbed angular gamma-gamma correlation technique it was shown than in both compounds the CDW is incommensurate in paramagnetic phase and becomes commensurate below Neel temperature.

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Magnetic ordering features of the $Co_{5-x}Zn_xTeO_8$ spinel-type series

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Spinel materials were always of considerable attention due to a rich variety of exhibiting phenomena, especially in the field of magnetism. For materials with general formula AB_2O_4 rather simple cationic arrangement gives rise to a numerous possible magnetic behaviour. $CoCr_2O_4$, for instance, possess a re-entrant spin glass ground state preceded by a commensurate ferrimagnetic transition at 93 K and incommensurate spiral at 27 K, which, in turn, locally breaks symmetry causing emerge of electrical polarization and therefore multiferroic type-II behaviour [1]. Moreover, magnetic dilution on both A and B sublattices leads to significant alterations of magnetic properties: while for tetrahedral A-sites Zn doping suppresses the spiral ordering [2] for octahedral B-sites, in turn, it increases an in-field magnetization and saturated electronic polarization [3].

The aim of the current work was to characterize a magnetic ordering of $Co_{5-x}Zn_xTeO_8$ spinel family. Depending on synthesis conditions two different polymorphs Co_5TeO_8 ($Co[Co_{1.5}Te_{0.5}]O_4$) may be obtained: classical "disordered" *Fd*-3*m* and "ordered" non-centrosymmetric $P4_332$ within which B-site Co^{2+} and Te^{6+} cations order in Kagome layer. Magnetic susceptibility measurements have revealed the same Curie-Weiss behaviour for both polymorphs with θ = - 148 K. Neutron powder diffraction at G4.1 powder diffractometer (LLB, Saclay, France) has shown that the "disordered" polymorph is a conventional ferrimagnet with T_C = 40 K, μ= -1.94(6) μ_B on A-sites and μ = 2.39(7) μ_B on B-sites at T = 1.8 K. The "ordered" one demonstrates more complex behaviour: below T_{C1} = 45 K the magnetic structure is conical and at T_{C2} = 27 K an additional ferrimagnetic component appears with an increasing of incommensurate k-vector **k** = (0 0 k_z) from k_z=0.086 to k_z=0.137. Moreover, NPD on the ordered Co_5TeO_8 has shown the presence of a strong magnetic diffuse scattering below 130 K which was studied by means of XYZ neutron polarization analysis at D7 spectrometer (ILL, Grenoble, France). Pure magnetic scattering in a wide range of temperatures obtained at D7 was then treated with the SPINVERT program [4]. Thus, the reverse Monte-Carlo simulations showed that short-range correlations presented in the system above 45 K have a conical character, indicating an important role of frustration of magnetic exchange interactions and anisotropy at temperatures significantly higher than T_{C1}.

Neutron and X-ray diffraction measurements for $Co_{5-x}Zn_xTeO_8$ exposed that for 0 < x < 1 magnetic dilution takes place exclusively at the A-site. In turn, magnetic susceptibility measurements revealed a decrease of both: the magnetic ordering temperature and the magnetic susceptibility itself upon the increase of Zn. To plot a magnetic phase diagram of $Co_{5-x}Zn_xTeO_8$ as a function of x, a series of experiments was performed at D1B powder diffractometer (ILL, Grenoble, France). Results of NPD agree with macroscopic measurements and show a total suppress of the ferrimagnetic component for x > 0.2 accompanied by a dramatic drop of the k-vector to k_z = 0.065. Upon further increase of Zn in the system k-vector increases up to k_z = 0.19 indicating a shortening of a conical modulation up to x = 1 at which no coherent magnetic scattering is observed down to 1.8 K, pointing out only a short-range ordering for Co_4ZnTeO_8.

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Magnetic frustration in $SrLn_2O_4$ compounds studied by magnetic PDF-analysis

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The Ln^{3+} magnetic ions in $SrLn_2O_4$ compounds reside on 2 sites (distinguished by their slightly different crystallographic environments) within distorted hexagonal planes that are connected perpendicularly via 1D chains and triangular ladders. Geometric frustration between next-nearest neighbors results in complex magnetic structures containing a certain degree of local spin disorder, thus leading to diffuse magnetic scattering of neutrons. The total magnetic scattering (both Bragg and diffuse) can be isolated from the neutron diffraction pattern and Fourier transformed to produce a magnetic Pair-Distribution Function or mPDF(r) [1], a real-space function of relative distance between magnetic ions (here only Ln^{3+}) that exhibits positive or negative peaks for ferro- or antiferro-magnetic alignment between spins, respectively. The local quasi-instantaneous magnetic structure reported by the mPDF(r) is complementary to the space+time averaged structure gained through Rietveld refinement of elastic magnetic scattering at Bragg peak positions, and has an additional advantage of revealing not only static spin-spin correlations below T_N, but also dynamic spin-spin correlations above T_N.

In the case of Ln = Gd, the temperature dependence of the mPDF(r) shows that the 1D chains order first and progressively as T decreases towards T_N = 2.7 K, followed by ordering between chains and within the hexagonal sheets once T_N is reached (see figures below). The positive slope in the mPDF(r) between 0 and 2.5 Å corresponds to the *collinear* ferromagnetic ordering within the 1D chains. The short range of the dynamic spin-spin correlations above T_N is immediately visible.

In the case of Ln = Nd (data not shown), the mPDF(r) exhibits both below and above T_N = 2.3 K a clear negative peak at 3.55 Å that corresponds to the *transverse* antiferromagnetic ordering along the 1D chains. As expected, a positive peak occurs at twice this distance, *i.e.* 7.1 Å, whose spin-spin correlations are however weaker above T_N due to the finite magnetic correlation length. In addition, a negative peak at 6.1 Å below T_N attests to the antiferromagnetic inter-ladder ordering of the long-range ordered magnetic phase whose two possible spin assignments were also distinguished, but with greater difficulty, using standard Rietveld refinement techniques.

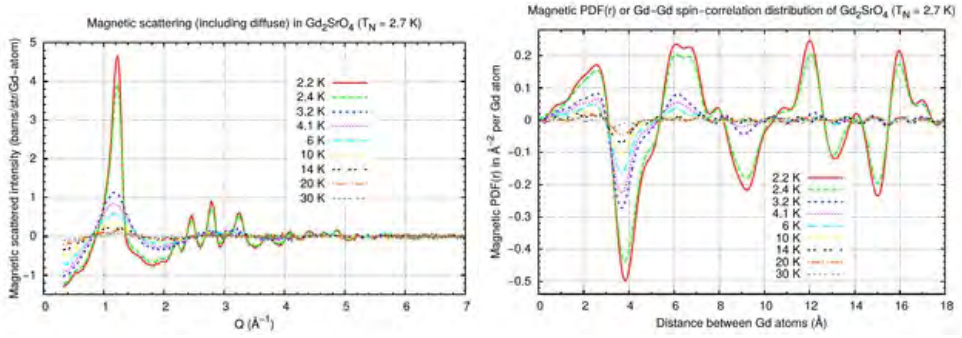

Figure 1: (Left) Magnetic Bragg peaks and magnetic diffuse scattering measured from a powder sample of $SrGd_2O_4$ with the D4c neutron diffractometer (wavelength = 0.5 Å) at the Institut Laue-Langevin. (Right) The corresponding magnetic Pair-Distribution Function or mPDF(r) obtained via Fourier transformation of the same diffraction data.

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Chiral spin liquid ground state in a highly frustrated extended kagome system

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A chiral spin liquid ground state is observed in the extended layered kagome system $YBaFeCo_3O_7$. This system is extremely frustrated with a Curie-Weiss constant of -2000K but there is no observed magnetic order at low temperatures.[1]

While classical Heisenberg models show the existence of an extended spin liquid phase due to strong geometric frustration effects for nearest neighbor antiferromagnetic interactions, [2] indeed the lack of inversion symmetry for these bonds allows for Dzyaloshinskii-Moriya interactions, which may add a specific chirality to the spin liquid state.[3]

As these properties were hidden to earlier powder diffraction, we studied a single crystal sample at low temperatures by neutron diffraction with polarization analysis, and separated the magnetic diffuse scattering further in contributions from in- and out-of (hk0)-plane components, including all possible chiral terms by additional polarization reversal.

By Fourier analyses of these diffuse scattering contributions the spatial correlation functions were obtained, which establishes the vector spin correlation function. The most significant correlation relates to a specific cycloidal chirality that indicates a triple-q vortex of rather short-period.

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Emergence of a dimer physics in the Cairo frustrated pentagonal magnet $Bi_2Fe_4O_9$

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The Fe^{3+} ions in $Bi_2Fe_4O_9$ materialize the first analogue of a magnetic pentagonal lattice [1]. The unit cell contains two different sites of four iron atoms each, which have different connectivities with the other irons (three or four neighbours for Fe_1 and Fe_2 respectively), and that form a lattice of pentagons. Because of its odd number of bonds per elemental brick, this lattice is prone to geometric frustration. The compound magnetically orders around 240 K: the resulting spin configuration on the two sites is the same, i.e. two orthogonal pairs of antiferromagnetic spins in a plane, with a global rotation between the two sites Fe_1 and Fe_2. This peculiar magnetic structure, which is the result of the complex connectivity and magnetic frustration, has opened new perspectives in the field of magnetic frustration.

Here, we present some consequences of the frustrated and hierarchical magnetic interactions in this original system. First, magnetization distribution maps have been obtained using polarized neutrons under an applied magnetic field at the Institut Laue Langevin (ILL). Remarkably, the magnetic moments of the Fe_1 sites, contrary to Fe_2, are extremely weakly polarized by the field both in the paramagnetic phase and in the ordered one. In order to understand this peculiar behaviour, the magnetic excitations have been investigated by inelastic neutron scattering using triple axis spectrometers at the LLB and the ILL. The confrontation of the experimental results with spinwave calculations allows to determine the Hamiltonian of the system and shows in particular that the Fe_1 forming the orthogonal pairs are coupled to each other by a strong antiferromagnetic exchange, thus materializing isolated singlet dimers in the paramagnetic state. Additionally, we found in the ordered state a second type of frustrated dimers of parallel Fe_2 whose signature is a flat mode in the magnetic excitations.

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Anharmonic magnon excitations in non-collinear and charge-ordered $RbFe^{2+}Fe^{3+}F_6$

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$RbFe^{2+}Fe^{3+}F_6$ is a charge-ordered antiferromagnet, belonging to the family of mixed-metal fluorides $AM^{2+}M^{3+}F_6$ (A = alkali metal or NH4; M is a metal). Although $RbFe^{2+}Fe^{3+}F_6$ is usually presented as a pyrochlore system [1,4], its structure can also be described as interpenetrating chains of corner-shared $Fe^{3+}F_6$ and $Fe^{2+}F_6$ octahedra, running along the b and a axes respectively. Neutron diffraction and magnetisation measurements show that this system orders below T_N = 16 K [1], where the spins associated to Fe^{3+} (S = 5/2) and spins associated to Fe^{2+} (S = 2) form a non collinear orthogonal structure. Moreover, the magnetic moment related to Fe^{3+} is significantly reduced in the ordered state. Inelastic neutron scattering on single crystals highlights two well separated spin wave bands due to the two charge-ordered chains. Interestingly, high resolution measurements show a broad continuum located at an energy scale of twice the lower spin wave mode, where two magnon processes are kinematically allowed. Taking into account the strong reduction of the Fe^{3+} magnetic moment, as well as the non-collinearity of the spin structure in this system, this continuum is interpreted as magnon decay, in agreement with theoretical views on non-collinear two dimensional antiferromagnets [2]. In this case, magnon decay is thought to arise from the interaction between the longitudinal fluctuations of the Fe^{3+} spins and the transverse excitations of Fe^{2+} spins, thanks to interchain interactions. $RbFe^{2+}Fe^{3+}F_6$ is therefore a unique example illustrating a coupling between charge and spin ordering through multi-magnon processes [3].

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Stabilizing magnetic spirals in layered perovskites far beyond room temperature

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In the past years, magnetism-driven ferroelectricity and gigantic magnetoelectric effects have been reported for a number of frustrated magnets with spiral magnetic orders. Such materials are of high current interest due to their potential for spintronics and low-power magnetoelectric devices. However, their low magnetic order temperatures (typically <100K) greatly restrict their fields of application.

Recently, we have established that chemical disorder is a powerful tool that can be used to stabilize magnetic spiral phases up to 310K [1]. Here we explore the design space opened up by this novel stabilization mechanism, recently rationalized in terms of random magnetic exchanges [2]. We show that in CuFe-based layered perovskites T_{spiral} can be further increased up to 400K, and we reveal a scaling law between this quantity and the spiral wave vector [3]. This linear relationship ends at a paramagnetic–collinear–spiral multicritical point, which defines the highest spiral-order temperatures that can be achieved in this kind of materials. Based on our findings, we propose a general set of rules for designing magnetic spirals in layered perovskites using external pressure, chemical substitutions and/or epitaxial strain, which should guide future efforts to engineering spiral phases with order temperatures suitable for technological applications.

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Control of magnetic chirality in $Nd_{1-x}Tb_xMn_2O_5$ by external electric field

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Manganite oxides family RMn_2O_5 (R – rare-earth element) represents prominent example of a multiferroics with extremely interesting and close relationship between magnetism and ferroelectricity [1-3]. The most significant issue in the studies of RMn_2O_5 is the understanding of the microscopic mechanisms responsible for spin-driven ferroelectricity in these compounds. In order to make a new approach to those mechanisms we performed the detailed investigations of the magnetic ordering in single crystals of multiferroics $Nd_{1-x}Tb_xMn_2O_5$ (x = 0, 0.2, 1) using both non-polarized and polarized neutron diffraction techniques.

In all the crystals, the chiral scattering originated from the difference between the population of right- and left-handedness chiral domains was observed. This difference can be controlled by the external electric field of few kV/cm revealing strong magnetoelectric coupling. The results are discussed within the frame of antisymmetric super-exchange model for Dzyaloshinsky-Moria interaction.

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Anomalous lattice dynamics in La(2-x)Sr(x)CuO(4+y): The role of static and mobile dopants

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The cuprate $La_{2-x}Sr_xCuO_{4+y}$ (LSCO+O) is an interesting model system for high-temperature superconductivity due to its relatively simple crystal structure and differences in the superconducting transition temperature, T_c, as function of strontium and oxygen doping. Hole-doping with Sr^{2+} (LSCO) creates a superconductor where T_c varies monotonically with doping. Doping with highly mobile, excess O^{2-}, in contrast, results in a bulk superconductor separated into two unique phases, regardless of strontium content: 1) An optimally doped, bulk superconducting phase (T_c = 40K)[1] with low pinning[2] and a 2) long-range modulated antiferromagnet with period ≈ 8 similar to the striped cuprates[3].

While both optimally doped LSCO and LSCO+O have similar superconducting properties, the specific role of the dopant ions on a microscopic scale is still unknown. Recently, an anomaly in the Cu-O bond stretching phonon was found to correlate with T_c in Sr-doped LSCO, indicating a coupling to a novel charge mode possibly related to stripes[4,5]. In order to distinguish between a lattice effect driven by the superconducting transition or a lattice anomaly introduced by Sr doping, we concentrated our research on samples that are strongly underdoped in terms of Sr ($x \leq 0.06$), but optimally superconducting (T_c = 40K) due to excess oxygen. Our neutron scattering measurements on x = 0.06 and x = 0 show phonon anomalies with similar strength to optimally doped LSCO as reported in literature (Figure 1A)[6], strengthening the argument for an electronic origin of the phenomenon. Strong magnetic fields are known to increase the volume fraction of the stripe-like magnetic phase in our samples[7] but reveal no effect on the phonon anomaly (Figure 1B). Our studies raise important questions to the significance of stripe order in the superconducting cuprates.

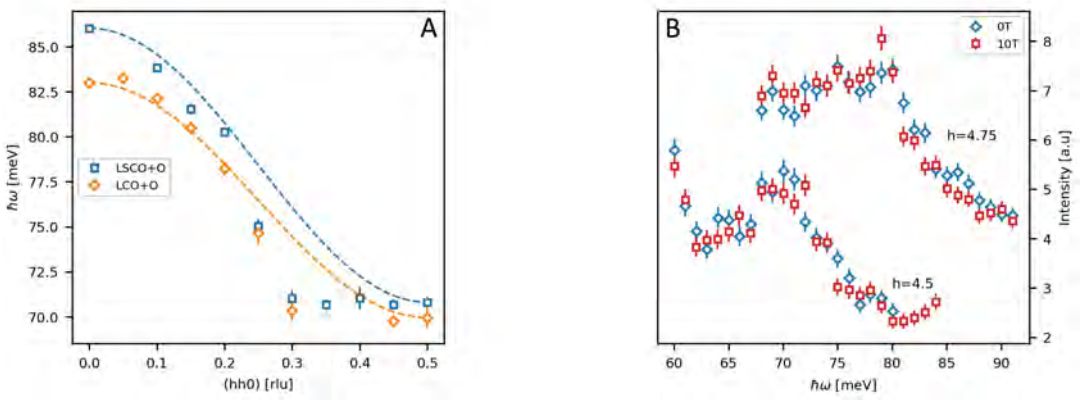

Figure_1: **(A)** Dispersion of Cu-O bond-stretching phonon in LSCO+O (x=0, x=0.06) as obtained from peak positions of individual spectra. Dashed line represents the "normal" sinosoidal dispersion. **(B)** Individual scans of LSCO+O (x=0.06) at normal (h=4.5) and anomalous (h=4.75) wave vectors in zero magnetic field and with H=10T.

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Magnetic and magnetoelectric phases of $LiNiPO_4$ up to 55T

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We present a study of the magnetic phases of orthorhombic $LiNiPO_4$ and their interrelation with magnetoelectricity. We have probed the magnetization and electric polarization along the a-axis for fields up to 55T applied along the c-axis [1]. These data reveal hitherto unknown magnetic phases above transitions fields 37.6T, 39.4T and 54.1T. In combination with earlier reports [2-5], the three phases reported here bring the total number of low-temperature magnetic phases of $LiNiPO_4$ to eight for fields smaller than 55T. Three of these phases, including the phase between 39.4T and 54.1T [1], display a pronounced magnetoelectric effect. To understand the coupling between magnetoelectricity and magnetic structure, we performed neutron diffraction experiments in static fields up to 26T at HFM/EXED Helmholtz Zentrum Berlin, and in pulsed fields up to 42T at NOBORU, J-PARC. We identified the magnetic propagation vectors in the field ranges 37.6T to 39.4T and 39.4T to 42T to be **k**=(0 1/3 0) and **k**= (0 0 0), respectively. We conclude that magnetoelectricity in $LiNiPO_4$ requires a magnetic structure with the same periodicity as the lattice. All phases not satisfying this criterion are non-magnetoelectric.

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Effect of chemical substitution on the magneto-electric coupling of the $(ND_4)_2[FeCl_5(D_2O)]$ hybrid multiferroic

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The hybrid system $(NH_4)_2[MX_5(H_2O)]$ (X = halide ion and M = magnetic metal) or ammonium ion) represents a new approach to obtain materials with strong magneto-electric coupling. In particular, $(NH_4)_2[FeCl_5(H_2O)]$, is a multiferroic material below *ca.* 6.9 K,[i] where multiferroicity stems from a cycloidal magnetic structure propagating in the *c*-axis with **k** = (0, 0, 0.23) and with the magnetic moments lying in the *ac*-plane that produces ferroelectric polarization through the spin-current mechanism.[ii]

The observation of giant spin-driven ferroelectric polarization under external pressure in an archetypical multiferroic as $TbMnO_3$, [iii] has stimulated the studies on the effect of applied pressure in multiferroics. An alternative to hydrostatic pressure is chemical pressure, which in this system can be achieved through partial substitutions of Cl^- by Br^- ions into the iron environment. The influence of the chemical pressure in the physical properties of the $(ND_4)_2[FeCl_{5x}Br_{5-5x}(D_2O)]$ series, for low values of x, has been studied combining magnetometry measurements, specific heat, X-ray and neutron diffraction experiments. By replacing Cl^- by Br^-, an increase in T_N is observed, suggesting a change in the magnetic structure, probably due to a decrease of magnetic frustration. Single-crystal neutron diffraction measurements have revealed a continuous change in the magnetic propagation vector **k** = (0, 0, k_z) for low values of x, followed by an abrupt change to **k** = (0, 0, 0) for higher substitution rates ($x \gtrsim 0.2$).

The inclusion of bromine produces a variation of the exchange-coupling scheme proposed for the $(ND_4)_2[FeCl_5(D_2O)]$ compound that allowed explaining the observed cycloidal magnetic structure. This exchange-coupling model involves a non-negligible frustration between the different iron centers, which is the final responsible of the magnetic moments configuration. The increase of T_N, suggests a decrease of this frustration, which is compatible with the occurrence of a magnetic propagation vector **k** = (0, 0, 0) for the higher values of x, as occurs by applying magnetic field[iv] or by changing the ammonium counterion by a monovalent alkali metal.[v]

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Proof of the elusive high-temperature incommensurate phase in CuO by spherical neutron polarimetry

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CuO is the only known binary multiferroic compound so far and due to its high transition temperature (230 K [1]) into the multiferroic state it has been extensively studied [2, 3]. Compared to other prototype multiferroic materials it shows close analogies with respect to the sequence of magnetic phase transitions and the nature of the involved phases. However, the nature and even the existence of the high-temperature incommensurate – so called AF3 – phase has been strongly debated [4, 5] – both experimentally and theoretically – since it is only stable for a few tenths of a Kelvin just below the Néel temperature.

Here we demonstrate the huge potential of spherical neutron polarimetry, firstly, in detecting changes in the magnetic structure which are not or weakly manifest in the intensity of the magnetic Bragg peaks and, secondly, in deducing the spin arrangement of the so far hypothetic AF3 phase. Using spherical neutron polarimetry, we have confirmed the extensively studied magnetic structures in the AF1 and AF2 phases [Fig. 1(a) and (b) respectively]. We have also derived unambiguous proof for the existence of the elusive AF3 phase in CuO by following specific polarization matrix elements - which are susceptible to the change in the magnetic structure - as a function of temperature. Furthermore, our data allows the exact determination of the magnetic structure.

This is the first neutron scattering study able to overcome the difficulties in observing this phase owing to a very small ordered magnetic moment (~0.06 m_B) and a stability range of only 0.5 K below an elevated T_N.

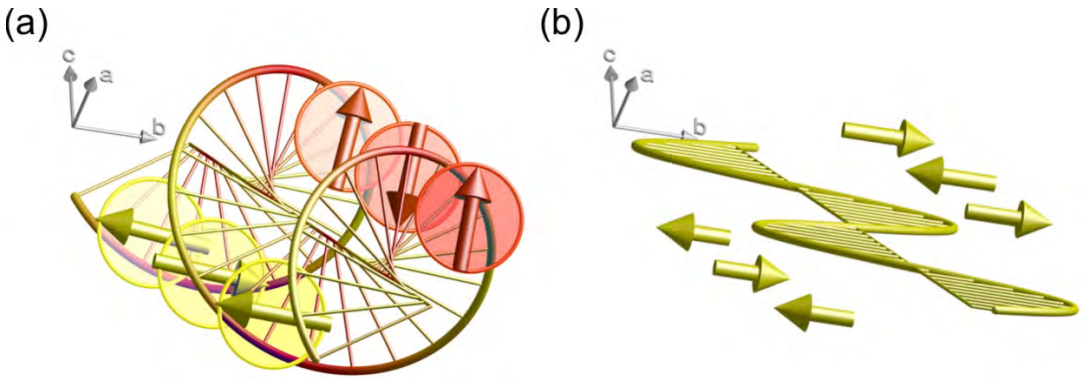

Figure 1: (a) Cycloidal magnetic structure in the AF2 phase, (b-d) Collinear sinusoidally modulated magnetic structure within the AF1 phase with magnetic moments along the b axis.

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Unusual Spin Structures in Quadruple and Simple Exotic Perovskites

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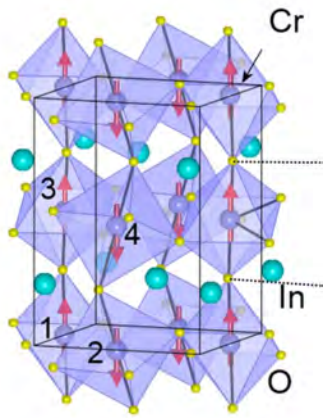
ABO_3 simple perovskites are usually formed with large A cations. However, it is possible to prepare the so-called 'exotic' perovskites with small A cations, such as, A = Mn^{2+}, Sc^{3+} and In^{3+}, using a high-pressure high-temperature method [1]. Due to large structural distortions/tilts of such perovskites at the B sites unusual physical properties are expected. There is a special class of the perovskite family - the so-called A-site ordered quadruple perovskites, $AA'_3B_4O_{12}$ - which also has very large structural distortions/tilts. $AA'_3B_4O_{12}$ perovskites are formed when the A' site is occupied by small Jahn-Teller cations (such as, Cu^{2+} and Mn^{3+}), and the A site has a large cation.

In this presentation, we show our results on magnetic structure determination and physical properties of a large number of quadruple perovskite manganites (e.g., AMn_7O_{12} (A = Cd, Ca, Sr, and Pb) [2] and RMn_7O_{12} (A = La, Ce, Nd, Sm, Eu, Y, and Bi) [3]) and simple perovskites [e.g., $ScCrO_3$, $InCrO_3$ [4] (a figure shows the C-type magnetic structure of $InCrO_3$), Sc_2NiMnO_6, and In_2NiMnO_6 [5]) prepared by a high-pressure high-temperature method. Many of these compounds show deviations from the Goodenough-Kanamori rules and counterintuitive magnetic structures. As a result of different types of competitions, they often exhibit a number of different magnetic transitions and spin-induced multiferroic properties.



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Neutrons as a key method for accessing magnetoelastic effects

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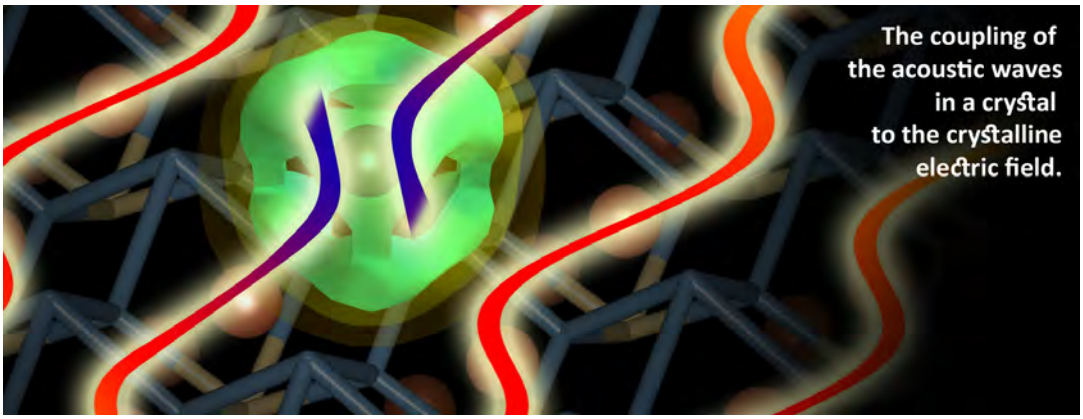
Nearly a century of research has established the Born–Oppenheimer approximation [1] as a cornerstone of condensed-matter systems, stating that the motion of the atomic nuclei and electrons may be treated separately. Interactions beyond the Born–Oppenheimer approximation are at the heart of magneto-elastic functionalities and instabilities. These effects are often neglected and believed non-important for overall system.

Recently, magneto-elastic (namely crystal-field - phonon) excitations are becoming topical in different groups of compounds, like the magnetoelastic interactions in pyrochlores [2], the phonon-crystal field bound state in NpO_2 [3] or the coupled modes in multiferroic rare-earth iron borates [4]. Still studied materials are considered as rare examples of the physics beyond Born-Oppenheimer approximation.

We will show you comprehensive neutron spectroscopy and ab-initio phonon calculations of the coupling between phonons and crystalline electric field in typical heavy fermion material $CeAuAl_3$ [5-6]. Our careful analysis of three axis spectrometer data reveals, that electron-phonon interaction can lead to creation of the new states in the matter, even in the case of weak interactions. Namely:

1) An anti-crossing between a crystal field excitation and acoustic phonons in the paramagnetic state of an intermetallic compound at zero magnetic field, observed for the first time.
2) The vibronic bound state driven by acoustic rather than optical phonons.
3) General observation of damping caused by the interaction with the conduction electrons.

Our observations imply that magneto-elastic hybrid excitations must be abundant and rather generic, establishing neutron spectroscopy as the only method for its direct detection. We expect that future studies will identify a large number of further examples of similar hybrid effects in seemingly harmless materials.



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Magnetic structure and magnetic excitations in the multiferroic pyroxene $SrMnGe_2O_6$

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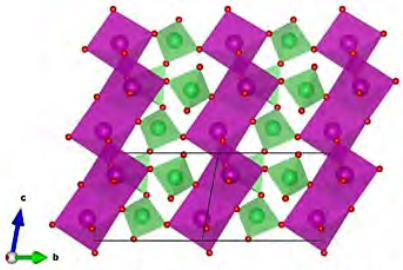
As a non-trivial magnetic system, pyroxenes with chemical formulas AMT_2O_6 (A = mono- or divalent metal, M = di- or trivalent transition metal, T = Si or Ge) containing magnetic cations have recently attracted revitalized interest because of their intriguing quasi-one-dimensional magnetic and multiferroic properties [1]. These properties are associated with the special atomic arrangement of the pyroxene crystal structure, where almost isolated zig-zag chains of edge-sharing MO_6 octahedra are bridged by corner linked TO_4 tetrahedra chains. The magnetic subsystem in pyroxenes is therefore quasi one-dimensional (fig.1). One aspect is here especially important, a “shifted” packing of neighboring M chains leads to the situation where every M ion is connected (via its own O and XO_4 tetrahedra) with two M ions in neighboring chain. Thus, the general topology of exchange interaction is triangular-like (see Fig. 1), and the magnetic system may be frustrated. We recently investigated the crystal structure and magnetic properties of a new clinopyroxene compound $SrMnGe_2O_6$ (*C2/c* monoclinic space group), by means of neutron powder diffraction and magneto-electric measurements [2]. A multiferroic behavior was revealed by the appearance of a spontaneous polarization at T_N where the incommensurate magnetic order appear. Recently, we have succeeded in growing large single crystal of $SrMnGe_2O_6$ by floating zone furnace technique. In this contribution, we will present elastic and inelastic neutron scattering experiment along with magnetization, heat capacity and pyroelectric current measurement. The neutron diffraction experiment allowed us to determine in detail the spiral magnetic structure and its polar symmetry and relate it to the measured electric polarization. The well-known inverse DM theory cannot explain fully the observed polarization in this system and we have to invoke also the extended inverse DM effect. Based on the inelastic scattering study of the magnetic excitations, which is the first one that has ever been performed in pyroxene compounds, we will discuss the microscopic mechanisms leading to the stabilization of the spiral structure and therefore to the multiferroicity in $SrMnGe_2O_6$.



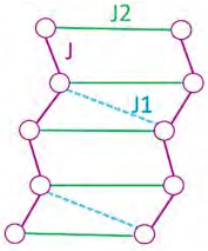


Figure 1: Left: Structure of $SrMnGe_2O_6$; right: the schematic drawing of triangular exchange interactions.

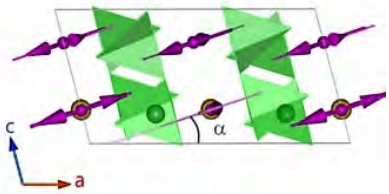


Figure 2: elliptical cycloidal spin structure of $SrMnGe_2O_6$

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Magnetism of rare-earth/transition metal multilayers

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Metallic magnetic multilayers composed of alternating layers of different metals are considered as a new class of artificial magnetic materials displaying a large variety of fascinating properties. Heavy rare-earth metals are known to display complex magnetic behavior in applied magnetic field and temperature. Magnetic multilayers having rare earth metals as a consistent are expected to show complex magnetic phases. Exchange coupling of magnetic nanolayers separated by nonmagnetic spacers is relatively well studied for purely rare earth systems or purely transition metal ones but little is known about interlayer exchange coupling rare earth and transition magnetic metals through spacers. In our presentation, we report results of neutron/X-ray combined study of several rare earth/transition metal systems as Fe/Pd/Gd, Fe/Cr/Gd, Dy/Co, Dy/Gd etc. By combining neutron and resonant X-ray reflectometry we found rich phase diagram of the nanostructures which arising due to the competition of exchange coupling, magneto crystalline anisotropy and Zeeman energy. The research was partly supported by RFBR under Grants No. 18-32-00197 and 19-02-00674.

Complex magnetic order in the $Nd(Tb)Fe_3(BO_3)_4$ multiferroic revealed by the single crystal neutron diffraction

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Magnetic structure of the substituted multiferroics-ferroborates $Nd_{0.9}Tb_{0.1}Fe_3(BO_3)_4$ and $Nd_{0.8}Tb_{0.2}Fe_3(BO_3)_4$ were determined in the framework of a self-consistent refinement of the single crystal neutron diffraction data. The small substitution of Nd for Tb leads to the reorientation of the main antiferromagnetic vector **L** from the basal plane towards to the hexagonal axis. The reorientation takes place via an angular structure for which **L** does not coincide with the principal crystallographic directions and evolves with temperature due to competing magnetic anisotropies of Fe, Nd and Tb subsystems. Our refinement at 2 K reveals the existence of distortions in the collinear antiferromagnetic Fe spin arrangement suggested before in other ferroborates. Therefore, besides the main antiferromagnetic vector **L**, the magnetic structure involves additional fine symmetrized combinations of spin components allowed by symmetry. They coexist with certain **L** components and could originate from the antisymmetric Dzyaloshinsky-Moriya Fe-Fe exchange interactions. At higher temperatures, the simple collinear model describes the magnetic structure, where the **L** vector is deviated from the hexagonal plane.

Evidence for new mechanism of antiferromagnetic domain selection driven by spin-orbit coupling

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The selection and switching of magnetic domains plays a key role in modern data storage and spintronics [1]. The selection of antiferromagnetic domains using magnetic fields is less straightforward than for ferromagnetic domains, and often relies on the Zeeman interaction. Recently, another selection mechanism involving spin-orbit interactions was proposed for tetragonal two-band metals featuring antiferromagnetic domains described by an ordering wave-vector k in the basal plane [2]. This applies to $CeCoIn_5$, where a spin density wave emerges in the superconducting phase with two domains $\mathbf{k}^{+-}$ = (q,+-q,0.5). A small rotation of the magnetic field direction around [1 0 0] is sufficient to lift the degeneracy of these two domains and provoke a switching [3]. A Zeeman-induced domain selection can be excluded as its origin, because the ordered moments are perpendicular to the field applied in the tetragonal plane. In this context, two other theories relying on the coupling of the magnetic order with superconductivity were developed to explain the phenomenon [3,4]. In order to distinguish these theories, we studied the k-domains in $Nd_{1-x}Ce_xCoIn_5$ for x=0.83 in the absence of superconductivity using neutron diffraction. We observe a domain selection in the normal conducting state, ruling out interpretations based on the coupling with superconductivity. This type of domain selection mechanism should be universal across multiband materials with high symmetry crystal structure displaying itinerant antiferromagnetism modulated in the basal plane. Our results emphasize the important role of spin-orbit interactions for $CeCoIn_5$.

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Zone center physics in magnetic diffuse neutron scattering

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Probing physical quantities using neutron scattering is crucial in many areas of physics. Magnetic neutron scattering measures a generalised magnetic susceptibility, but which susceptibility is actually measured as the scattering vector Q -->0? We consider the case of spin ice, which lends itself well to such a study as it obeys both the static approximation of neutron scattering, the classical fluctuation-dissipation theorem and it also has an extremely large paramagnetic susceptibility. By comparing a direct magnetic measurement using a SQUID magnetometer and a neutron scattering measurement near a Brillouin zone center, we show that the external susceptibility is recovered rather than the intrinsic one. Theoretically we investigate this result by Monte Carlo simulations of the spin ice Hamiltonian with different boundary conditions. Our conclusion is that when measuring the paramagnetic structure factor for a Brillouin zone center point in Fourier space, a demagnetising transformation may be needed in order to recover the intrinsic susceptibility of a magnetic material.

Rietveld method for polarized neutron powder diffraction

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Neutron diffraction is particularly powerful when used with polarized neutrons. Polarized neutron diffraction can provide information about the atomic site susceptibility tensor χ_{ij} characterizing the magnetic response of individual atoms to an external magnetic field [1]. The six independent atomic susceptibility parameters (ASPs) can be determined from polarized neutron flipping ratio measurements on single crystals and visualized as magnetic ellipsoids which are analogous to the thermal ellipsoids obtained from atomic displacement parameters (ADPs) [2, 3]. Recently it has been demonstrated that the information about local magnetic susceptibility can be obtained from polarized neutron diffraction on magnetized powder samples [4]. However, due to the absence of a general Rietveld type software adapted to the analysis of diffraction profiles of polycrystalline samples the polarized neutron diffraction is hardly applicable to a number of highly interesting materials like molecular magnets or nanoscale systems. We describe an implementation of the Rietveld method in the analysis of polarized neutron powder patterns, realized in the newly developed software RhoChi (http://www-llb.cea.fr). Architype spin-ice compound $Ho_2Ti_2O_7$ was used as a benchmark for the software. In result the susceptibility tensors of $Ho_2Ti_2O_7$ obtained by the Rietveld analysis at various temperatures and fields were found in perfect agreement with these found earlier in single crystal experiments [2]. Moreover, the procedure of powder averaging described in Ref. [4], formulated for a case of vertical magnetic fields and the neutron scattering in the horizontal plane, has been generalized for an arbitrary scattering geometry. This should open route to PNPD for data from large area detectors commonly used at modern neutron sources.

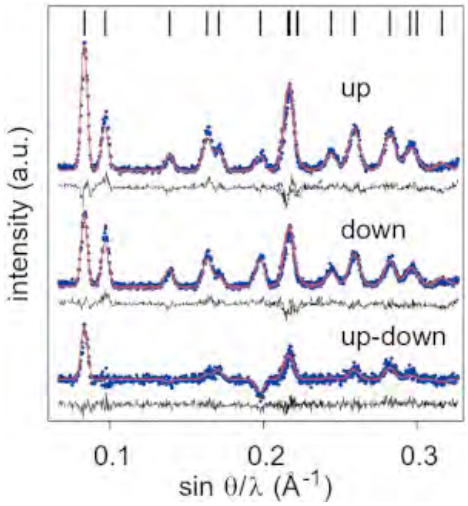

Figure: profile analysis of neutron diffraction patterns of $Ho_2Ti_2O_7$ measured at 5 K, 1 T (diffractometer 6T2, LLB) with the neutron polarization ‘up’ (top), ‘down’ (middle) and its difference (bottom). The row of bars marks the positions of Bragg reflections.

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Embossing induced internal stress in electrical steel sheets

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In electric machines, electrical steel sheets are used to guide the magnetic field. The energy loss due to reversal of magnetism is strongly dependent on the mobility of the magnetic domains. The magnetic domain mobility is in turn influenced by the treatment of the elctrical steel sheet during fabrication. Internal stress induced during the manufacturing (e.g. by blanking the sheets) causes, due to the magneto-elastic effect [1,2], a degradation of domain wall mobility. Consequently the overall energy loss increases. This is evident from larger hysteresis losses in classical magnetization measurements. However, there is a shortage of spatially resolved techniques allowing to probe the magnetic domain constellation in bulk samples of technically relevant dimensions.

Based on the high penetration of neutrons in electric steels and their high sensitivity to magnetic fields, Neutron grating interferometry (nGI) is the technique of choice for analysing the local effect of induced stress on the magnetic properties of a material [3].

nGI simultaneously gathers information about the neutron transmission (TI), the phase shift of the neutron wave inside a sample (DPC) and the amount of ultra-small-angle-neutron scattering (USANS) caused by a sample [3]. Particularly the contrast generated by USANS has aroused high interest, as the resulting dark field image (DFI) is sensitive to the distribution of magnetic domain walls, which serve as scattering centres. Hence, the DFI signal is influenced by the local distribution and size of magnetic domains inside a sample.

In our contribution we will show how stress induced by the manufacturing process locally degrades the mobility of the magnetic domains in electrical steel sheets. In contrast to previous works, we use this degradation of the magnetic domains to actively guide the magnetic flux in an electrical steel sheet. The guiding is performed by embossing a structure on the sample, which locally induces stress. This eliminates the need to cut out areas of the electrical steel sheet to guide the magnetic flux and therefore lowering the mechanical stability. This allows to use electrical steel sheets which have lower losses during the reversal of magnetization due to their material composition, but as a trade off have a lower yield strength. This leads to an increase of efficiency of high speed electrical engines, where the yield strength of an electrical steel sheet is a crucial design parameter.

We will show how different embossing types lead to varying effects on the magnetic properties of an electrical steel sheet. We will show how the evaluated effect of the internal stress correlates with simulated internal stress patterns of the performed embossings.

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Using polarized neutron reflectometry to study the layer integrity of annealed MgO/CoFeB magnetic tunnel junctions with W diffusion barriers

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Magnetic tunnel junctions (MTJ) are an integral component of modern spintronics devices, including the recently commercialized magnetic random access memory. In state of the art MTJs, MgO and CoFeB have become the materials of choice for the thin insulating barrier and ferromagnetic electrode, respectively, forming the core structure of the junction [1]. Typically, a post growth annealing process is performed to maximize the tunneling magnetoresistance and perpendicular magnetic anisotropy, but the exact processes are far from being understood [2]. High annealing temperatures are favorable leading to improved crystallization of CoFeB and MgO, but can be detrimental to the layer structure due to enhanced elemental diffusion [3]. Here we study W diffusion barriers [3] as a method to stabilize the MTJ's layer structure at high annealing temperatures and compare the diffusion processes to conventional structures.

We use the high depth sensitivity of polarized neutron (PNR) and x-ray reflectometry (XRR) to elucidate the layer composition, magnetism and interface structure as a function of annealing temperature. The data of the two probes is co-refined to obtain neutron and x-ray scattering length density profiles revealing the magnetic and elemental distribution in thin layers below nanometer length scales. We compare diffusion processes at temperatures from 250°C to 450°C in MgO/CoFeB/Ta/Pt and MgO/CoFeB/W/Ta/Pt type junctions [3]. Of all elements, the Pt and Ta capping layers are observed to show the largest diffusion, with direct impact on the MTJ performance. In addition, our analysis suggests a substantial Fe out-diffusion towards the capping layer. The W-spacer layer acts as a diffusion barrier for Ta and Fe, leading to an improved magnetic profile up to 450°C annealing. Our results enable a quantitative understanding of the MTJ performance behavior upon annealing with and without diffusion barriers.

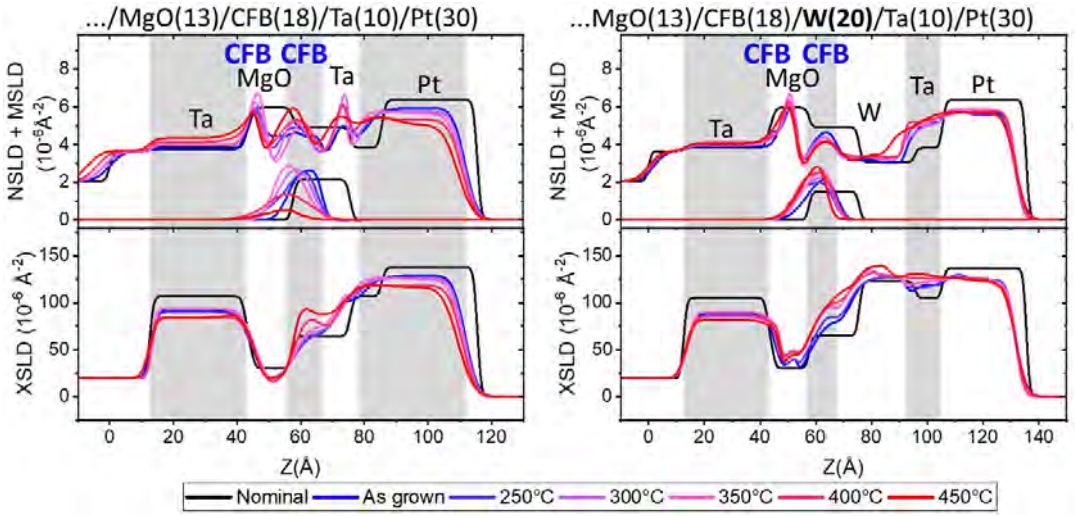

Figure 1: Nuclear (NSLD) and magnetic (MSLD) neutron and x-ray (XSLD) scattering length density profiles at different annealing temperatures. The labels in the graph indicate the intended layer composition based on the as-grown profile.

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Skyrmion lattice in Fe-doped MnGe compounds

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We have grown $Mn_{1-x}Fe_xGe$ compounds with x = 0.0, 0.1, 0.2 and 0.3 using high pressure synthesis [1]. It is well known that the magnetic system of $Mn_{1-x}Fe_xGe$ B20-type solid solutions with $x < 0.4$ orders into helical structure with a wave vector $k \approx 2$ nm^{-1} at low temperatures [2]. The analysis of the evolution of the FeGe compound under external magnetic field revealed the appearance of the skyrmion lattice (SkX) within the specific field range at temperatures close to T_C [3]. The formation of the SkX is an inherent feature of all helical magnets based on Dzyaloshinsky-Moriya interaction (DMI) studied up to now. Only the presence of the SkX in pure bulk MnGe has not been clearly established.

The evolution of the magnetic system of the $Mn_{1-x}Fe_xGe$ compounds with x = 0.0, 0.1, 0.2 and 0.3 under external magnetic field has been studied using small-angle neutron scattering. As the result the (H-T) phase diagram has been plotted for each compound. The skyrmion lattice (SkX) was not found for MnGe compound within the range 0 T < H < 10 T and 5 K < T < 200 K. However the A-phase has been observed for compounds with x = 0.1, 0.2 and 0.3 from very low temperatures almost up to T_N. As to the field range, the existence of the SkX increases linearly with x up to 1.5 T for $Mn_{0.7}Fe_{0.3}Ge$.

We suggest that the appearance of the SkX and the increase of the field range of its presence is connected to the linear increase of the DMI in $Mn_{1-x}Fe_xGe$ with increase of Fe concentration [4-6]. The *ab*-initio calculations predict almost zero value of the DMI for pure MnGe that, to our opinion, correlates with the absence of SkX for pure compound. The temperature range of the presence of the SkX is most likely connected to the intrinsic instability of the magnetic structure found for MnGe and Fe-doped compounds [7]. Another intriguing feature of SkX is the relatively large deviation of the wave vector value for SkX and for the helical structure. It is found to be not less than 10 %. We suggest the DMI serves as an instrument for destabilization of the ordered helical structure upon increase of x and as the main reason for the appearance of the A-phase in $Mn_{1-x}Fe_xGe$ solid solutions with $x > 0.1$.

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Complementary study of magnetic frustration in $Co_7Zn_7Mn_6$ chiral magnet by muons, neutrons and x-rays

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The competition between the magnetic interactions in non-centrosymmetric compounds results in complex phase diagrams. Thus, the interplay between exchange interaction, antisymmetric Dzyaloshinskii-Moriya interaction (DMI) and anisotropy can stabilize long range modulated magnetic phases hosting helical, conical and skyrmion lattice (SkX) orders. Skyrmions are of particular interest since they can be manipulated easily by external current pulses with ultra-low current densities, microwave fields and temperature gradient. Moreover, the typical size of a skyrmion varies in range from a few to a few hundred nm making them promising candidates for spintronics applications [1]. Recently a class of chiral magnets with β-Mn structure was found to be skyrmion-hosting where, moreover, SkX formation in CoZnMn compounds occurs close to the room temperature or even above [2]. Frustration of the Mn site in Co-Zn-Mn alloys results into the spin-glass transition observed at Tg~10 K in Co8Zn8Mn4 and at Tg~30 K in Co7Zn7Mn6 [3,4,5]. Moreover, a low-temperature frustration-induced equilibrium skyrmion phase has been recently found in the latter [4].

We report on complementary study of dynamical frustration effects in Co7Zn7Mn6 by muon spin relaxation spectroscopy (μSR), diffuse wide-angle neutron scattering (DNS) and resonant elastic small-angle x-ray scattering (RESAXS). The μSR experiment revealed the increment of the relaxation rate just above the temperature of the spin-glass transition caused by frustration-induced dynamics. This additional fluctuation regime is reminiscent of the thermal fluctuations near Tc and triggers stabilisation of the disordered equilibrium skyrmion phase. Analysis of magnetic DNS on powdered sample suggests that a *quasi-static* magnetic disorder persist in Co7Zn7Mn6 up to the room temperature. Finally, element-specific RESAXS data points to the unambiguous conclusion that the frustration is driven by Mn sublattice, while Co atoms keep long-range helimagnetic order even below the spin-glass transition temperature.

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The power of small angle neutron scattering for the study of skyrmionic systems

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Magnetic Skyrmions are vortex-like arrangements of spins that constitute a new topological state of matter. They are at the centre of great research efforts because they are considered possible new information carriers in newly developed spintronic devices.

Skyrmions were first observed with Small Angle Neutron Scattering (SANS) in MnSi in 2009 [1], since then, they have been observed in other materials with the same space group [2,3], in noncentrosymmetric compounds [4,5], in thin films [6,7], and recently also in frustrated magnets [8].

In bulk materials, skyrmions form only under specific conditions of temperature and applied magnetic field, which correspond to a small region in the magnetic phase diagram, the skyrmion pocket. The small dimensions of this region constitute one of the major drawbacks for possible technological applications. For this reason, in bulk materials, it is crucial to understand how to manipulate the dimensions of the skyrmion pocket, and how its extent is linked to the underlying crystal structure.

One way in which it is possible to enlarge the skyrmions' region of stability is via rapid field cooling through the skyrmion pocket [9]. In this way, a metastable skyrmion state is formed, which decays over time into the conical state, and extends down to low temperatures and for a wide range of applied magnetic fields; however, the possible technological exploitation of this metastable state is closely related to its lifetime. In Cu_2OSeO_3, it has been shown that it is possible to significantly enhance this lifetime through the controlled chemical substitution of Cu ions with non magnetic Zn ions [10].

The observation of such metastable state comes with questions about the nature of its decay process, and how this process is influenced by the increased disorder provided by chemical substitution.

In this context, SANS is a powerful technique that can directly probe the ordering of the magnetic state, allowing a clear identification of the observed magnetic phase. While this is extremely useful for the comparison with results from other techniques, such as AC susceptibility, SANS provides also unique evidence on the correlation lengths of the system, allowing the extraction of information on the perfection of the skyrmion lattice, thanks to the neutron's long penetration depth and their high sensitivity to magnetic fields.

In our work, we have used SANS to study the time dependent behavior of the metastable skyrmion lattice structure in Zn substituted Cu_2OSeO_3. We have been able to observe the decay of the metastable skyrmion state in the conical ground state of the system, gathering structural information on the characteristic correlation lengths of the system.

In this talk, we will present the possibilities offered by SANS for the study of the skyrmionic magnetic texture, with particular focus on how to extract information both on the disorder of this lattice, and on the mechanism through which it decays into the conical state. Any time dependent behavior of the correlation lengths would be useful for the understanding of the decaying process, and for the development of a model to describe it.

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Kinetic small-angle neutron scattering of skyrmion lattice order in chiral magnets

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Skyrmions are topologically non-trivial spin textures that attract great interest, offering a possible avenue towards novel spintronics applications, e.g., in skyrmion-based racetrack memory [1]. A key feature that motivates this interest is related to an exceptionally efficient coupling of skyrmion lattice order to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe and $Cu_{2}OSeO_3 $(CSO), respectively [2, 3, 4, 6, 7]. Another property of great interest for applications is the spectrum of helimagnon excitations and putative solitary excitations [8, 9]. This raises the question for the microscopic mechanisms that control the pinning and the elasticity modulus of the skyrmion lattice as well as the elasticity moduli of skyrmion lattices in chiral magnets.

We report kinetic studies of skyrmion lattice order by means of Time-resolved Small Angle Neutron Scattering (TISANE). We compare the characteristics of skyrmion lattices in metallic systems such as MnSi, where spin transfer torques are dominated by spin-polarized charge currents, with insulating materials such as Cu_2OSeO_3 (CSO), where the spin transfer torques are due to magnon currents. This provides direct insights into the pinning mechanisms and elasticity moduli as a precondition for the development of spintronics devices.

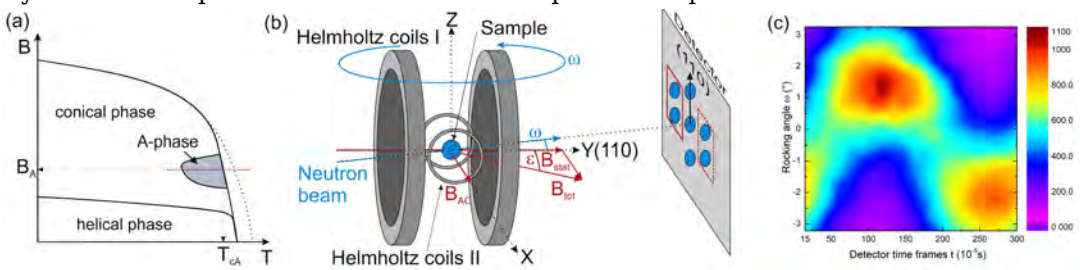

Fig. 1. (a) Schematic depiction of the magnetic phase diagram. (b) Illustration of the experimental setup with the orientation of the static and excitation magnetic fields. (c) Typical time resolved rocking maps of the unpinning of the skyrmion lattice in Cu_2OSeO_3.

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Polarization analysis of the skyrmion dynamics in MnSi

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The itinerant-electron compound MnSi features a skyrmion order [1] for temperatures in the range $T \approx 28 - 29$ K and for magnetic fields $B \approx 0.16 - 0.21$ T. Its non-centrosymmetric $P2_13$ space group has profound consequences for spin-wave dynamics in all ordered magnetic phases of MnSi. Namely, it introduces a Dzyaloshinskii-Moriya term which – at reduced momentum transfers parallel to a helimagnetic propagation vector – leads to magnon creation at energies that are different from the energies for magnon annihilation at the same momentum transfer q. The dynamical magnetic structure factor $S(\boldsymbol{q}, E, \boldsymbol{B})$, with $\boldsymbol{q} = \boldsymbol{Q} - \boldsymbol{G}$ and lattice vector $\boldsymbol{G}$, is thus asymmetric ("non-reciprocal") with respect to changing the sign of either the reduced momentum transfer $\boldsymbol{q}$, the energy transfer E, or the magnetic field $\boldsymbol{B}$, but is symmetric upon interchanging the signs of two of these variables [2]. Such an asymmetric behavior could be observed for the field-polarized [3, 4], the paramagnetic [5], the conical [6], and the skyrmion [2] phase of MnSi.

In a recent series of experiments at the instrument ThALES [7], we discovered an asymmetric separation of the non-reciprocal skyrmion dynamics into different polarization channels, which signify a flip from spin-down to spin-up ("SF-+"), from up to down ("SF+-") or no spin-flip ("NSF"). Theoretically, we succeeded to describe our results utilizing a mean-field linear spin-wave model. Correcting the theory for instrumental resolution effects yields a virtually perfect quantitative agreement between experiment and theory.

Our new results are intriguing, as they not only confirm the previously determined [2] asymmetric nature of the skyrmion dynamical structure factor with respect to $\boldsymbol{q}$, E, and $\boldsymbol{B}$, but moreover extend the asymmetry to the flipping direction of the spin. We could furthermore show a close relationship between dynamics in the skyrmion phase and all other ordered magnetic phases in MnSi.

Upcoming publication: T. Weber, D. Fobes, J. Waizner, L. Beddrich, P. Steffens, G. Tucker, R. Bewley, R. Georgii, A. Bauer, C. Pfleiderer, P. Böni, M. Janoschek, and M. Garst, in preparation. (The present work will be published as part of a general investigation into skyrmion dynamics.)

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Multiple-q noncollinear magnetism in the itinerant hexagonal magnet $Y_3Co_8Sn_4$

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Multiple-*q* spin order, i.e., a spin texture characterized by a multiple number of coexisting magnetic modulation vectors *q*, has recently attracted attention as a source of nontrivial magnetic topology and associated emergent phenomena. One typical example is the triple-*q* skyrmion lattice state stabilized by Dzyaloshinskii-Moriya interactions in noncentrosymmetric magnets, while the emergence of various multiple-q states of different origins is expected according to the latest theories. Here, we investigated the magnetic structure of the itinerant polar hexagonal magnet $Y_3Co_8Sn_4$, in which several distinctive mechanisms favoring multiple-*q* states are allowed to become active [1]. Small angle neutron-scattering experiments suggest the formation of incommensurate triple-*q* magnetic order with an in-plane vortex-like spin texture, which can be most consistently explained in terms of the novel four-spin interaction mechanism inherent to itinerant magnets. The present results suggest a new route to realizing exotic multiple-*q* orders and that itinerant hexagonal magnets, including the $R_3M_8Sn_4$ family with wide chemical tunability, can be a unique material platform to explore their rich phase diagrams.

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Spin textures induced by quenched disorder in a reentrant spin glass: vortices versus frustrated skyrmions

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Disorder plays a central role in the advent of the most spectacular quantum phenomena observed in condensed matter. Reentrant spin glasses (RSG's) are nice playground to study the influence of disorder on frustrated ferromagnets, and see how it affects topological defects. RSG's develop vortex-like textures under magnetic field [1,2], which we investigate in comparison with the frustrated skyrmions predicted by theory [3,4].

Our recent study of a $Ni_{1-x}Mn_x$ single crystal by small angle neutron scattering [5] clarifies their internal structure and shows that these textures are randomly distributed. Using two magnetic field geometries, we found that transverse spin components rotate over length scales of 3-15 nm, decreasing as field increases from 0 up to 8 T according to a scaling law .

Monte-Carlo simulations reveal that the internal structure of the vortices is strongly distorted and differs from that assumed for frustrated skyrmions. The pattern of topological charge density depends on the bond distribution. The vortices keep an anisotropic shape on a 3 dimensional lattice, recalling "croutons" in a "ferromagnetic soup". Their size and number can be tuned by the magnetic field and concentration x (or heat treatment), respectively. This opens an original route to understand and control the influence of quenched disorder in systems hosting non trivial spin textures.

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Liquid crystalline structures and elasticity in a cubic chiral helimagnet

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Condensed matter provides convenient ways to observe and manipulate a large variety of complex long-range orders. Currently, a strong focus is put on the study of chiral magnets belonging to the so-called B20 family, such as MnSi, FeGe, MnGe, *etc.* These alloys indeed display a plethora of multiply modulated phases, including the topologically non-trivial *skyrmion* (SK) lattice, and a constantly improved understanding of their microscopic properties is required.

Using small-angle neutron scattering on $Mn_{1-x}(Co,Rh)_xGe$ solid solutions, we have recently discovered that MnGe undergoes a doping-induced transition from helimagnetism to weak ferromagnetism through a mixed-state. Within this intermediate phase, topological defects -akin to SK-anti SK pairs- proliferate, even in zero field [1]. The formal equivalence between the latter and the "*twist-grain boundary*" (TGB) phase already evidenced in certain chiral liquid crystals [2] underscores the deep connections between the two classes of systems.

In turn, this analogy implies that the helimagnetic (HM) ground state should support low-energy *phason* modes [3], but their observation has remained elusive in B20 compounds. We have used a cutting-edge quasi-elastic scattering method, the so-called MIEZE spectroscopy [4], to verify this prediction. Our study of the temperature-dependence of the HM order lifetime in pure MnGe revealed that it is *finite* in a large temperature interval below the macroscopic ordering temperature $T_N \approx 170$ K down to $T_{com} \approx 30$ K [5]. This finding suggests that the ground state is dominated by non-linear excitations, which destabilize the long-range order. They could be connected to the large topological Hall effect observed in this compound [6].

Altogether, our work shows that there exists an amazing landscape to be explored in chiral magnets, beyond the physics of skyrmions. Neutron scattering will keep on playing a key role in this adventure.

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Cluster-like structure of Fe-based alloys with enhanced magnetostriction

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The discovery of a manyfold increase in magnetostriction of Fe-*x*Ga alloys comparing with pure α-iron stimulated a plenty of theoretical and experimental investigations. At present this enhanced magnetostriction is addressed in several studies to the formation of a heterogeneous state of a ferromagnetic material. Typical example of inhomogeneity – phase separated states – is well known in physics of complex oxides in which unusual properties are observed and widely studied by neutron diffraction. In this paper the structure and microstructure of several Fe-based alloys with phase separated structure have been studied by neutron diffraction with high $\Delta d/d$ resolution and with high-intensity continuous scanning in a wide temperature range. Complex analysis of several Fe-based alloys allowed establishing that their microstructure is organized as nanoscopic-sized clusters with a better ordered atomic structure coherently embedded in a disordered or less ordered matrix. The characteristic size of the clusters depends on the state of the alloy and the temperature, and ranges in size from 100 to 1000 Å. The dispersed cluster formation in Fe-based alloys may be indicated as systematic “order-disorder” phase separation in terms of coexisting regions that differ in the degree of atomic order. One of the factors stabilizing the phase-separated state in a compositionally homogeneous medium can be local composition fluctuations at the level of elementary cells, which in turn leads to fluctuations in the interactions of neighbouring pairs of atoms.

$Fe_{3-x}Mn_xBO_5$: an extraordinarily rich magnetic phase diagram

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Ludwigite oxyborates $M_2M'BO_5$, where M and M' are divalent and trivalent 3*d* metal ions, respectively, have an intriguing orthorhombic crystal structure made of interconnected low dimensional units in the form of three-leg (3LL) ladders, 3LL1 and 3LL2 [1]. The existence of two crystallographically distinct sublattices is not anodyne : in Fe_3BO_5, Mössbauer and X-ray diffraction studies at room temperature have evidenced that Fe^{3+} species occupy preferentially 3LL1, while 3LL2 is occupied by Fe^{2+} [2]. In addition, a charge ordering transition has also been observed at T_{CO} = 283 K [1], [3], resulting from the ordering on 3LL1 of the extra itinerant electron within each Fe^{3+} triad. This also impacts the magnetic properties : according to neutron diffraction results, 3LL1 and 3LL2 magnetically order, but independently, at T_{N1} = 112 K and T_{N2} = 70 K, respectively, with orthogonal propagation vectors.

In the presented work, the isostructural system $Fe_{3-x}Mn_xBO_5$ has been studied by electron microscopy, neutron scattering, and Mn and Fe *K*-edge X-ray absorption, combined with physical properties measurements. The heterometallic ludwigite system $Fe_{3-x}Mn_xBO_5$, recently investigated for its ferroelectric properties, has been studied using synchrotron and neutron diffraction, combined with XANES and magnetisation measurements. The results show the *Pbam* ludwigite crystal structure is preserved with little structural distortions up to x = 1.5, and that divalent Mn is substituted preferentially on the 3LL2 sub-lattice unit. As x increases, and up to Fe_2MnBO_5, the two sub-lattice magnetic order of Fe_3BO_5 is preserved : magnetic order on 3LL1 (k = (0 0 0.5), moments along b) survives with reduced magnetic moment, while the correlation length of the magnetic order on 3LL2 (k = (0 0 0), moments along a) decreases. In contrast, for x = 1.5, a new k = (0 0 0) magnetic ordering, coupling both sub-lattices, is observed, with all moments aligned along c. These results provide new insight on the physical properties of the system, which are discussed in terms of three parameters : (i) competing easy-axis anisotropy and magnetic exchanges along the 3LLs legs in the decoupled sub-lattice regime, (ii) non-linear evolution of the substitution on each sub-lattice, and (iii) changes in the direct-exchange and super-exchange couplings as Mn^{2+} ($3d^5$, isoelectronic with Fe^{3+}) is introduced in the structure. These three parameters at play in the $Fe_{3-x}Mn_xBO_5$ system are at the origin of an extremely rich (x, T) magnetic phase diagram. ¶

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Magnetism of surface modified and gallium doped magnetite particles

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Results of X-ray and neutron diffraction, small angle neutron scattering (SANS), transmission electron microscopy (TEM), magnetization and Mössbauer spectroscopy measurements on $Ga_xFe_{3-x}O_4$ (x= 0.2, 0.4, 0.6, 0.8 and 1.0) nanoparticles are presented. The systems crystallize in the inverse spinel type structure, and their unit cell volumes are practically independent of the gallium concentration. X-ray and neutron diffraction techniques confirmed the phase homogeneity of all the samples. Diffraction and Mössbauer measurements disclosed that with increasing magnetite doping up to x=0.6, nonmagnetic Ga expels the magnetic Fe cation from A-positions while above this content up to x=1.0 gallium cations occupy A and B - positions and change the magnetic interactions drastically. All presented systems have been quickly saturated disclosing neglectable coercive fields. Gallium doped magnetite nanoparticles belong to soft magnetic materials with a phase transition temperature above 350 K.

Spherical particles based on iron oxides form a group of innovative nanomaterials with wide prospects of applications. A growing interest in nanotechnology causes development of big variety of isostoichiometric materials of different shapes in nanoscale. SANS and TEM measurements confirm the change in the shape of nanoparticles from parallelepiped to spherically symmetrical ones. Dependently on gallium content (x = 0.2, 0.4, 0.6, 0.8 and 1.0) in the $Ga_xFe_{3-x}O_4$ samples and its location at the core or shell respectively, particles of the sizes from 3 nm to 30 nm were obtained.

Studies of thermal behavior of gallium doped iron tetroxide particles became the subject of fundamental research and in perspective biomedical applications. The phenomena of magnetic nanoparticles thermal effects, as a reaction on alternating magnetic field application and its modulation by particles size, type and as well as modified field frequency are investigated in details. Depending on the conditions of preparation the shape and size of the variously ordered particles of ferrites manifests differently strong magnetic nature. The very similar ionic radius of the iron (III) and gallium (III) cation results in a poorly sensitive unit cell parameter versus gallium content. A diversity of magnetic properties is caused by a peculiarity of distribution of gallium cations between two crystallographic A and B positions with tetrahedral and octahedral oxygen coordination in the inverse spinel type structure.

Structure and Texture of Nanosized Magnetic Hexaferrites

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Thorough investigations have been carried out on the hexagonal ferrite $SrFe_{12}O_{19}$, a hard magnetic material which crystallizes in the space group $P6_3/mmc$ with unit cell parameters ab=5.88 Å and c=23.09 Å. To improve the magnetic performance it is important to control the atomic structure, the size and shape on the nanoscale and the relative orientation of all nanocrystallites in the magnetic ensemble. Only by controlling the structure over eight orders of magnitude is it possible to prepare magnetic materials with optimized performance.[1] A large fraction of the parameters are controlled through the synthesis conditions, here we have developed different synthesis approaches, which allow excellent control over the size and shape of the nanocrystallites. The methods include hydrothermal synthesis using flow and batch reactors, sol-gel, and modified sol-gel.[2, 3, 4] The situation is illustrated in Figure 1.

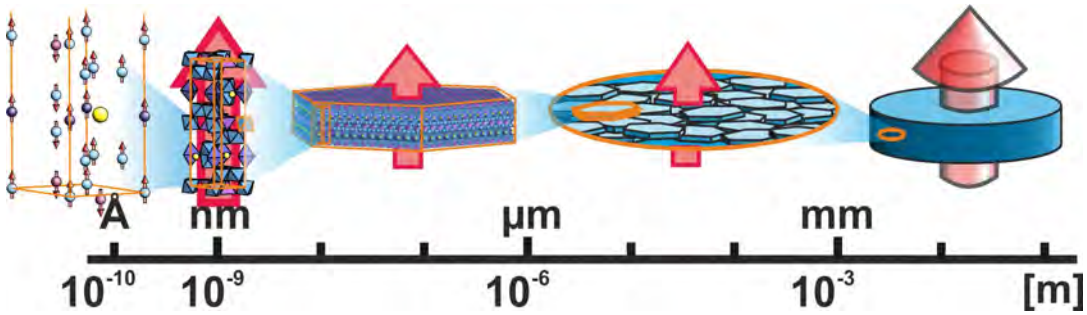

Figure 1: Correlation between magnetism and structure throughout ten orders of magnitude.

The prepared nanocrystallites are varied in their morphology by controlling the aspect ratio A/C, where A is the size along the crystallographic *ab*-axis and C is the size along the *c*-axis. To obtain bulk magnets for actual applications, it is necessary to compact the size-controlled nanocrystallites. Controlling the pressing process is paramount, as heat and pressure may alter the nanocrystallite structure, composition, texture and thus magnetic properties of the resulting magnet.[5] We have used Spark Plasma Sintering to prepare the final magnets. The as-prepared magnetic nanopowder has been investigated by neutron powder diffraction, likewise has the final pellet been investigated by neutron pole figure measurements to extract the texture information. The neutron data clearly demonstrated a correlation between the aspect ratio of the starting nanoplatelets and the alignment of the crystallites in the produced magnets. The insight gained through these neutron studies is vital for the design of materials, the improvement of sample processing and the enhancement of magnetic performance.

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Powder and single crystal neutron diffraction in ferromagnetic shape memory alloys: structure vs magnetism

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Ferromagnetic Shape Memory Alloys (FSMAs) are a group of active materials that undergo martensitic transformations induced by temperature, stress and/or magnetic fields, which result in large recoverable mechanical deformations [1]. Their fast response and high energy density make them ideal candidates for implementation in sensors and actuators. The magnetic properties of FSMAs depend on the interactions between the magnetic moments of atoms that, in turn, depend on the atomic positions within the lattice [2, 3]. Here we present a combination of powder neutron diffraction experiments in a series of polycrystalline samples of 6-element FSMAs with varied Fe content, where the alloys present actuation at temperatures around 370 K. Their atomic site occupancies, the ratio c/a and, therefore, the maximum achievable deformation ε, are calculated for each alloy [4]. Based on the atomic site occupancies and additional measurements of the saturation magnetization in each sample, the influence of the structure and chemical order on the magnetism in these samples is presented. This study is complemented by the single crystal polarized and non-polarized neutron diffraction experiments in one of the samples used for the powder neutron diffraction measurements, from which a single crystal was grown. Together with the atomic site occupancies in the single crystal, the analysis of the polarized neutron diffraction measurements provides us with information about the magnetic moment distribution in each atomic position present in the unit cell of the single crystal.

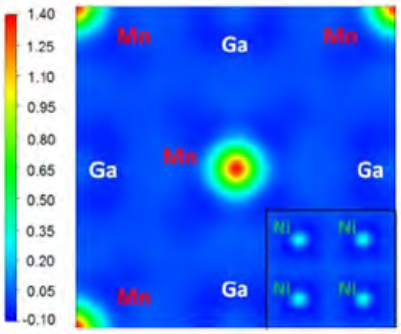

Fig.1: Magnetic moment distributions of the Fe5 single crystal at z=0 (main) and z=0.25 (inset) planes measured in D3, where z is the unit vector along the c axis of the unit cell. The colour code units are $\mu_B/Å^3$.

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GISAS studies of the shape, size and layout of silicon nanowhiskers

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Nanowhiskers (NWs) are unique 1D structures that can be used as a basis for memory elements, chemical sensors, solar energy cells [1]. Understanding the full-scale sample morphology and controlling over the entire growth process is of primary importance for successful integration of the nanostructures in modern nanoelectronic devices. Grazing incidence small-angle scattering (GISAS) provides data on sample morphology averaged over the whole sample surface.

Silicon NWs with the different compositions of catalytic nanoparticles (pure Au and Au:Cu (60:1)) have been produced by pulsed laser deposition technique. Laboratory research methods (SEM, TEM and AFM) provided information about shape and size of NWs from local areas. It was observed that depending on the addition of Cu, the final structures formed as a prism or a pyramid [2].

In the present contribution, shape, size and layout of NWs have been studied by GISAS technique. GISAXS measurements have been done at the laboratory small angle X-ray scattering instrument GALAXI (Jülich, Germany) [3]. GISANS studies have been carried out at very small angle scattering diffractometer KWS-3 (Garching, Germany) [4]. The analysis of GISAS data has been performed with BornAgain software [5]. The first type of NWs has a shape of hexagonal prism (average height about 340nm, width of side face about 150nm) with an elongated hemisphere cap on the top (average height about 200nm, radius about 150nm). The second type has shape of a hexagonal antiprism with negligible top base (average height about 150 nm, width of bottom base about 150nm, tilt of side face about 75°). On GISAXS patterns, hemispherical reflexes have been observed. Our previous research has revealed the presence of nanoparticles of metal-catalyst on the NWs side. We suppose that the aforementioned reflexes correspond to these nanoparticles. Both, GISAS and imaging techniques show the broad size distribution of NWs, but the mean particle size differs. Thus, GISAS measurements are very important for comprehensive studies of growth mechanisms of NWs.

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Insights into the magnetocaloric effect in $MnFe_4Si_3$ gained with inelastic neutron scattering

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The magnetocaloric effect (MCE) is the temperature or entropy change of a material subject to a variation of magnetic field and is the basic principle of magnetic refrigeration.
This technique is considered as promising for a more environmentally friendly and efficient use of energy. However, the fundamental mechanisms at play are to be revealed and the key ingredients are to be identified in order to design new materials.

The model system MnFe4Si3 exhibits a transition to the ferromagnetic state at Tc=305K and shows a moderate direct MCE (cooling with adiabatic demagnetization) at low magnetic fields of 2T.

To get insight into the microscopic mechanisms of the MCE inelastic neutron scattering (INS) single crystal studies under different temperatures and magnetic fields have been employed using polarized and unpolarized neutron techniques.

Magnetic excitation spectra were collected in the ferromagnetic phase as well as in the paramagnetic (PM) state, in order to understand the nature of the magnetism in MnFe4Si3.
Spin wave measurements reveal a strong anisotropy between in- and out-of-plane magnetic exchange interactions which manifests itself also in the q-dependent linewidths of the fluctuations in the PM state.

The correlation lengths point to the importance of short-range order in this system.
Around Tc in- and out-of-plane spin-fluctuations are found to be isotropic. In addition the critical fluctuations in the PM state show a strong response to a magnetic field of 2T [1].

While no clear evidence for magnon-phonon interaction has been detected, a full phonon intensity cancellation in one of the two non-spinflip polarization channels has been observed in a transverse acoustic phonon branch employing longitudinal polarized INS and a magnetic field of 1T. This intensity cancellation is considered as coincidental and is explained with the nuclear magnetic interference between the nuclear one-phonon and the magnetovibrational one-phonon scattering cross sections (creation or annihilation of phonons via the elastic magnetic interaction) [2].

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$FAPbBr_3$ – about the influence of deuteration: A temperature dependent neutron diffraction study

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Perovskite materials - which due to their chemical diversity reveal an intriguing amount of physical properties - have recently gained renewed interest following the discovery that hybrid perovskites are attractive materials for photovoltaic applications due to their high energy conversion efficiencies.

Just like the “classic” oxide perovskites with its ABX_3 stoichiometry hybrid perovskites show corner sharing BX_6 octahedra networks. In contrast to the inorganic $A^{[XII]}$ cation in the oxide perovskites the hybrid perovskite’s A cation is an organic molecule which is surrounded by 12 halide anions (X).

One of the materials with record-breaking solar energy conversion efficiencies of 22.1 % (1) is methylammonium lead iodide ($CH_3NH_3PbI_3$ - $MAPbI_3$). Solid solutions with either substitution of the organic molecule, the halide anion or both, give the opportunity to further tailor and improve physical properties.

The substitution of the A cation by formamidinium ($CH(NH_2)_2$ - FA) and the iodine by bromine leads to formamidinium lead bromide ($FAPbBr_3$) which gained interest as a material used as a wide bandgap [2.27eV(2)] absorber material in tandem solar cells. Although thin film synthesis and optoelectronic properties are known only a minor emphasis is put on the influence of the crystal structure and the interplay of octahedral tilting and organic unit.

We present a study about the crystal structure determination of $FAPbBr_3$ over a range of 3 – 300K using neutron- and X-ray diffraction techniques (HZB, BERII – E9 and BESSYII – KMC-2) with emphasis on the different orientation, and orientational disordering of the formamidinium molecule in dependence of partly deuteration of the formamidinium molecule.

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Water captured in the polysaccharide network of chia mucilage

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Mucilage is a natural hydrogel, which is vital for plants [1] and highly relevant for industry (mainly food and pharmacy). The most important properties are the huge water holding capacity and slow water transport, which is dominated by water diffusion and polymer relaxation [2]. Mucilage is an amorphous material, containing mainly polysaccharides [3]. The polysaccharide chains form a hydrogen-bonded network of fibrils, which are in the order of 100nm thick [4]. Dynamics of hydrogels have been already studied by QENS and other techniques [e.g. 5]. The novelty of this study is to use rehydrated freeze-dried samples to minimize the contribution from bulk-like water (which dominates the QENS spectra in the original state) and simultaneously preserve the open porous structure and high surface area of the hydrogel. Currently we work on chia seed mucilage, which is one of the most studied mucilages in the literature due to its industrial relevance and simple extraction.

QENS and FWS measurements have been performed at the FOCUS and MARS spectrometers at PSI and at IN13 at ILL. Samples hydrated with H_2O and D_2O was used to separate water and polymer contributions. Despite of the complexity of the sample, the mucilage dynamics can be described by a single process on the ps time scale, which we attribute to localized motions of the sugar rings around the glycosidic linkages. Furthermore, we find that the whole polysaccharide is mobile on the ns time scale. Surprisingly, we did not observe long range translational diffusion of water, although part of the water can crystallize. On the other hand, strong dynamical coupling between polysaccharide and water molecules is evidenced. The frequently used mucilage analogue, polygalacturonic acid showed remarkable similarities but also significant differences.

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Next generation solar cells studied with GISANS

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Next generation solar cells such as for example organic solar cells are an interesting alternative to conventional silicon based solar cells as they feature new possibilities introduced by using a different class of materials namely polymers. Instead of expensive ultra-high vacuum technologies, fabrication can be done at room temperature, using wet chemical processing, and thereby enabling usage of methods such as roll-to-roll printing. As a consequence, the production of organic solar cells has the potential to become very cheap and easy. Moreover, the use of polymers allows for flexible solar cells and light weight devices, which will be usable in a very different fashion as compared to the immobile silicon solar panels. In addition, the energy payback times of organic solar cells are significantly shorter as compared to the today's silicon solar cells. However, despite all these significant advantages of organic solar cells, still fundamental knowledge is very limited.

In particular, it is challenging to detect the complex morphologies, which are necessary to have high efficiency organic solar cells. The combination of grazing incidence small and wide angle x-ray and neutron scattering (GISAXS, GISANS and GIWAXS) allows for overcoming these challenges. Selected examples will be shown to illustrate the possibilities arising from using the advanced scattering techniques in particular highlighting the use of GISANS.

Neutron imaging study of degradation in commercial Li-ion batteries

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Rechargeable lithium-ion (Li-ion) batteries are nowadays widely used as power sources, for instance powering phones, laptops, electrical vehicles. Therefore, researching the degradation mechanisms is essential to overcome the present limitations, such as ageing. Ageing is identified by capacity fading and an increase in resistance, irrespective of whether the battery is cycled or not. During charging and discharging, Li-ions are inserted into and extracted out of the crystal structures of two electrodes. However, repeating this process gradually degrades the crystalline electrode materials over time, thereby causing battery degradation, loss in capacity and lifetime.

In our most recent neutron imaging study we have investigated four IFR 10440 $LiFePO_4$commercial batteries with 3.2 V nominal voltage. We have observed the differences between one pristine battery and three cycled batteries, with three distinct cases of cycling behaviors. Two out of the three cases were systematically cycled, one in the full potential window (2.5 V – 3.36 V) and one in a partial potential window (3.08 V – 3.45 V). For the third battery the potential limits were randomized to simulate the daily use of a rechargeable battery. Data sets were acquired at NEUTRA and ICON beamlines at Paul Scherrer Institute. During the neutron imaging study, we have acquired three tomographies per battery at 0% state of charge (SoC), 50% SoC, and 100% SoC. Each tomography was reconstructed, with MuhRec [1], from 375 radiographies collected over 360 degrees. Here, we will present the results of our investigation.

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Characterisation of hydrogen storage materials with neutron imaging and scattering techniques

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Hydrogen can be stored safely and reversibly at high volumetric densities in hydrogen storage tanks filled with light metal hydrides. Reactive Hydride Composites (RHCs) are metal hydride mixtures that are very promising hydrogen storage materials due to high hydrogen densities, stability and safety. The hydrogen sorption kinetics of the RHCs is distinctly improved by high-energy ball milling and the addition of suitable additives.

Due to the sensitivity of neutrons towards hydrogen, in situ Neutron Radiography (NR) is the ideal technique for time-resolved investigations of the hydrogenation process of metal hydride powder beds and pellets inside a hydrogen storage tank. Neutron Computerized Tomography (NCT) provides additional 3D information about the material structure and hydrogen distribution. I*n situ* NR measurements of hydrogen storage tanks filled with RHCs were performed at the instruments NECTAR and ANTARES at MLZ/FRM II. Combining cold and fission neutron spectra and using a new method for the quantitative investigation of neutron imaging data, a precise study of the hydrogen distribution in the metal hydride material is possible [1]. Effects of temperature field and material packing density were investigated. The 3D structure was analysed additionally by NCT. The results allow the optimization of the hydrogen storage systems in terms of capacity, kinetics and safety [2].

In addition, different scattering methods with neutrons and X-rays were used to study phase transformations and changes in the nanostructure in different RHC systems in order to get a deeper insight into the complex hydrogen sorption processes [3-5]. Dynamic processes in the hydrogen storage materials were studied by inelastic neutron scattering investigations at the instrument TOFTOF. For the characterisation of hydrogen storage materials at high pressures and temperatures, a high-pressure cell for *in situ* neutron studies at pressures up to 700 bar and temperatures up to 500°C was used at different neutron instruments, e.g. at SANS-1 at MLZ/FRM II.

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Local structure and dynamics of metal hydride-reduced BaTiO3 samples investigated with inelastic and quasielastic neutron scattering

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Perovskite-type oxyhydrides, of the form $BaTiO_{3-x}H_x$, represent a highly interesting, emerging class of materials that have been recently shown to exhibit hydride-ion (H^-) conductivity at elevated temperatures [1], which is of relevance for, e.g., the development of electrolytes for all-solid-state batteries and fuel cells. However, the coordination of hydride-ions and the underlaying mechanism of hydride-ion conduction and how it depends on temperature and oxygen vacancy concentration remain unclear. In this contribution, we will present data from inelastic and quasielastic (INS and QENS, respectively) measurements [2] aimed at revealing the local coordination and dynamics of three metal-hydride reduced $BaTiO_3$ samples which are characterized by the simultaneous presence of hydride ions and oxygen vacancies. INS measurements at low temperature (< 10 K) show the presence of two main vibrational modes of the hydride ions, manifested as local Ti-H vibrational modes perpendicular and parallel to the Ti-H-Ti bond direction, and, because no traces of O-H species are found, confirm that the hydride ions are located on vacant oxygen sites of the perovskite host lattice, as suggested elsewhere. Measurements of elastic fixed window scans upon heating reveal the presence of quasielastic scattering due to hydride-ion dynamics for temperatures above ca. 200 K. Analysis of QENS spectra measured at "low" temperature (225 and 250 K) and at "high" temperature (400 - 700 K) show that the dynamics can be adequately described by established models of jump diffusion. At low temperature, < 250 K, all the models feature a characteristic jump distance of about 2.8 Å, thus of the order of the distance between neighbouring oxygen atoms or oxygen vacancies of the perovskite lattice and a mean residence time between successive jumps of the order of 0.1 ns. At higher temperatures, > 400 K, the jump distance increases to about 4 Å, thus of the order of the distance between next-nearest neighbouring oxygen atoms or oxygen vacancies, with a mean residence time of the order of picoseconds. These new results can be expected to be useful for developing new efficient synthesis routes and novel applications for oxyhydride materials.

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Nanoscale structure of electrochemical interfaces for lithium power sources by neutron scattering

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The performance characteristics of modern and advanced lithium power sources such as energy capacity, power, stability of operation, service life, etc., are largely determined by the processes occurring at charge separation interfaces including the evolution of the structure, composition and chemistry of electrodes and electrolytes. The report presents how neutron scattering techniques allow monitoring and studying the structure of interfaces of different types in the course of their operation in model electrochemical cells under potential. High penetrating power of thermal neutrons makes it possible [1,2] to probe buried electrochemical interfaces by different neutron scattering methods such as reflectometry applied to planar boundaries and small-angle scattering used in the study of developed pore structures. Potentials of these methods are demonstrated by experimental examples which deal with the general problems of the formation and evolution of solid electrolyte interphase layer and lithium plating on metal anodes contacting liquid electrolytes, as well as the pore filling by products of electrochemical reactions in carbon fiber based electrodes for actively studied lithium-sulfur and lithium-air batteries. An essential feature of lithium containing depositions with respect to the application of neutron scattering is a low scattering length of lithium, which makes the use of deuterated electrolytes in contrasting the products of electrochemical reactions to be very efficient in the detection and analysis of the corresponding formations at the interfaces.

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Residual stress measurements using correlation RTOF (Fourier) diffractometry at long-pulse neutron source

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The diffraction of thermal neutrons is a powerful tool for investigations of residual stresses in various structural materials and bulk industrial products due to the non-destructive character of the method and high penetration depth of neutrons. Therefore, for conducting experiments in this research field, the neutron Fourier stress diffractometer FSD has been constructed at the IBR-2 pulsed reactor in FLNP JINR (Dubna, Russia). Using a special correlation technique at the long-pulse neutron source - fast Fourier chopper for the primary neutron beam intensity modulation and the reverse time-of-flight (RTOF) method for data accumulation, a high resolution level of the instrument has been achieved over a wide range of interplanar spacing at a relatively short flight distance between the chopper and neutron detectors ($L \approx 6.6$ m): $\Delta d/d \approx 2.3 \cdot 10^{-3}$ for backscattering detector and $\Delta d/d \approx 4 \cdot 10^{-3}$ for both ±90°-detectors at $d = 2$ Å and at a maximum rotation speed of the Fourier chopper $\Omega_{max} = 6000$ rpm.

The FSD design satisfies the requirements of a high luminosity, high resolution, and specific sample environment. The collimator system guarantees a minimum gauge volume of 2x2x2 mm^3 with precise sample positioning by 4-axis (X, Y, Z, Ω) HUBER goniometer. To study the behavior of structural materials under external load *in situ* in a neutron beam, an uniaxial mechanical-type loading machine LM-29 is used; it provides any required combination of external load (up to 29 kN) and temperature (up to 800 °C), which considerably extends the range of possible experiments on the diffractometer.

Using RTOF technique at pulsed neutron source allows recording the complete pattern with many diffraction peaks in wide range of interplanar spacing at fixed scattering angles. This makes possible to study polycrystalline materials with a rather complex structure, including multiphase ones, under various external conditions on the sample. In addition, high resolution level and symmetrical Gaussian shape of the instrument profile allows one to estimate the microstrain level and the size of coherently scattering domains in studied material.

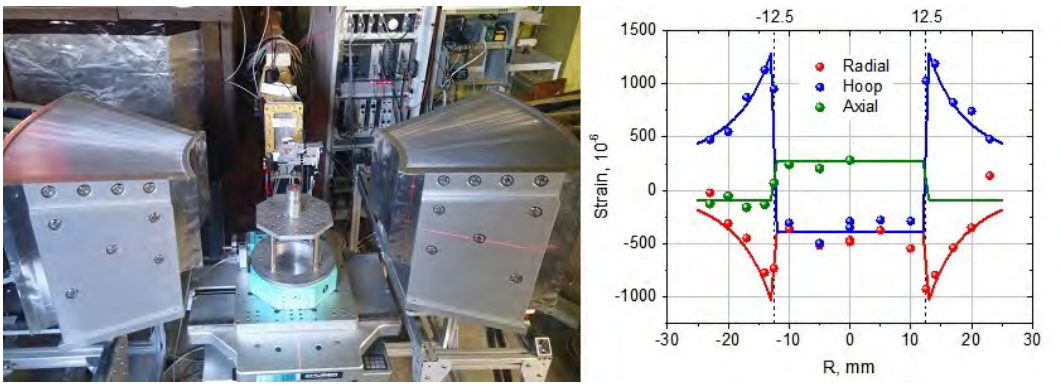

Fig. 1. Left: Sample place at the FSD diffractometer. Huber goniometer, the incident beam diaphragm, and two radial collimators at the scattered beams are visible. Right: Residual lattice strain measured in VAMAS shrink-fit ring and plug sample (set #1).

Neutron Imaging study of Strontium Chloride Ammine system for Heat Storage

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Salts of strontium chloride ammines ($SrCl_2$ / $SrCl_2(NH_3)_8$) can store and release heat based on exo-/endothermal ab-/desorption of ammonia. They are therefore promising materials for potential Thermochemical Heat Storage (THS) applications such as reutilization of industrial, low-grade waste heat and for district heating. The successful application of the $SrCl_2$ / $SrCl_2(NH_3)_8$ system depends not only on its heat storage capacity, but also on structural and microstructural changes that occur within the salts during NH_3 ab-/desorption processes. At the same time, the design of the THS reactor is crucial for the efficient transfer of heat to/from the salts.

In this work, strontium chloride ammine powders contained in a THS prototype reactor cell were studied by neutron imaging. The neutron imaging experiments were performed at the NECTAR facility located at the FRM-II reactor in Münich, Germany. The high neutron scattering cross-section of hydrogen allowed us to observe the NH_3 uptake and release within the salt. 2D neutron radiography images were taken during NH_3 absorption/desorption cycling at selected temperatures and pressures of ammonia. The salts were embedded in a stainless-steel honeycomb structure, in order to facilitate the heat conduction from a heating element to the opposite regions of the cell.

Absorption and desorption profiles for different regions of the THS reactor were obtained for each cycle by neutron radiography. The results of image analysis are discussed with respect to the homogeneity of the ab-/desorption process over the volume of the cell and how this is affected by the degree of compaction of the powder, as well as how efficiently the stainless-steel honeycomb structure conducts the heat during ammonia desorption. Tomography experiments were also performed. Swelling of the salt was observed during the first ammonia cycles which resulted in the evolution of a porous structure in the $SrCl_2$ salt.

1D Imaging of Flocculating and Sedimenting Particles

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Flocculants are usually polymeric molecules which cause the aggregation of particles in suspensions and will modify the sedimentation of particles. The gravitational field and the hydrodynamics of the aggregates result in a situation where larger aggregates sediment more quickly for less efficient packing and smaller particles will sediment more slowly. Such considerations are important in the formation of filter cakes where the porosity of the structure is critical for the transport of water and the hydraulic conductivity. Here we consider the structural profile of flocculated $CaCO_3$ particle suspensions under the influence of gravity and a commercial flocculant in the direction of the gravitational field. Dark field imaging[1] provides high resolution structural imaging of the structures formed by sedimented particles over a limited range of length-scales. We also consider spatially resolved USANS of the same suspensions after sedimentation which can consider an extended range of length-scales but have limited spatial resolution.

High-resolution residual strain mapping by energy-dispersive neutron imaging

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High resolution Bragg edge neutron transmission has emerged as a useful strain imaging technique for engineering samples, facilitated by the recent installations of neutron imaging beamlines at pulsed sources and the developments of time-resolving detector technologies. It measures shifts of lattice spacings in Bragg edge spectra, produced by the back-scattering of neutrons traversing polycrystalline materials. The transmission geometry preserves the information in real space, therefore the technique can produce a high-resolution maps with suitable imaging detectors, e.g., a micro-channel plate (MCP) detector.

Over diffraction-based techniques (neutron & X-ray), Bragg edge strain imaging offers the advantage of measuring hundreds of thousands of points in a single exposure. This become especially useful to perform strain mapping on samples with complex geometries, albeit only one through-sample averaged strain component is measured at a time. Experiments have been performed on the new IMAT imaging beamline at ISIS, UK, to study the residual strain profile generated by different manufacturing processes. One of them involved a complex-shaped, laser-peened steel sample, used for power generation applications, Fig. 1(A). Laser shock peening (LSP), a process which introduces beneficial compressive residual stress near the surface of the component, is normally applied to a flat surface, but it was extended to concave and convex surfaces in this study, Fig. 1(B). Transmission spectra were produced, and the Fe {*110*} Bragg edge was analysed, Fig. 1(C) to yield the reconstructed strain map presented in Fig. 1(D), where compressive residual strain profile can be clearly observed under the peened surface. Picking up a strain profile with high resolution (300-600 με) would be a challenge for a diffraction based technique. This test study emphasises the advantages of Bragg edge strain mapping for engineering applications. Other energy-resolved imaging examples, including strain mapping on cold-expanded holes and recrystallization of aluminium in high temperature will be presented.

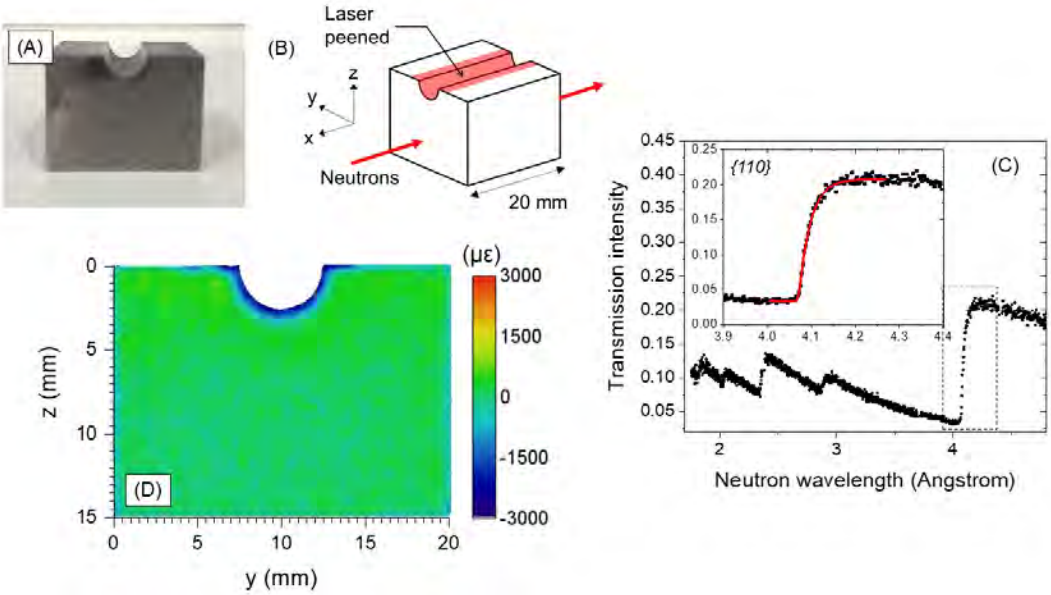

Figure 1. (A) Complex-shaped, laser-peened steel sample, used in power generation application; (B) laser peening was applied to a concave surface, the neutrons were transmitted parallel to the peening strip; (C) neutron transmission spectrum, with Fe {*110*} highlighted; (D) reconstructed strain map, showing compressive strain below the peened surface.

In-situ neutron diffraction study of Ni-addition influence on phase transformations in Co-Re-Cr high-temperature alloys

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Amongst new alloy systems being developed to supplement Ni-based superalloys in gas turbine application, the Co-Re-based alloys show promise because of their excellent specific strength and relatively high melting range (1490°-1560°C) [1]. Alloying elements with various functionality are added to these alloys. For example, Re to increase melting temperature, Cr, Ni, for oxidation resistance, C, Ta to produce high-temperature strengthening phase (TaC) or boron (to improve ductility). The effects of these elements on structure and microstructure were intensively investigated in the past by neutron scattering and other techniques [2-3]. Moreover, since the Co matrix undergoes an allotropic transformation from the low temperature closed packed hexagonal (hcp) structure to the high-temperature face centred cubic (fcc) structure, a two-phase matrix exists in Co-Re alloys at intermediate temperatures [4].

Like other Co-based superalloys presently used in gas turbine static components, the Co-Re alloys use Cr to provide oxidation resistance [5]. Cr addition above 20 at.%, however, pose a challenge – namely the formation of topologically closed packed Cr_2Re_3-type σ-phase. It is generally avoided in high-temperature alloys as its presence causes brittleness. The Co-Re alloys designed presently at TU Braunschweig are now being investigated for improving oxidation resistance and, simultaneously, suppression of σ-phase. It is intended to achieve this goal by a partial replacement of Cr by Ni atoms.

To fully reveal changes in polycrystalline bulky samples over the whole volume, in-situ neutron diffraction measurements were performed during heating to high temperatures (up to 1500°C) and cooling for a various Ni (8, 15 and 25 at. %) and constant Cr (23 at.%) content alloys. The allotropic transformation of the Co-matrix and the evolution of the low-temperature hexagonal and high-temperature cubic Co phases were studied. A surprising observation was the splitting of the fcc Co phase peaks [6] at high temperature during heating as well as cooling. The phase evolution was monitored, and an appearance of the secondary fcc phase could be linked to the formation of the σ phase associated with a compositional change in the matrix due to diffusion processes at high temperatures. At a lower-content of Ni (8 and 15 at.%), the secondary fcc phase transforms to secondary low-temperature hcp phase with the different chemical composition compared to the primary one. The σ-phase formation and its influence on the matrix phase separation – two fcc/hcp phases – in Co-Re-Cr-Ni alloys are an important discovery for the Co-Re alloy development and deserve further investigation.

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Cement-based materials for the conditioning of low and intermediate level radioactive waste: neutron scattering studies

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Cement-based materials are used in the predisposal of radioactive waste, in the conditioning phase, either to incorporate the wastes or to prepare the shieldings. Beyond the conditioning phase, they must comply with the disposal waste acceptance criteria (WAC) in terms of stability for 300 years [1, 2]. For obtaining a suitable cement matrix to be used for metallic radioactive aluminum conditioning, new chemical formulas are developed with the addition of inorganic [3] or organic [4, 5] components into the cement paste in order to reduce the corrosion rate in alkaline solutions and to obtain a low permeability rate [6]. The internal structure of several such cement-based materials for the conditioning of low and intermediate level radioactive waste (LILW) were studied using neutron tomography [7] and diffraction [8] in order to assess the effectiveness and stability of the hardened cement matrix, taking in consideration the need for long term durability in disposal conditions.

Two sets of samples were prepared based on two types of cement matrices which demonstrate good mechanical behavior, CEM V-A and CEM III-A. The neutron experiments have been carried out at the neutron radiography and tomography facility and texture diffractometer SKAT placed at the 14^{th} and respectively 7^{th} beamlines of the high flux IBR-2M pulsed reactor. The obtained experimental tomography 3D data were used to analyze the spatial arrangement of pores containing free water and aggregates, as well as inner pore structures [7]. In order to evaluate the stability of the hardened cement matrix and for taking into consideration the need for long-term durability in disposal conditions, the samples of CEM III cement-based materials were measured each year, in the period from 2016 to 2018, at the SKAT instrument.

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Non-destructive neutron surface and high spatial resolved residual stress analysis

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Diffraction is a powerful tool for investigation of residual as well as applied stresses in engineering materials and components. Both x-ray and neutron diffraction can be used for this purpose. The interest in neutron stress analysis stems from the high penetrating power of neutrons when compared to x-ray sources, i.e. several cm instead of tens of µm in metallic materials. This contribution gives an overview on current instrumental and methodical developments for non-destructive neutron through surface and high spatial resolved strain measurements.

Recent examples of high spatial resolution measurements in a three superimposed AISI 316L (ITER) weld passes using a mechanized tungsten inert gas (TIG) process, an (electron beam) EB welded austenitic and ferritic steel plates as well as in gold bracelets will be presented. These examples picture the current limit of residual stress analysis with neutrons.

Neutron imaging at long-pulse sources: opportunities, results and perspectives

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The neutron radiography and tomography method is a powerful tool of non-destructive analysis, which plays an important part in industrial and scientific research. The fundamental difference in the nature of neutron interaction with matter compared to X-rays provides additional benefits to neutron methods, including sensitivity to light elements, notable difference in contrast between neighboring elements like nickel and iron and high penetration ability. All these features make neutron tomography an attractive tool with a growing range of applications in industry, archeology and geophysics.

The neutron radiography and tomography facility located at the beamline 14 of the high-flux pulsed IBR-2 reactor was put into operation a few years ago. The facility provides possibilities for studies by means of neutron radiography and neutron tomography methods. The energy-selected neutron radiography techniques are also developed.

A specially designed detector module with two mirrors scheme for reduction of radiation damage effects is used for data collection. The camera based on Hamamatsu CCD chip with 2048 ×2048 pixels and precision remote control digital system of confocal coated lens provide the ability to vary the field-of-view of detector from 20×20 cm to 5×5 cm and clip of imaging data depending on the experimental requirements.

The neutron radiography and tomography methods are currently used in a wide range of research including engineering sciences, cultural heritage, paleontology and materials studies. In the present report, the recently obtained results are overviewed. The hardened cement samples with selected compositions as prospective construction materials for radioactive waste stores were studied. The spatial distribution of composition components and the geometric arrangement of pores and voids inside cement matrixes have been obtained. In addition, the real-time measurements of hardening of the cement pasta were performed. The internal organization of cultural heritage objects from collections of the Institute of Archeology RAS (Moscow) was also studied.

One of the benefits of the pulsed operation regime of the IBR-2 reactor is opportunities for implementing an energy-resolving mode in the neutron radiography experiments. The relevant results and prospects are presented.

Further development of neutron radiography and tomography techniques at IBR-2 reactor is also discussed. In particular, the project of cold neutron radiography facility at the beamline 10 of the IBR-2 reactor is being realized.

Detector developments in BrightnESS: beyond the limits of the current detector technologies for neutron scattering science.

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The BrigthnESS European funding (EU Horizon 2020, INFRADEV-3-2015, 676548) has given a significant contribution to the development of new neutron detector technologies for neutron scattering applications. Some of these detector technologies existed as a demonstrator before BrightnESS and they were boosted, moving from a technology feasibility study to an actual deployment of a detector into a real instrumental environment, leading to a scientific output and to a direct comparison with the state-of-the-art detectors. Others, instead, were created brand-new and developed from scratch thanks to this funding.

He3 and scintillators have been the main actors in neutron detection for years. In the last ten years many research centers were looking at new detector technologies for two main reasons. On one hand, the feasibility of large area (several square meters) neutron detectors was, and it is still, impossible due to He3 shortage problem and budget issues. On the other hand, even if the He3 or scintillators for small area detectors (from one square meter and below) would be available and affordable, a performance issue makes these technologies obsolete since they cannot cope with the requirements set by the upcoming instruments.

Nowadays neutron sources, such as the ESS, are more and more bright and their instruments require more performing detectors, mainly in terms of counting rate capability and spatial resolution. The He3-based technology is actual hitting its fundamental limits.

BrigthnESS work package 4 (WP4) was focused on the innovation of key neutronic technologies such as detectors and moderators. Four out of the five tasks in this WP were about detectors and they led to three novel detectors for neutron scattering which will be employed in six instruments at ESS.

These detector developments will be presented.

The first detector is the Gd-GEM [1,2], based on the GEM (gas electron multiplier) technology and Gd as a neutron converter, it replaces image plates and cameras to challenge the spatial resolution needed in Laue diffractometers. Typical state-of-the-art detectors with timing resolution are presently limited in spatial resolution to approximately 1 mm. So far, no time resolved detectors are commonly used with a position resolution between 100 micron and 1 mm.

The second is the Multi-Blade [3-5] B10-based detector and it aims to surpass the limits of He3 detectors for neutron reflectometers which are already at saturation at current neutron sources. A sub-millimeter spatial resolution and a much larger counting rate capability is needed compared to the state-of-the-art detectors in order to enable new science.

The third is the Multi-Grid [6] detector which is also based on B10 layers and it will be employed in the chopper spectrometers. Large area (several square meters) detectors have traditionally been built using the isotope He3. However, He3 is no longer available or not affordable, and here the Multi-Grid represents a strategic challenge for Europe.

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Using Light to see Neutrons: a new 2D detector with high resolution.

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The evolution of light sensors enjoyed unprecedented growth in the last 20 years. This evolution is such that the camera of a smartphone can be used for Raman spectroscopy [1] or to detect atrial fibrillation in medicals. We will illustrate how these recent advances in light sensors revolutionize the observation in physics. Today the technology is sufficiently powerful to be exploited quantitatively in neutron spectrometry for the study of both elastic or inelastic scattering (time of flight). The two-dimensional high resolution neutron detector, called Barotron [2] (from the name of the inventor) is derived from this technology [3].

With a basis of 250 000 pixels, a resolution of 16 bits for each pixel, a very low detection limit (<< 1 / cm^2 / s), a high dynamic (16 bit) and an excellent spatial resolution (0.5 * 0.5mm^2), the Barotron performances compete the best current two-dimensional gas detectors. This new technology presents the huge advantage of being constantly upgraded by replacing the sensor. This development opens a new generation of high-performance neutron detectors, versatile and adapted to new spallation sources for an ever more precise characterization of the properties of the samples.

We will give some examples of exploitation of the high resolution detector including imaging, diffraction or SANS.

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Development of a large cylindrical Trench-MWPC detector for XTremeD neutron diffraction instrument

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A large cylindrical detector is under fabrication for the XtremeD neutron diffraction instrument which will be installed at ILL after the upgrade of one of the neutron guides [1]. XtremeD instrument will be dedicated to neutron diffraction by powder and crystal samples under extreme conditions. In order to maximise the count-rate capability of the detector, the Trench Multi-Wire-Proportional-Chamber (Trench-MWPC) was proposed as an alternative to more standard MWPC configurations [2]. In the Trench-MWPC design, anode wires are stretched along trenches machined in a stack of aluminium plates. The presence of cathode trench side-walls surrounding anode wires improves the collection of ions produced during the gas avalanche process; this configuration contributes to a reduction of space-charge effects which usually limit the maximum local count rate of MWPCs. The advantages of the Trench-MWPC were demonstrated using a proof-of-concept detector which was filled with a gas mixture of ^{3}He, Argon and CO_2 at a pressure of 7 bar to reach the specifications of XtremeD detector in terms of detection efficiency (80% at 2.5Å) and spatial resolution (0.15° longitudinally and 0.2° vertically). The design of this detector will be presented together with the main results obtained during a detector characterisation campaign performed on CT2 neutron detector test beamline at ILL. The XtremeD detector will contain 9 modules mounted side by side on a radius of 76 cm to produce an angular coverage of 130° horizontally by 24° vertically. The technical challenges and solutions regarding the mechanical design, fabrication and testing of this detector will be presented.

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The SoNDe high-flux neutron detector

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New high-flux and high-brilliance neutron sources demand a higher count-rate capability in neutron detectors. [1] In order to achieve that goal, the Solid-State Neutron Detector (SoNDe) project is developing a scintillation-based neutron detector. It is capable of fully exploiting the available flux at small-angle neutron scattering (SANS) instruments at high brilliance sources, such as SKADI at the European Spallation Source (ESS). The read-out of the scintillator is based on a pixelized multi-anode PMT (MaPMT), where each pixel is treated separately. In addition to enabling higher achievable count-rates, one of the design goals was to develop a modular and scalable solution that can also be used in other instruments or different contexts, such as for laboratory setups. This has been achieved by combining the complete read-out electronics along with the MaPMT into modules that can be controlled and read-out individually via a network without additional any infrastructure.

Since higher brilliance and flux sources call for detectors that can handle high-flux, especially when considering pulsed sources with high peak-flux, the requirements for the development of the SoNDe detector were defined as

- Possible to handle a flux of 20 MHz on a 1x1 m^2 detector area, about four times maximum peak flux achieved today
- Pixel resolution down to 3x3 mm^2
- Neutron detection efficiency higher than 80%, good gamma-discrimination
- ^{3}He independence
- µs time resolution
- consisting of individual modules to allow for simple repair and maintenance and avoid long down times.

The requirements as posed here were all achieved or exceeded. In order to do so, a small pixelization of multi-anode photomultipliers (MaPMTs) is combined with a ^{6}Li-glass scintillator as well as high-capacity read-out electronics that is built to fit completely behind the MaPMT so as to form a single module that can be tiled to cover an arbitrarily formed surface. [2]

Countrates of 250 kHz per module were measured under primary beam conditions at neutron scattering experiments. Combined with the high area coverage of the square modules and the high efficiency of the scintillator this allows to use high flux neutron sources to capacity. In areas where the high count rates are not strictly necessary, still the handling of a single module (5 cm x 5 cm x 20 cm) can be used for applications such as laboratory bench measurements as well as handheld devices.

During scaling up also modules with 10 cm x 10 cm surface coverage were constructed. Those reduce the power usage when compared to the single module devices, since the controlling FPGAs can be shared between several MaPMTs. These are also used to construct the 1 m x 1 m large-scale detector, which is currently assembled.

The SoNDe project has achieved its development goals and is now in the construction phase of the large-scale detector. In this contribution we want to give an overview of the development during the final stage of large-scale construction of the neutron detector.

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New prospects in 3He detector techniques

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A large number of projects in the Endurance program rely on the development of ^{3}He detectors for new instrumentsor for improving performance on existing instruments. The completion of 3 detectors is planned for 2019: the XtremeD instrument will be equipped with a trench-MWPC, containing a new cathode design to improve the counting rate capability of MWPCs; the PANTHER TOF instrument will use a MultiTube detector with a large sensitive area, and a high efficiency MAM (Monoblok Aluminium MultiTube) is in fabrication for the D3 diffractometer. Several otherprojects have been launched recently: the D11 and D22 SANS instruments will be equipped with linear PSDs; a large area trench-MWPC is in development for the D16 instrument; and a new version of the D20 detector based on the trench-MWPC technique, is under study. Beside the Endurance program, ^{3}He detectors are also developed in the SINE2020 project for high counting rate, high spatial resolution applications, and a MAM detector has been completed for the Platypus reflectometer at ANSTO. This paper will cover the recent development performed at the ILL in the field of ^{3}He detectors, with the objective to show that they remain the optimal choice for several applications in neutron scattering science.

PIK reactor neutron guide system

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This year the ramp up of the PIK reactor – the most powerful steady state neutron source in the world - has finally started. The instrumentation suite is now under design and construction.
12 instruments are to be fed with cold neutrons. All of them will be placed at the beamtube Channel-3 equipped with the cold neutron source. An extensive guide system is being created to transport neutrons from the beamtube to above mentioned instruments in the neutron guide hall. Main feature of
this system is the adaptation of beam properties to the instrument requirements.
The neutron guide system consists of 6 primary guides, some of which are branching downstream to provide additional end stations. Several guides are equipped with focusing noses for increasing the neutron flux density at sample positions.
The final configuration of the guide system is presented, as well as its design features and simulation results. Currently the technical drawings are ready and the production of the guide system has started.

ILL Modernisation Programme: Endurance. The ambitious renewal of the H15 cold neutron guide and instrumentation

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The ILL has begun a second phase of ambitious upgrades to scientific instruments and infrastructure under the Endurance programme. Endurance 2 (2019 - 2023) will involve the upgrade of many instruments including a number of large detector projects and with a main focus on the upgrade and re-modelling of instruments on the Vercors side of ILL 7, including a complete renewal of the H15 cold neutron guide. The massive scope of the H15 project aims to provide dedicated beam positions for the new or upgraded SHARP/RAMSES time-of-flight spectrometer, the polarised diffuse scattering instrument D7+, an upgraded D11 small-angle scattering (SANS) instrument as well as positions for additional instruments, GAPS (cold triple-axis spectrometer) and SAM (SANS). The conceptual design of the renewed H15 guide is highly complex, both in terms of its novel curved diverging trumpet expansion and the engineering constraints in the separation of six independent neutron guides and placement of instrumentation. Phase-space analysis shows how the diverging curved trumpet best allows for an optimal expansion of the initial high-m neutron guide and provides additional angular separation for the down-stream instrument branches. The Endurance programme, with a particular emphasis on the H15 guide project, will be presented.

Mirror flippers: experiments and possible applications

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Neutron spin optics (NSO) [1-3] based on quantum aspects of the neutron interaction with magnetically anisotropic layers signifies the expansion of polarized neutron optics from 1D (spin selection, as in conventional polarizers and analyzers) to 3D (spin manipulation). It may essentially widen the functionality of neutron optics. Basic elements for innovative neutron devices include mirror spin turners ($\pi/2$- and π-turners, in the first place). Experiments with the multilayer-backed flipper for monochromatic beams will be discussed. Such neutron reflectors may also be used as spin $\pi/2$-turners. Mirror flippers open new possibilities, one of which is a beam hyperpolarization, when the separation of neutrons with the opposite spins is followed by flipping the 'wrong' spins. The possibility to implement precessing spin neutron reflectometry will also be considered. The contribution was supported by the Federal target program of Ministry of Education and Science of Russian Federation (project No. RFMEFI60717X0194).

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Neutron guide design optimization of MIRACLES, the time-of-flight / backscattering spectrometer at the European Spallation Source

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A neutron transport system for MIRACLES, the time of flight / backscattering spectrometer at the European Spallation Source (ESS) has been proposed. Functional requirements derived from the science case of MIRACLES and construction constraints have determined the final design of the 160-meter neutron beamline. This included not only optimizing the transport of cold neutrons at quasielastic neutron scattering (QENS) energies (elastic wavelength, λ = 6.27 Å) but also extending this optimization to inelastic neutron scattering (INS) energy range for cold neutrons λ > 2 Å. The overall neutron intensity estimated at the sample position increases by more than 30% when compared to the original proposal. When studying the neutron beam extraction system, several options have been considered for the vertical geometry, and a solution involving a modified elliptical profile, aiming to an improved collection of cold neutrons from the source, has been selected. The horizontal geometry in turn is much simpler and consists of a slightly convergent tapered guide downstream to the pulse shaping chopper to match the essential requirement for high resolution of the instrument. A curved guide segment has been chosen to filter cold neutrons with wavelength λ > 2 Å. The long straight guide segment starts with a divergent guide section; this narrows the divergence distribution to maximize the neutron transport through the rest of the beamline. The focusing guide is designed to fully illuminate samples of 3x3 cm^2, while additional calculations resulted in a possible exchange of the 1-meter end segment in order to illuminate samples of 1x1 cm^2, reaching an increasing flux at the sample position of 70% at the elastic peak energies.

Recent achievements in Neutron Optics at the I.L.L.

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The Neutron Optics Service plays an active part in the modernisation programmes Millennium and Endurance phase 1 at the I.L.L., with the production of new optical components such as crystal monochromators and supermirrors. In addition, an innovative research programme in the field of polarising neutron optics is currently under way with the aim of developing advanced tools for neutron instrumentation. An overview of some recent achievements and recent advances in neutron optics is presented.

The neutron spin analyser for the new spin echo spectrometer WASP has been successfully completed. More than 3500 double-sided m=2.8 Co/Ti supermirrors have been in-house manufactured. Recently mounted onto the instrument for the commissioning phase, it will cover a detection angle of 90°.

Several monochromators are under preparation at the I.L.L. Two Large double-focusing monochromators composed respectively of HOPG and Cu mosaic crystals have been constructed for the new thermal time of flight spectrometer PANTHER. The Endurance1 project also involves the upgrade of the D10+ single crystal diffractometer, the IN13+ backscattering spectrometer and a new extreme conditions powder and single crystal diffractometer XtremeD. Each instrument will benefit from new monochromator optics developed at I.L.L.

The fundamental physics instrument PF1B has been equipped with a new type of solid-state broadband neutron polariser composed of 880 Fe/Si/Gd supermirrors coated on sapphire substrates. It should deliver cold neutron beams with very high polarisation up to 99.9 % for wavelengths in the 2-20 Å wavelength range.

XYZ polarisation analysis using ^{3}He spin filters has therefore been further developed through improvements to the performance of the so-called PASTIS system by increasing the helium-3 relaxation time up to 100 hours. Finally, to cope with an expected rise in demand for ^{3}He spin filters, the group has begun work on upgrading the filling station known as “Tyrex” in order to increase its production capacity by a factor of 2.

Project of advanced solid-state polarizer for PF1B

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The polarized neutrons beam line for Fundamental Physics PF1B operates with one of cold-neutrons beams at Institute Laue-Langevin. An essential component of PF1B is a neutron polarizer that produces a large-area, well-polarized neutron beam over a broad range of neutron wavelengths (0.2-2nm). The present polarizer is based on "classical" polarizing bender design [1-3]: 30 channels of 80 cm length, air gaps of 2 mm , borated glass substrates 0.7 mm thick, m=2.8 Co/Ti Super-Mirror (SM) coating, The transmission of the polarizer was measured ~ 50% for a "good" spin component and 98.5% polarisation [4]. When an Ultra-High polarisation is requested a second polarizer of the same type and properties is added in "Crossed configuration" [5] delivering P = 99.7% polarization with the 25% of transmission. During more then 15 years of successful exploitation the polarizer was irradiated by high integral neutron flux (> 2 10^{18} n/cm^2) which yields in high neutron activation of Co (decay constant $T_{1/2}$ =5.7 year), and significant neutron induced radiation damages of the mirrors. We present project of advanced polarizer for PF1B with significantly improved polarization performance [6] and free from radiation damages.

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New neutron supermirror polarizer

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New neutron supermirror polarizer is proposed [1]. The possibilities of using this polarizer in the neutron experiment are discussed. The proposed polarizer is compared with well-known supermirror polarizers, including the V-cavity [2].

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Mass production of neutron polarizing supermirrors for the WASP instrument at the ILL

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The neutron instrument WASP (Wide Angle Spin Echo) at the ILL [1] is in commissioning phase, and will soon accept its first users. This instrument is unique worldwide, and its unprecedented performances are expected to open new horizons in the investigations using the neutron spin echo technique. One critical optical component of this instrument is its wide-solid angle and broad-band spin-polarization analyzer [2]. It consists in 90 benders like the one illustrated on Figure 1b, each of them covering an angle of 1 degree 3 meters away from the sample. Each bender contains 36 C-shaped polarizing channels made out of double-side magnetic multilayer coated mirrors operating in reflection. The coating design is a Co/Ti/Gd 541-layer supermirror with anti-reflecting/absorbing layer. The production of these supermirror coatings, covering a total area of 239 m^2, spanned about 10 years and is now over. The design principle of the analyser will be briefly given, together with some intermediate characterisation of the benders and preliminary results from the first available neutrons on WASP.

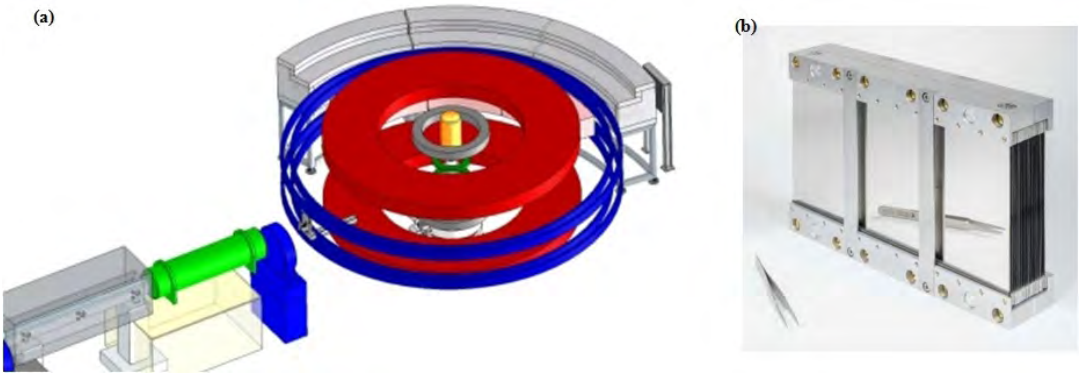

Figure 1: (a) General scheme of the WASP instrument, showing the 90° analyser bank.
(b) Analyzer bender covering horizontally 1° from the sample.

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Development and first test on large angle RF-flipper.

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The increase of count rate of the neutron resonance spin-echo spectrometer (NRSE) MUSES can be achieved by using a multi-detector system [1]. In this case acceptance angle of the second arm of NRSE should be increased according to the new detector bank. The curved resonance spin-flippers will be used to keep equal field integral for all scattered neutrons in large solid angle corresponding detectors acceptance one. In this work we present the development and first tests on the curved resonance flipper with the shorter radius of curvature which is most difficult one to realize with good field homogeneity. The results of field homogeneity measurements of curved RF-coil as well as results of the flipper efficiency test are presented for different scattering angles and frequencies.

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Ultra Wide angle 3He polarization analysis for neutron spectroscopy, PASTIS on NEAT

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Polarized 3He holds potential for difficult applications of polarization analysis in neutron scattering. One such application is the analysis of very wide angle detector banks in wide angle neutron spectroscopy. We have applied our so called "PASTIS" system, polarization analysis on a thermal inelastic spectrometer, in development for TOPAS at the MLZ on the NEAT chopper spectrometer at HZB. We have successfully implemented the system, and performed first scientific measurements. The installation provides analysis over nearly the full NEAT detector bank which covers over 240 degrees in the horizontal plane and 40 degrees vertically. We will describe the performance of the PASTIS system and show results of processed data from measurements using both uniaxial polarization analysis for separation of coherent and incohernt scattering, and also full XYZ polarization analysis on magnetic single crystals.

Uniaxial polarization analysis on the LET time-of-flight spectrometer: first results

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LET is a cold time-of-flight chopper spectrometer installed on the second target station at the ISIS facility. With nearly π st. of continuous detector coverage, it is primarily used to map excitation spectra in single crystals of magnetic materials. Beyond this application, its high resolution makes it well suited for quasi-elastic scattering (QENS) studies of energy materials, soft matter, and biological systems. Here, we present the design, construction, and commissioning of a uniaxial polarization analysis option for LET. The polarized beam is generated by a supermirror "V"-cavity polarizer, which is immediately followed by a Mezei-type precession coil flipper. Analysis of the scattered beam is achieved using a wide-angle ^{3}He spin filter, which provides access to the full LET detector. The potential of the instrument to carry out polarized QENS is illustrated by the example of a solar cell polymer blend, where the separation of the coherent and incoherent components of the cross section **[Fig. 1]** provides information on the motion of the polymer backbone and protons, respectively.

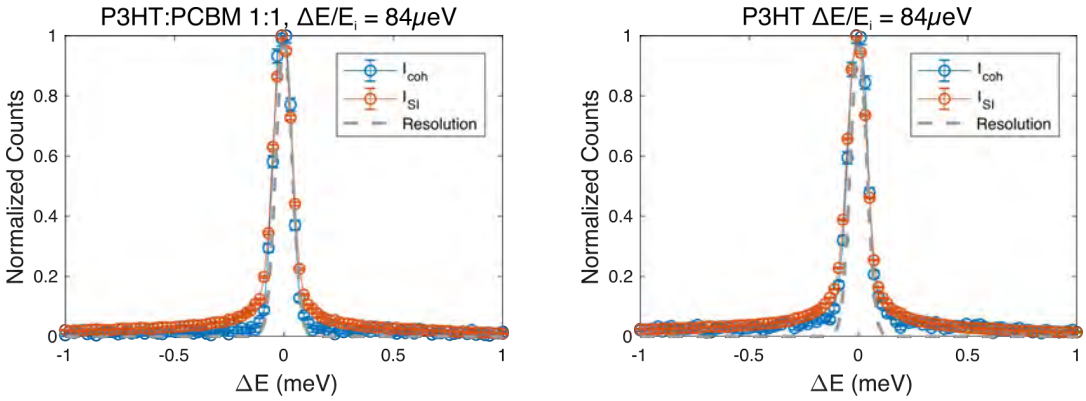

Figure 1: Coherent and incoherent QENS for a solid polymer-fullerene blend (left) and a pure polymer (right), as separated by uniaxial polarization analysis on LET. A significant narrowing in the coherent QENS is seen on blending, reflecting a slowing down in the motion of the polymer backbone.

Development of hyperpolarized helium-3 spin-filters for polarised neutron experiments at the ISIS neutron and muon source

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Hyperpolarized ^{3}He gas offers the possibility of polarizing or analyzing neutron beams across broad ranges of wavelength and solid angle, all without deviating the beam. This makes it ideally suited for applications like direct geometry time-of-flight spectroscopy [1] and small-angle neutron scattering. A particularly important property of hyperpolarised ^{3}He is its longitudinal relaxation rate $1/T_1$, where T_1 describes the time for the gas to depolarise. This is less formally described as the life-time, and is limited due various relaxation mechanisms; often, the dominant term is depolarisation due to interactions with the container/vessel wall.

Consequently, it is essential to understand the surface properties of the container wall, including its roughness, defect chemistry, and reactivity. A common vessel material for hyperpolarised ^{3}He spin-filters is fused quartz (SiO2), which contains very few magnetic impurities, but even with a highly polished surface gives an experimentally unviable T1 of 6 hours. In order to achieve longer ^{3}He life-times, it is therefore necessary to coat the surface; indeed, it is possible to achieve an improved life-time, often exceeding 100 hours, by coating the cell with caesium metal [2]. However, the hazards and practical difficulties associated with this procedure motivate the search for other coating materials, which should, as a minimum, provide competitive lifetimes to caesium (for our purposes, a minimum of 60 hours). This search has concentrated on siloxane-based coatings because of the long wall relaxation rates observed for polarized ^{129}Xe storage cells [3]. For the purpose of ^{3}He cells, simple organosilicon reagents such as dichlorodimethylsilane and trimethylchlorosilane are being explored as promising coating agents.

This presentation aims to address the following two topics: the surface chemistry of fused quartz-based ^{3}He cells, and the application of organosilicon coatings to both quartz and silicon containers to improve ^{3}He life-time. The techniques used are atomic force microscopy, X-ray and neutron reflectometry and X-ray photoelectron spectroscopy. Results indicate that the surface quality of quartz depends crucially on the type of manufacturing procedure used. Here, the observations made are decreased surface homogeneity as a function of chemical polishing, and doubled surface roughness as a function of hot working. With regards to the organosilicon coatings, a partial surface coverage has been achieved, and we will report prelimary results regarding the life-time of quartz and silicon containers.

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Novel type polarization analysis using multi-analyzer setup @ PUMA, FRM II

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The thermal triple-axis-spectrometer PUMA at the neutron research reactor FRM-II (MLZ) is one of the most robust and yet extremely flexible instruments worldwide of its kind. In addition to the "*normal triple axis*" set up, PUMA delivers a good number of unique features to meet the ever-growing demands of the scientific community worldwide. Multiplexing, using the multi-analyzer and multi-detector systems is one of them, which consists of eleven arbitrarily configurable analyzer-detector channels. In particular, single shot kinetic experiments are well suited as the setup allows the realization of an entire ($\boldsymbol{Q}$,$\boldsymbol{\omega}$)-scan within a time scale even less than a minute as a function of any external stimulant [1]. Moreover, the same set up can be used for polarization experiments very efficiently. By directing the spatially separated different spin-states of the scattered neutrons into the different analyzer channels, the spin flip (SF) and the non-spin flip (NSF) components can be simultaneously determined and to best of our knowledge none of the conventional existing neutron instruments collects both spin-states at the same time [2]. Especially in case of kinetic time-resolved experiments, where both spin states need to be registered synchronously at the same state of the sample, this set up is of absolute necessity. To allow an easy and efficient operation of this sophisticated polarization set up and provide support for subsequent data analysis, we have developed GUI based MAX-PA software. In this talk, I will report on the details of the current polarization analysis setup at PUMA and show results from the pilot experiments.

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Polarized pulsed neutrons using a 3He spin filter with an in-site SEOP method

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A 3He spin filter is a neutron polarization device composed of polarized 3He gas and alkali metal encapsulated into a special glass cell, which does not include boron. 3He has a very large absorption cross section (10666 barn) for anti-parallel neutrons; nevertheless the absorption cross section for parallel neutrons is approximately zero, and the neutron beam is polarized passing through a glass cell into which polarized 3He is encapsulated. 3He nuclei are polarized irradiating a circularly polarized laser (SEOP method). The 3He spin filter has a large acceptance and can polarize neutrons for a wide energy range. Therefore it is a useful neutron polarization device for pulsed neutron sources.

We are developing the 3He spin filter at J-PARC for fundamental physics, neutron scattering, neutron imaging, and so on. A 3He polarization system which can install neutron beam lines, so-called in-situ SEOP, are important to obtain stable neutron polarization during neutron experiments. A compact laser system whose size of 60cm x 60cm was developed at J-PARC. We installed the system to NOBORU beam line at the material life science facility in J-PARC, and succeeded to supply pulsed polarized neutrons. The pulsed polarized neutron beam was evaluated by transmitted neutrons measured with a Li-glass pixel detector and 3He polarization measured with EPR and AFP-NMR.

We will talk about the development of the in-situ SEOP system and the detail of the experiments result.

Fluorinated nanodiamonds as unique neutron reflector

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With the pronounced, worldwide trend of increasing the range of useful neutrons towards smaller energies—driven in particular by large-scale structure diffractometers, reflectometers, time-of-flight and spin-echo techniques as well as by particle physics—progress is limited by the low fluxes of the less energetic part of the cold neutron spectrum. One fundamental reason lies behind this drop in flux: regardless of the choice of materials for neutron reflectors, they are all composed of atoms. Atoms in solids and liquids are separated by distances of a few tenths of nm. If the neutron wavelength is larger than that, neutrons are weakly scattered by atoms/nuclei and the diffraction is limited by the inter-plane distances available; thus, neutrons pass through a reflector with low interaction with its material and are lost.

To construct efficient slow-neutron reflectors, currently there is no alternative other than to mimic conventional reflectors by replacing atoms/nuclei with nanoparticles of low absorbing, highly scattering materials—thereby changing the characteristic length scale and consequently the neutron wavelength corresponding to efficient neutron reflection [1]. Nanodiamonds [2] are an obvious choice for the material of such reflectors, as the cross-section of absorption in carbon is exceptionally low, the coherent scattering length is very high and the volume density is higher than that for other carbon materials. The characteristic sizes of available nanodiamonds are found to be in the range of optimum theoretical values. In addition, the reflectivity of available nanodiamonds has been assessed to be much higher than that of any alternative reflector [3]; however, it remained low for neutron velocities above 160 m/s, mainly because of the high content of hydrogen impurities. We overcome this principal difficulty by using fluorinated nanodiamonds [4] and proposed a new class of reflectors, based on designed fluorinated nanodiamonds, that can provide a continuous reflectivity curve with high albedo, thus minimising the existing ‘leak’ of neutrons through the so-called reflectivity gap. This high diffusive and quasi-specular reflection will dramatically improve the performance of neutron sources, the efficiency of neutron delivery and thus the fluxes of slow neutrons in neutron instruments. It might also allow a new generation of neutron sources and experiments to be designed.

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MARIA – The high-intensity polarized neutron reflectometer of JCNS

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The high-intensity reflectometer MARIA of JCNS is installed in the neutron guide hall of the FRM II reactor in Garching and is using a velocity selector (4.5Å<λ<40Å) as a primary wavelength filter with a resolution of 10%. In combination with the optional Fermi-Chopper the wavelength resolution can be increased to 1% or 3%. The full cross section of the beam is optionally polarized by a double-reflecting super mirror (4.5Å<λ<12Å) and in the vertical direction the elliptically focusing neutron guide increases the flux at the sample position and consequently reduces the required sample size or measuring time. A flexible Hexapod, as sample table, can be equipped with an electromagnet (up to 1.1T) or a cryomagnet (up to 5T), low temperature sample environment, a UHV-chamber (10^{-10} mbar range) for the measurement of Oxide MBE samples (transfer forth and back) and last but not least with various soft matter solid/liquid interface cells connected to a “sample robot” for automatic solvent contrast exchange and remote controlled heating/cooling. Together with the 400 x 400 mm² position sensitive detector and a time-stable ^{3}He polarization spin filter based on Spin-Exchange Optical Pumping (SEOP), the instrument is well equipped for investigating specular reflectivity and off-specular scattering from magnetic layered structures down to the monolayer regime. Furthermore the GISANS option can be used to investigate lateral correlations in the nm range. Due to the large detector even grazing incidence diffraction measurements are possible. All the options, like GISANS, polarization and ^{3}He polarization spin filter can be moved in and out of the beam in seconds by remote controlled push button operation and do not require any realignment.

MARIA is a state of the art reflectometer at a constant flux reactor. It gives the opportunity to investigate easily reflectivity curves in a dynamic range of up to 7-8 orders of magnitude including off-specular scattering and GISANS measurement. Furthermore the high intensity allows for kinetic measurements down to a few seconds over a dynamic range of 3-4 orders. In the case where dynamic ranges in the order of 4-5 orders need to be accessed, the measurement time is in the few minutes range.

Exploring dynamic functionality at nanoscale using high power neutron spectroscopy

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Keywords: neutron spectroscopy, instrumentation, dynamics

Direct geometry neutron time-of-flight spectrometers allow us to probe dynamic phenomena directly in wide-ranging time and length scale domains. Hence the range of application is very broad, stretching from investigations of spin dynamics in magnetic system to molecular or ionic transport in novel functional materials and to investigation of proteins and soft matter. Here we report the results of the full upgrade of TOF spectrometer NEAT in Berlin [1], developed to address the user community needs in more powerful instrumental capabilities. Using modern technology and innovative instrument design the upgrade resulted in 300 fold count rate increase. The high flux is combined with unprecedented instrumental flexibility which, on the one hand, allow us to best adapt to various user requirements and, on the other hand, does not compromise instrument performance. The upgrade placed NEAT on the similar level of performance as the world leader spectrometer IN5 at ILL despite of the order of magnitude lower cold neutron flux at the reactor in Berlin. The regular user operation has been started successfully in January 2017, just couple of month after the installation of the last key parts of the instrument.

The advanced features of the new instrument include novel integrated guide-chopper system with implemented options for high intensity and high resolution conditions. An additional option is the “inelastic” chopper configuration, which allows for further increase of the detected neutron intensity at larger energy transfers in neutron energy loss regime. NEAT neutron guide deliver neutrons to the sample with flexible beam properties: either homogeneous beam over 10 cm^2 cross section with low divergence for single crystals studies or “hot-spot” neutrons with enhanced intensity for small samples. Thanks to the high flux, the sample amount could be strongly reduced. The accessible wavelength range of the instrument from 1.3 Å to 20 Å is significantly extended towards shorter wavelengths compare to predecessor making NEAT a truly bispectral spectrometer. As a result the frequency range at neutron energy loss is doubled providing better experimental conditions in particular for low temperature studies. Large coverage of the detection angle has been achieved using state-of-the art ^{3}He position sensitive detectors placed at 3 m from the sample and equipped by modern electronics and event recording data collection [2]. The entire secondary flight path is non-magnetic and allows for applications of high magnetic field sample environment up to 15 T. Novel feature of NEAT is the polarized neutron spectroscopy option which has been implemented in collaboration with scientists from JCNS in Germany, ESS project in Sweden and Wigner Research Center in Hungary [3], [4].

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Bambus: a new inelastic neutron multiplexed analyzer for Panda at MLZ

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Cold-neutron triple-axis spectrometers (TAS) are dedicated to the investigation of low-energy excitations in a wide area of condensed matter physics, from quantum magnetism to unconventional superconductors. This technique allows us to measure individual points in the large *(**Q**,E)* space for one instrument setting, in particular at very low temperatures and high magnetic fields. New engineering solutions were recently developed in order to increase the useful signal on TAS. With this purpose, the multianalyser Bambus is being constructed at the cold-neutron triple-axis spectrometer Panda at MLZ, in cooperation with TU Dresden, and financial support from the BMBF project 05K16OD2. Its concept lies in collecting data at a certain energy transfers along a curved path in ***Q*** space, with the aim to construct broad reciprocal space maps at multiple energy transfers in a reliable, easy-to-use setup without movable axes. Hence, experiments will provide an overview in a large *(**Q**,E)* space, in order to get insights of broad features at low energy or study complex dispersion laws. Because this spectrometer is designed as a complementary option to the normal TAS mode, a fast switch between the two setups is foreseen. The general concept will be presented together with the final design, the different key components, and the results obtained with two prototypes.

PANTHER: the new thermal time of flight spectrometer at the ILL.

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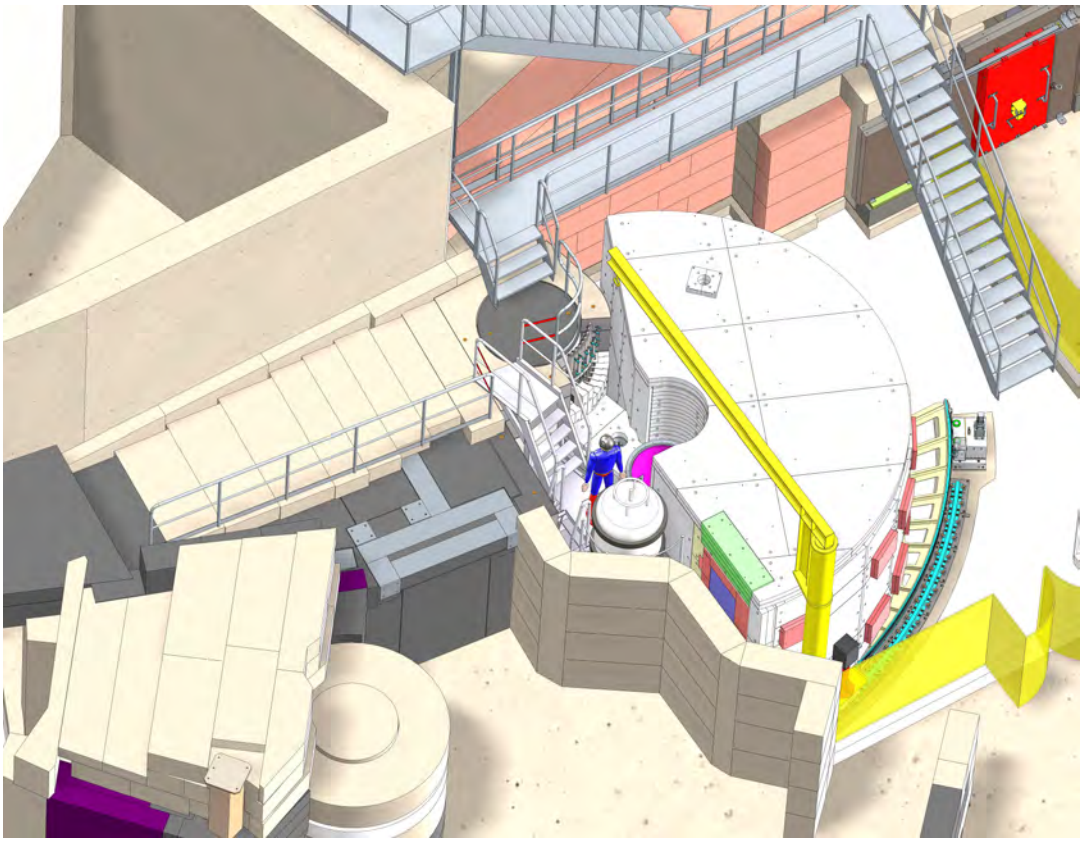
PANTHER (Polarization ANalysis on a THERmal time-of-flight) is a multi-purpose direct geometry thermal neutron time-of-flight (TOF) spectrometer optimized for studies of magnetism, single crystals, and small samples. Its high neutron flux, medium resolution, large detector coverage, and wide span of incoming energies allows for fast mapping of magnetic and structural excitations over a large range of wave-vector and energy transfers. PANTHER will allow for the use of complex sample environment, including the 10 Tesla « IN5 » magnet. It will also be equipped with full longitudinal polarization analysis using a 3He-filter device (PASTIS-3). The instrument is under construction at the H12 beam tube and will replace IN4C.

Compared to IN4C, the main improvements are the use of position-sensitive detectors (PSD), a well-shielded flight chamber connected to a wide-diameter sample area with a common vacuum, fully double focusing monochromators, additional background choppers, and non-magnetic construction materials. This will lead to a gain in flux of about two, an increased solid area of a factor of three, and a reduced background by a factor of ten. The improved signal-to-noise ratio of 60 will be profitable for studies of magnetism, lattice dynamics, and vibrational spectroscopy in the incoming energy range 6-120 meV. The use of ^{3}He PSD's will allow for single-crystal studies.

In this presentation we will review most of the critical aspects of this project, from the focusing principle to the description of the last generation of background choppers to be installed on PANTHER. We will also discuss PANTHER’s timeline, from the present state to the first experiment in the user program.



IN16B - a most versatile high flux neutron backscattering spectrometer

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IN16B, a latest generation neutron backscattering spectrometer at the ILL reactor [1], offers today the highest energy resolution [2], the best signal-to-noise ratio [3] and with its recent time of flight backscattering option BATS also the widest dynamic range [4,5]. The flexible instrument concept of IN16B has enabled both, new instrument developments and heavy user operation as a classical reactor backscattering instrument with sub-µeV energy resolution.

We review the instrument design of IN16B, which for Si (111) backscattering crystals IN16B achieves an energy resolution of 0.3 - 0.7 µeV in a Q-range from 0.2 - 1.9 $Å^{-1}$ and with Si (311) crystals a resolution of 2 µeV in a Q-range from 0.7 - 3.5 $Å^{-1}$. New instrument developments are the recent inverted time-of-flight backscattering option BATS with 1.5 - 8 µeV energy resolution and a wide energy transfer range (up to ~700 µeV) [5] or the extremely high energy resolution GaAs (200) prototype (78 neV FWHM) [2].

We further review the user operation of IN16B with applications in a wide field of science. The research addressed in parallel to instrument commissioning and development during the five years of user operation ranges from molecular spectroscopy and magnetism to material science for energy materials and biology. We highlight a few examples and feature the popular use of alternating fixed elastic and inelastic scans [6], which for now is unique on IN16B.

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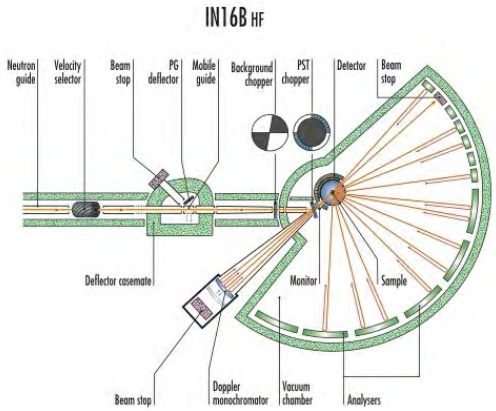

CAMEA - A novel neutron spectrometer for extreme environment investigations

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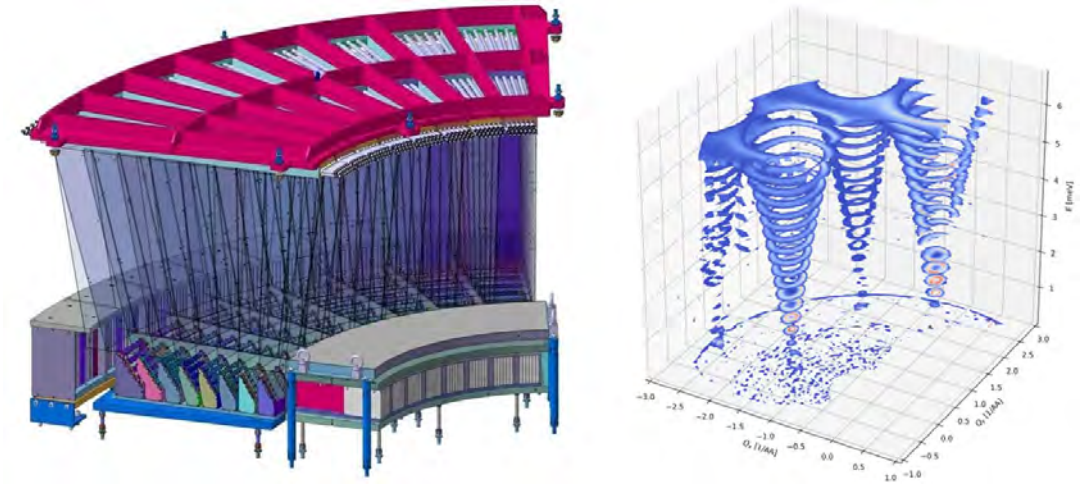
Modern triple axis spectrometers are workhorses of neutron scattering used to map both the static correlations and elemental execitations in condensed matter materials. These measurements are in general flux limited, and there are continuous efforts to improve the sensitivity: Increase the number of neutrons created at the source, increase the number of neutrons reaching the sample by better better neutron transport, detect as many of the scattered neutrons as possible covering a large part of reciprocal space.

In this presentation we report on the commissioning of the new secondary spectrometer upgrade of RITA2 at SINQ with the multiplexing secondary spectrometer, CAMEA [1]. With 104 position sensitive detectors and more than 600 analyser crystals a large part of reciprocal space is covered within the scattering plane making CAMEA ideal for experiments with extreme environments, such as magnets and pressure cell. First data taken with the new spectrometer demonstrate the enormous advance for the mapping of elementary excitations. Being the first instrument to utilize the prismatic analyser concept [2] and due to the similarities with the upcoming BIFROST spectrometer at ESS [3], CAMEA will pave the way for the next generation of secondary triple axis spectrometers. With the added complexity new challenges arise in terms of data treatment and visualization software. This is the goal of the new software package MJOLNIR.



Left: Secondary spectrometer CAMEA with the 104 position sensitive detector tubes radially placed above an array of pyrolitic graphite analysers covering 60 degrees in scattering angle and 8 fixed final energies. **Right:** Example of spin wave data measured in MnF2 single crystal during commissioning.

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Crystal Analysers for Indirect-Geometry Broadband Neutron Spectrometers: Adding Reality to Idealised Design

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The recent trend for indirect-geometry broadband neutron spectrometers to fully exploit available neutrons at pulsed spallation sources seeks to improve their performance via the use of large-area curved analysers, which focus neutrons in time, energy and space. Herein, we describe ongoing and joint efforts between CNR (IT) and ISIS (UK) aimed at future upgrades of TOSCA at ISIS [1, 2] as well as for the design and subsequent construction of VESPA at the ESS [2, 3].

To achieve high resolution over the entire spectral range of 0 – 500 meV, time-focusing of neutrons from the sample to the detector must be achieved within tight tolerances. To optimise the design of the secondary spectrometer, extensive neutron-transport simulations, using McStas [4], and baseline studies of neutronic response have been performed [5, 6]. Additionally, a quantitative assessment and benchmarking of the mechanical properties and neutronic response of construction materials (e.g. graphite tiles, glues, substrates, etc.) is in progress. The effect of graphite mosaicity and its variation from crystal to crystal across the whole analyser, as well as the impact of manufacturing tolerances on instrument performance will be presented.

In the case of VESPA, we show that an unprecedented coverage of more than five steradians is well within reach. For TOSCA, feasibility studies [7] indicate an order-of-magnitude gain in performance when compared to the current configuration following the recent guide upgrade [8]. Such an improvement in performance arises from both a larger detector coverage using a curved geometry as well as the appropriate tuning of crystal mosaicity.

We gratefully acknowledge financial support from the VESPA Project, the STFC, the 2014-2020 CNR-STFC agreement for collaborative scientific research at ISIS, and the STFC SCARF HPC cluster.

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The BATS option for inverted TOF-Backscattering on IN16B: Design, performance and ongoing upgrades with variable focusing optics

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The BATS (Backscattering And Time of flight Spectrometer) option for inverted TOF spectroscopy on IN16B at ILL extends the accessible energy transfer of the instrument from presently ±30 µeV to a full window of 340 µeV. Two counter rotating disc chopper pairs with multiple slits provide high flexibility for varying the instrumental resolution in seven steps between 1.5 and 9.8 µeV, with the additional possibility for inelastic offsets [1]. In our contribution, we review the design of the BATS option, its performance during hot commissioning in 2018 [2] (see Figure) and focus on the ongoing upgrade of the neutron optics system.

The chopper system for BATS consists out of two counter rotating pairs of novel oriented Carbon Fibre Reinforced Polymer discs with 750 mm diameter and 4 differently sized slits each, attaining 19000 rpm. The largest slits correspond to the 90 mm wide IN16B neutron guide and the smallest slits need to be reduced down to 10 mm to achieve the necessary short pulse lengths. To optimize the neutron transmission for each slit width, we developed the concept of a 10 m long adaptive horizontally focusing and defocusing guide system with 18 sections. This allows to realize any guide shape with widths between 90 mm and 10 mm as piecewise linear approximation. As any of the counter rotating pairs can act as pulse chopper while the other one takes the role of a suppressor chopper, the focusing must be adaptable on either chopper pair. The variable guide allows to tune the level of beam compression depending on the selected slit width.

Optimisation of the variable focusing guide system has been done by combining ray-tracing simulations with a particle swarm algorithm. These calculations help to obtain the best guide profiles, and the necessary m-values of the supermirrors can be estimated by examining reflections in the focusing segments. While the smallest chopper slit width uses only about $^1/_8$ of the available guide cross section, the simulations show that an intensity factor of more than five can be gained back. The construction of the variable focusing system is ongoing with its installation envisaged for 2020.

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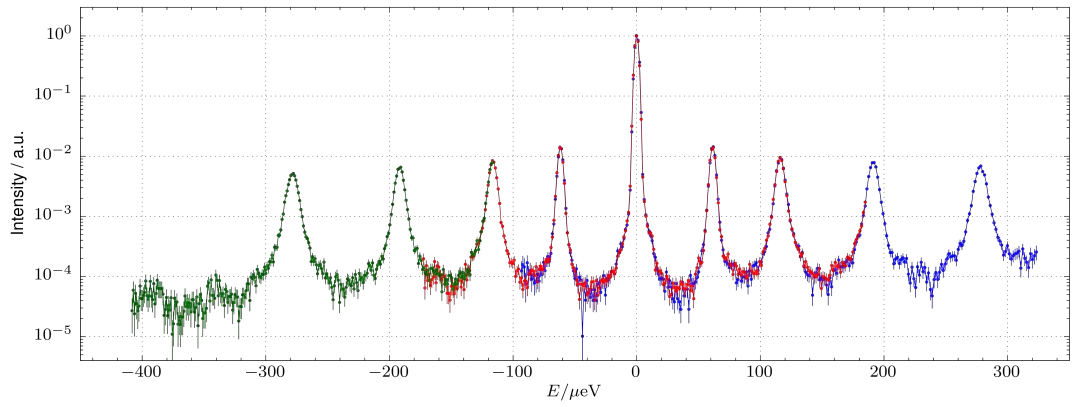

Fig. 1: Tunneling spectrum recorded on γ-picoline-N-oxide at T = 1.8 K with BATS (from Ref. [2]). Three consecutive measurements with different offsets of the observed energy transfer window are shown in different colors. The resolution FWHM at the elastic peak is 3.8 µeV.

LARMOR a TOF instrument with many modes

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LARMOR is a neutron scattering instrument at ISIS, that is partially financed by a Dutch "NWO groot" grant. The basis is a competitive Time-Of-Flight SANS instrument with polarized neutron capabilities. The SANS mode has been developed by ISIS and is in operation since summer 2015. The instrument has the flexibility in space and electronics to accommodate a rich flavour of Larmor labelling techniques, that have been developed within the Dutch contribution and significantly increase its functionality.

The modes that are presently tested and operational are: SANS, Polarized SANS, Diffraction, Spin Echo SANS (SESANS), Spin Echo Modulated SANS (SEMSANS), Time Of Flight Larmor precession (TOFLAR) and Modulated Intensity by Zero Effort (MIEZE). The near future will see the commissioning of High Resolution Larmor Diffraction (HRLD) and Neutron Resonance Spin Echo (NRSE). Some of these different techniques may be combined, like SANS and SEMSANS, simultaneously and will allow to investigate phenomena from nanometre to micrometre scales.

The Larmor labelling components have been developed and produced at Delft University of Technology, which together with the University of Groningen and Eindhoven has launched a scientific program to exploit the capabilities of the instrument.

We would like to present an overview of the development of the Larmor labelling features of this instrument.

Background suppression in neutron scattering experiments at the pulsed IBR-2 reactor by set of choppers

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Delayed neutrons emitted by neutron rich fission fragments are the most important source of the background at neutron scattering instruments at a pulsed neutron reactor. Being emitted any time up to a few minutes after the fission event, they are the source of a continuous neutron irradiation superimposing the time-structured neutron beam.

The flux of delayed neutrons amounts to 3-5% of the mean neutron flux of the pulsed neutron beam. Such a high background of delayed neutrons is a serious drawback of the pulsed reactor sources, particularly the pulsed reactor IBR-2 [1] and a new pulsed neutron source under considerations in JINR (Dubna, Russia) [2]. Especially suffering are neutron reflectometry and small-angle neutron scattering, where such background is practically limiting measurements of weak scattered signals already at the level of 10^{-4}.

Here we suggest a possible way for the solution of this problem. The idea is to convert the continuous background of delayed neutrons in a pulsed neutron beam superimposing neutron pulses from the reactor. This can be achieved by a mechanical chopper placed at about 5m from the reactor core (i.e. beyond the reactor shielding) that creates the pulses of the delayed neutrons with the time width of about few milliseconds, which is much higher than the width of neutron pulses, however matches well to requirements of low-resolution reflectometry and SANS experiments. In this case the delayed neutrons are contributing to the useful signal rather than to background.

The efficiency of the suggested method is illustrated by VITESS simulations of a virtual neutron reflectometry experiment at IBR-2.

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FARO: A new type of neutron spectrometer with Flux And Resolution Optimised

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A new type of high intensity and high resolution time-of-flight neutron backscattering spectrometer is presented which is capable of an energy resolution of 4.0 μeV with a data collection rate an order of magnitude larger than current backscattering spectrometers capable of this resolution. The design is unusual in that it goes against two norms of high resolution indirect neutron spectrometers; it uses large mosaic pyrolytic graphite (PG) (002) crystals instead of nearly perfect silicon (111) crystals to select the final neutron energy and it operates well away from the normal backscattering condition $2\varphi \approx 180°$, instead using $2\varphi = 160°$. The presentation describes the methodology behind this spectrometer along with full ray-tracing simulations of the instrument using the *McStas* program.

Quasielastic Neutron Scattering - is there another way?

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Incoherent diffusive-motion is usually measured using quasielastic neutron scattering (QENS). It is difficult to extract dynamical information directly from the experimental QUENS energy-spectrum (S(q,w)), so either analytical or molecular-dynamics models are typically used to understand the measured dynamics in the time-domain (I(q,t)). Currently, only neutron spin-echo can measure the decay of atomic position (or correlation) in the time-domain directly, and were motivated by that approach to explore other methods that might access dynamics directly in the time-domain.

In practice the measured polarisation in NSE remains on the elastic condition, and this bears a tantalising similarity to the technique “resolution elastic neutron scattering” (RENS), which used the integrated elastic intensity to the probe probability of position decay within the experimental resolution-time. RENS results are restricted to overall relaxation and are intractable for obtaining I(q,t) because when existing time-of-flight (TOF) and backscattering (BS) instruments are used for RENS the sample dynamics are convoluted with resolution elements of the primary and secondary spectrometers. We will present an instrument concept, based either on back-scattering (BS) or time-of-flight (TOF), that makes RENS-like scan, but overcomes the limitations above to measure dynamics in the time-domain that do provide straightforward access to (I(q,t).

Three basic principles (not specific to TOF (direct or inverted) or BS) are required:

Firstly, either the primary or secondary resolution needs to remain fixed the best achievable level, whilst the other resolution is scanned. The two alternatives are conceptually equivalent, but one may have practical advantages over the other.

Secondly, the resolution is best scanned in equal steps as dynamics-time resolution, not equal steps in energy resolution. Measure constant time-bins or re-bin from constant energy-bins.

Finally, under these conditions, at each resolution point (at t) we measure the integral of (I(q,t)) up to t, so the experiment provides the travelling-integral of I(q,t). Differentiation of this signal provides I(q,t) and we will discuss practical ways of obtaining this derivative.

Although QENS and our concept are formally equivalent, the practical experiments are not:

Firstly, advantages depend on what is to be measured. For example, our method prevails where no appropriate dynamical model exits, whilst QENS would be better for a rapid spectral overview.

Secondly, we are trading the need to obtain a derivative from data with statistical noise (in our case) against the need for a Fourier transform of data with statistical noise and limited range (in the QENS case). The relative merits and limitations of each need to be considered case-by-case.

Finally, with our concept it is easy to adjust the counting-time at each point so that the errors in I(q,t) are uniform, thus maximising efficiency. This is difficult (in some cases impossible) to achieve with QENS where errors increase substantially with increasing t, parts of the spectrum being over-counted whilst others are under-counted.

The new high-resolution neutron spin echo spectrometer J-NSE "PHOENIX" at MLZ

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Neutron spin echo (NSE) spectroscopy provides the ultimate energy resolution in quasi-elastic thermal and cold neutron scattering spectroscopy. In terms of Fourier-time (τ) – or equivalently in terms of the accessible energy (E) – high resolution means the extension of τ (respectively E) into to the regime of μs (neV). In 2017 the Jülich neutron spin echo at MLZ went through a refurbishment of the secondary spectrometer: The old normal conducting main-precession coils have been replaced by a new set of fringe-field compensated, superconducting magnets that were realized following the results obtained for the design of ESSENSE, the proposed high-resolution NSE spectrometer at the ESS. One of the most innovative characteristics of the coils is their optimized geometry that maximizes the intrinsic field-integral homogeneity along the flight-path of the neutrons and that enhances the resolution of a factor 2.5, as the first experiments could already confirm. The installation of the new magnets was finalized in September 2017 and since 2018 the J-NSE is back in user program. The new configuration yields an improved resolution that may be exploited to reach larger Fourier-times and/or to benefit from significant intensity gains if shorter neutron wavelengths are used at a given Fourier-time. Thus the new J-NSE Phoenix meets the needs to look into the microscopic dynamics of soft- or biological matter with enhanced and new quality. Here we present the results on the performance of the spectrometer after the refurbishment and some selected examples from the realm of soft matter dynamics that largely rely on the enhanced properties of the new J-NSE.

WASP, the Widest Angle SPin echo spectrometer

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All functioning Neutron Spin Echo spectrometers essentially use the IN11A design where the precession field is generated by long solenoids along the neutron beam. This construction limits the angular coverage and count rate of the instruments. Last century there have been two tries to make a wide angle coverage neutron spin echo instrument. IN11C at ILL is equipped with a flattened solenoid and has been in use since its creation. It has a 30 degree-wide angular coverage but a very limited resolution. This instrument was practically trading intensity for resolution. The SPAN instrument at HZB used a pair of coils in the anti Helmholtz configuration creating an azimuthally symmetric magnetic field; which, in theory, could allow a nearly 360 degree detector coverage. WASP will use an improved SPAN construction, and it aims to have a 500 times higher detected intensity than IN11A while the resolution remains the same.

The long construction has finished in 2018, and the three weeks of commissioning were promising. We have echo in all detectors up to one third nominal field integral, and the detected intensity is 500x of IN11A. By the time of the conference we hope to present even more promising results on this new flagship instrument.

Mapping Small Angle Scattering with Image Resolution in Dark-Field Contrast Imaging

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Neutron imaging is well known as a technique to map macroscopic inner structure based on local beam attenuation. However, this image has changed significantly in recent years with the introduction of a number of novel imaging modalities, building on inherently differing contrast mechanisms. While conventional attenuation contrast neutron imaging provides up to 5 micrometer resolution nowadays, dark field contrast imaging enables to go significantly beyond this limit. Dark-field contrast detects small angle scattering with the spatial resolution of neutron imaging [1]. However, in each pixel of the image a small angle scattering function can be extracted and analysed, thus providing structural information significantly below the direct image resolution [2,3].

Dark-field imaging is based on spatial beam modulation, which allows despite full field illumination of the sample to measure the local small angle scattering with remarkable angular resolution. Small angle scattering manifests as loss of visibility of the beam modulation, which can be detected locally with the spatial resolution of the imaging set-up [1]. Hence, spatial variations in scattering and hence microstructure are detected easily and enable straightforward observation. Prominent examples are porosity variations in engineering materials [4] but in particular also visualisations of magnetic domain networks [5].

Based on successful qualitative studies an approach could be developed which allows to systematically probe the scattering related to specific correlation lengths and length ranges and thus quantitative assessment of microstructures in dark-field contrast imaging [2]. Examples range from spatially resolved observations of sedimentation and quasi-crystallisation of microparticles [6] and the breakdown of fractal networks in cohesive powders. Here the technique, recent developments and application results will be presented.

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Neutron Microtomography

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Recent detector developments lead to enhancement of spatial resolution capabilities of neutron imaging to single digit micrometres level. At PSI, a device that enabled imaging with better than 5 micrometres spatial resolution was developed within the framework of a Neutron Microscope project and is now available to a broad neutron imaging user community at various beamlines. The available field of view of such high resolution imaging detectors is usually limited to several tens of square millimetres thus covering similar lengthscales as corresponding set-ups used in X-ray imaging. Consequently, the samples imaged with such a high spatial resolution neutron detector are also limited to some millimetres in thickness.

In this regime of sample dimensions, X-ray microtomography is still best suited for the majority of materials due to the higher available flux and generally higher availability of sources/instrumentation. However, neutron microtomography excels in the numerous cases of high-Z materials due to superior transmission of such materials for neutrons.

Several applications of neutron microtomography for structural characterization of samples of high-Z materials will be presented in this contribution. Applications include but are not limited to porosity in gold and additively manufactured gold alloys, dendritic structures in high-Z eutectic alloys (e.g. In-Bi, Au-Pb, etc.) and defects, such as pores and cracks in uranium oxide tristructural-isotropic (TRISO) fuel particles.

New instruments for materials engineering STRESS and DRAKON at reactor IR-8: performance and first results

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Reactor IR-8

Research reactor IR-8 (maximum power 8 MW) at NRC "Kurchatov Institute" has thermal neutrons flux in the reactor core ~ $2 \cdot 10^{14}$ $ncm^{-2}sec^{-1}$. There are 12 horizontal channels in reactor for neutron beams. The neutron flux at the outlet of the channels is ~10^{10} $ncm^{-2}sec^{-1}$. Usually reactor is running at a power of 6MW.

Diffractometer STRESS

The STRESS diffractometer is designed to study internal stresses in various polycrystalline materials. Unlike most stress diffractometers, the instrument uses a double-crystal monochromator. This allowed creating a compact and high luminosity instrument, which is comparable in its characteristics to stress diffractometers at more powerful reactors. Main characteristics of the instrument and examples of researches of stress distribution in thick (~45mm) steel weld and thin (~2 mm) plates, produced by additive manufacturing are reported.

Imaging station DRAKON

Imaging station DRAKON is designed for non-destructive analysis of internal structure of various objects by neutron radiography and tomography. Neutrons can be extracted through 3 different channels. The first channel, directed to the reactor core, provides "white" neutron beam. The second channel with double-crystal monochromator PG002/PG002 provides monochromatic neutrons with wavelength in the range from 1.6 to 6 Å for energy-selective neutron imaging. The third channel provides monochromatic neutrons with wavelength of 0,9Å, reflected from the first PG monochromator at take-off angle 15^0. The examples of researches, conducted at the station for solving actual problems in science and industry are presented.

New developments in the fast neutron powder diffraction instrument ErwiN at MLZ

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The development of the ErwiN – **E**nergy **r**esearch **wi**th **N**eutrons – neutron powder diffraction (NPD) beamline is presented with three possible advancements: Firstly, the primary beam optics will be replaced to bring this diffractometer to the same level as the high flux and high resolution instrument D20 at the ILL. The ErwiN instrument will be used for the investigation of energy storage materials, also integrated in complete components and under real operating conditions. Thus, it is possible to scan a large parameter space (e.g. temperature, state of charge, charge rate, fatigue degree) for the investigation of modern functional materials in kinetic and time-resolved experiments. Diffraction data will be obtained from the entire sample volume or in a spatially resolved mode from individual parts of the sample. ErwiN is designed for different scenarios: for very fast measurements at medium resolution, for medium fast measurements at higher resolution and for very high resolution still at a reasonable time frame. The final commissioning and integration of ErwiN is the second important objective which will be addressed, while thirdly, the integration of newly developed and strongly needed sample environment, e.g. H_2-gas system, will enhance the attractiveness for a wider community in energy research as well as materials science while furthermore developing novel methods for the neutron science community.

MAGiC: a polarized diffractometer at ESS

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The European Spallation Source is now well advanced in its construction phase, with the first neutrons expected on the instruments in mid-2022. On the instrumentation side, the first 8 instruments, covering most of the needs of the scientific community (imaging, SANS, inelastic neutron scattering, diffraction, reflectometry), will be opened to international users along 2023 and 2024.

Among those, MAGiC is a polarized diffractometer designed with a specific attention to the broad case of magnetism in single crystals in mind. The instrument will allow the refinement of magnetic properties (structure, local susceptibility, magnetic diffuse scattering, spin density) on sub-mm^3 and thin-film samples on a daily basis. The scientific case covers systems with strong potential applications such as multifunctional materials, molecular magnets and superconductors as well as fundamental materials such as quantum spin liquids, skyrmions and strong spin-orbit coupling materials.

To do so, MAGiC will make full use of the ESS high brilliance on the thermal and cold spectra, both permanently polarized thanks to the use of FeSi coated super-mirrors. Two detectors will ensure high-efficiency date collection with a 0.8 sr area detector for half-polarized experiments and a 120°x10° detector for polarization analysis on the cold spectrum experiment. The polarization analyzer will be based on Si blades coated with FeSi and accompanied by a XYZ setup ensuring data collection on all available channels.

Simulations of the MAGiC performance, with the help of the McStas software package, on single crystals and powder samples show an expected gain compared to state of the art polarized diffractometer of 1 to 2 orders of magnitude.

The instrument is now in its detailed design phase with a start of installation scheduled for mid-2020, a hot commissioning in 2023 and an opening to users in 2024.

In this talk, we will present the scientific case supporting the instrument construction, the details of the instrument design and its current status in the ESS installation plan.

DN-6 diffractometer for studies of microsamples at ultrahigh pressures

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A DN-6 neutron diffractometer allows investigating the magnetic and crystalline ordering of polycrystalline samples in a wide range of pressures and temperatures. The neutron diffraction experiments can be carried out with very small samples of the order of 0.01 mm^3 due to the high neutron flux on the sample and the wide solid angle of the detector system. Satisfactory diffraction patterns from such small-volume samples make it possible to use both anvils made of synthetic sapphire single crystals and small diamond anvils to create and achieve pressures up to 50 GPa. A closed-type refrigerator can cool high-pressure sapphire and diamond anvils cells down to 4 K, and thus the investigation of the simultaneous influence of low temperatures and high pressures on the structure of the compounds can be obtained.

The technical design, basic parameters and current capabilities of the DN-6 diffractometer are described.

A brief overview of recent results is given.

Neutron Larmor Diffraction on samples in magnetic field

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Neutron Larmor diffraction (LD) is a high resolution diffraction technique based on the Larmor precession of neutron spins in magnetic fields along the beam path, similar to neutron spin-echo [1]. Lattice spacings in single- and poly-crystalline materials can be measured with a relative resolution ~10^{-6}. Typical experiments include thermal expansion under extreme conditions [2], accurate determination of lattice parameters [3,4], magnetic and structural domain sizes [5], and lattice distortions related to phase transitions [6].

LD is well established, but currently available only at a few spin-echo three-axis instruments, such as the TRISP spectrometer at the FRM II, and the FLEXX spectrometer at HZB. Currently, the technique is limited to samples in zero magnetic fields, which is a severe limitation for the study magnetic phases.

There are two proposals for modified LD allowing for sample fields in the Tesla range. The first is Rekveldt - van Well single arm Larmor diffractometer [7,8], the second is is based on an intensity modulation technique based on radio frequency spin flippers [9]. We will discuss the specific advantages of the latter technique and the resolution properties in practical applications.

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Nonmagneic high pressure piston-cylinder type clamp cells for neutron scattering.

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Pressure is an important thermodynamic parameter like temperature and magnetic field.The increased interest in quantum phase transitions and study of the new magnetic state-skyrmions under pressure demands the creation of new non-magnetic high-pressure cells. High pressure clamp cells made of hard nonmagnetic alloys (Al, 40HNU (NiCrAl), CuBe, TiZr) for use by TOF-method on pulse and reactor neutron sources (SNS-[1], ILL-[2], SINQ-[2,3] and other) are presented in this report. The cells fit for powder and single crystal studies for neutron scattering. They can be placed in typical cryostats (as well as in dilution fridge insert-ISIS) and high magnetic field cryostat-ILL.

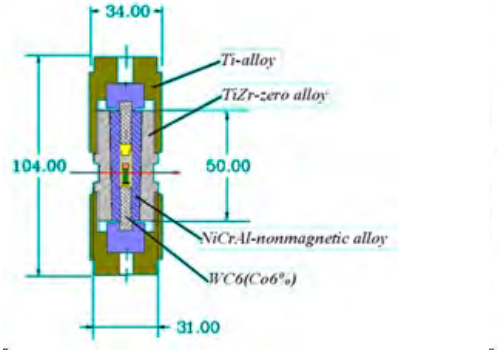

Fig.1. Sketch of the high pressure cell HPC40-ILL-D3 (max. up to 40kbar)

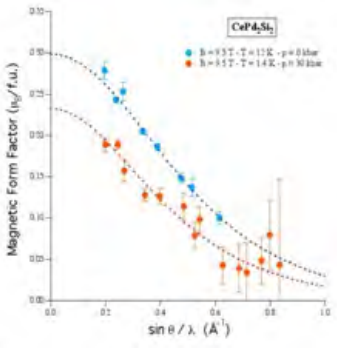

Fig.2. Change Magnetic form factors Ce in the CePd2Si2 under pressure. The Polarised Neutron Beam Facility D3(ILL).

1. Pressure effect on hydrogen tunneling and vibrational spectrum in α-Mn.
A. I. Kolesnikov, A. Podlesnyak, R. A. Sadykov, V. E. Antonov, M. A. Kuzovnikov, G. Ehlers, and G. E. Granroth.
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R A Sadykov, Th. Strassle, A Podlesnyak, L Keller, B Fak, J Mesot,
IOP Conf. Series: Journal of Physics: Conf. Series 941 (2017) 012082 doi :10.1088/1742-6596/941/1/01208
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M. E. Zayed, Ch. Rüegg, J. Larrea J., A. M. Läuchli, C. Panagopoulos, S. S. Saxena, M. Ellerby, D. F. McMorrow, Th. Strässle, S. Klotz, G. Hamel, R. A. Sadykov, V. Pomjakushin, M. Boehm, M. Jiménez–Ruiz, A. Schneidewind, E. Pomjakushina, M. Stingaciu, K. Conder & H. M. Rønnow.
Nature PhysicsVOL13(2017) OCTOBER2017 pp962-967,doi:10.1038/nphys4190

Visualization and Processing of Single-Crystal Diffraction Data Measured with a Point Detector using Davinci Software

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Nowadays, area detectors are among the standard equipment for X-ray diffractometers at synchrotron facilities as well as for many instruments at neutron sources. However, point detectors provide often more accuracy to measured intensities, especially in the case of neutrons with short wavelengths. Therefore, point detectors are still in use at hot-neutron diffractometers, such as HEiDi and POLI at MLZ, etc. Data reduction software for neutron diffractometers with point detectors is often a locally-developed instrument-specific console program hard-coded with instruments geometry and measured data format.

This contribution presents *Davinci* (http://davinci.sazonov.org), a software for the visualization and processing of single-crystal diffraction data measured with a point detector. Currently, the software supports data collected at POLI, HEiDi and MIRA at MLZ as well as 6T2 at LLB and Zebra/TriCS at PSI. *Davinci* allows to extract the experimental structure factors from the measured scans of Bragg reflections for further analysis with crystallographic software, such as FullProf, Jana, ShelX, etc. In the case of polarized neutron diffraction, the *Davinci* allows to obtain the experimental flipping ratios. With this software, the treatment of both the whole data set and individual peaks is noticeably simplified due to the convenient and intuitive graphical user interface. *Davinci* is an open source software developed in C++ using the modern multi-platform Qt framework and available for macOs, Windows and Linux operating systems.

Neutron Diffraction Stress Analysis Down Under: 10 Year Experience in Industrial and Scientific Applications

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Although 10 years has passed since residual stress diffractometer KOWARI started its operation, it still remains one of the newly built instruments in its class in the world. It is based at the OPAL 20 MW research reactor of the Australian Nuclear Science and Technology Organisation (ANSTO) and one of the suite of instruments (more than a dozen strong) available at the Australian Centre for Neutron Scattering (ACNS). Since then the instrument proved its high performance and high throughput owing to its design, including large monochromator, large detector and high-capacity sample stage. As result the major features of the instrument are high neutron flux (2x10^6 n/cm2/s), which equals the most intense residual stress diffractometers in the world, while having low ambient background, that makes possible experiments with high spatial resolution (down to 0.1 mm) and high accuracy (< 5 MPa).
Considering the advantages of the instrument, the scope of the scientific and industrial applications and projects that has become traditional on the instrument includes modern manufacturing technologies (including the most popular recently topic of additive manufacturing of different kinds), surface engineering (coatings or surface treatments), composite materials, etc. Few topics that are unique for KOWARI include residual stress analysis in geo-materials, materials with complex microstructure (e.g. lattices made by additive manufacturing) and granular materials.

Neutron Optics And Instrumentation

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[5]*Elettra Sincrotrone Trieste*
[6]*ESRF*
*Corresponding Author: cubitt@ill.fr

Optics has many applications to help us improve the performance of our neutron instruments from complex guide geometries to focusing mono-chromators. I will present examples of how optics has improved the performance of large scale structure instrumentation at the Insitut Laue Langevin (ILL). A focusing prism has been shown to be a very effective method of measuring the wavelength on the reflectometer D50 exploiting the mean ILL flux with good resolution and no limit on the bandwidth. Specular reflectometry has also gained from exploiting the fact that upon interacting with the sample, information about the neutron path is preserved, meaning that the angular uncertainty of a beam is not as large as has been often thought. The instrument D17 has been exploited using the full angular range available without any loss of resolution, vastly improving the performance. It might be thought that the time for a chopper blade to cross such a wide guide would tend to loosen the resolution but this can also be resolved in data reduction without any loss of resolution by the same principle. Finally the ILL possesses the only gravity limited SANS instrument in the world (D11) where the total length is such that gravity prevents any transmission through the collimation above a certain wavelength and the beam can also fall off the bottom of the detector, with both effects limiting the minimum q we can measure. With a trick learned from the vertical reflection plane reflectometer, FIGARO, both these effects can be undone, allowing a minimum q of 7e-5 Ang.$^{-1}$.

Fast heating - Sample Environments for for High Brightness Sources

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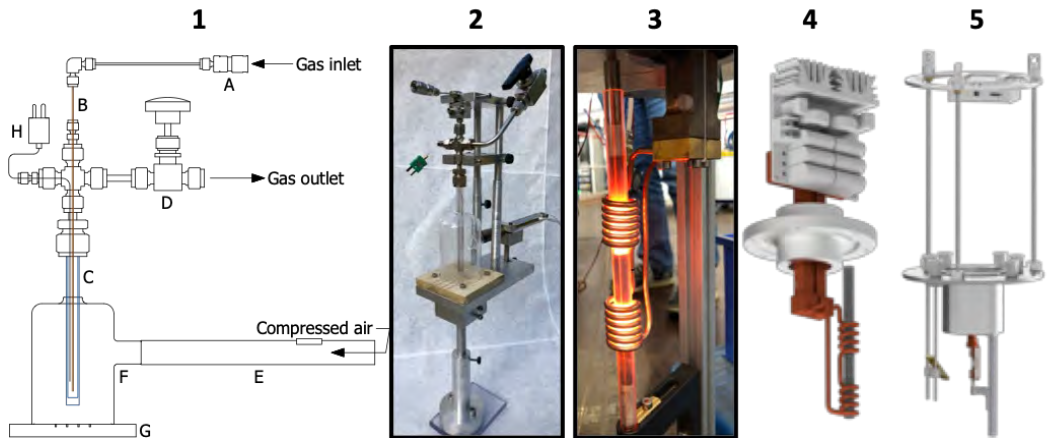
In order to take full advantage of the significantly increased data collection rates expected at the European Spallation Source (ESS), it is paramount that new sample environments are developed to match the performance of the coming instruments. Here, we present two newly developed sample environments for neutron powder diffraction:

1. A single crystal **S**apphire **A**ir gun **H**eater **S**etup (SAHS), specially designed for solid-gas *in situ* angular dispersive neutron powder diffraction, has been developed [1](picture 1 and 2). Heating is provided by an air gun heater, allowing the sample to reach temperatures of up to 700°C within less than 5 min. The setup is based on a single crystal sapphire tube, which is oriented to give a very low and smooth background.

2. An induction furnace has been developed in a collaboration with Chalmers (SE), ISIS (UK) and the ESS (SE) (picture 3, 4 and 5). A fully functioning prototype has been built for the Time of Flight (ToF) diffractometer POLARIS at ISIS and will lead to a second version for the diffractometer/Small Angle Neutron Scattering (SANS) instrument HEIMDAL at ESS. The heating is based on an induction element, which allows for an extremely fast and efficient way of heating and can reach temperatures of up to 1600°C in less than 5 min. Furthermore, the setup works both in vacuum and under ambient conditions and requires no heat shielding, thus both reducing the beam attenuation and lowering the levels of background scattering.

Both setups offer high temperatures, fast temperature stability, large sample volumes and very low attenuation of the beam. The setups have proven to be ideal for carrying out investigations of advanced materials under realistic conditions. The ability to investigate real materials, in real time under realistic conditions, is a huge advantage for scientific as well as for industrial applications.



1-2: Schematic and picture of the SAHS. Gas flows through the system in the following order: **A** Quick fit connector, **B** Fused silica tube, **C** SCS sample container, **D** Outlet valve. The heater airflow goes through: **E** Hi-Heater airgun, **F** heat confinement quartz dome, **G** Ceramic insulator with air outlet grooves. **H** Thermocouple. **3-4:** The induction furnace heat element. **5** The full induction furnace setup.

[1] Ahlburg, J. V., In review, Journal of Applied Crystallography, **2019,** ref number in5023

Non-magnetic goniometer for dilution refrigerators

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For Neutron scattering experiments at ultra-low temperatures the thermal response of the sample as well as the cryostat increase. Subsequently, sample equilibration as well as the cooling and warming of the cryostat occupy a sizable part of the measurement time.

Moreover, the use of complex sample environment, such as cryo-magnets, call for the possibility to reorient and align of the sample inside the running sample environment, i.e. at low temperatures or at high magnetic fields.

We present our progress on the development of a miniature low- temperature goniometer, which will allow for a reorientation of samples at ultra-low temperatures.

This work is part of the SINE2020 work package on sample environment.

Scientific software developments at the European Spallation Source

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The European Spallation Source (ESS) is the largest investment in European Neutron scattering since the construction of the Institute Laue Langevin. The Data Management and Software Centre (DMSC) is responsible for the delivery of the scientific computing and data management for the ESS. In this presentation the current status of the ESS project will be discussed in relation to the development of scientific software for the ESS instrument suite.

The performance of a next generation neutron spallation source, the first one with long pulse characteristics, creates specific requirements for the data acquisition system, data processing and data analysis software. These requirements will be presented along with the design choices, prototype performance and test results for the core DMSC systems which are geared towards a paradigm where the core neutron detection technology has shifted from 3He to 10B. The contribution will also detail what is being done to be prepare ESS for the broader European desire for open access to research data and sustainable software projects.

The ESS is a pan-European project with 15 European nations as members and Sweden and Denmark as host nations. The role and benefits of collaborative open source software development will be examined in relation to the advantages and challenges for scientific software development at a green field research infrastructure.

Neutron Resonance Spin-Echo Spectrometers at BL06 VIN ROSE at J-PARC MLF

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High Energy Accelerator Research Organization (KEK) and Kyoto University have jointly installed resonance-type neutron spin echo spectrometers at BL06 of the Materials and Life Science Experimental Facility (MLF) at J-PARC. BL06 has two beam branches for NRSE (neutron resonance spin echo) and MIEZE (modulated intensity with zero effort) spectrometer (Fig. 1), hence the name “Village of neutron resonance spin echo spectrometers: VIN ROSE”. NRSE aims for the study of slow dynamics of soft matters with a high-resolution realized by ellipsoidal focusing supermirrors. MIEZE aims to expand the scope of neutron spin-echo spectroscopy by its specific advantages such as the flexibility of sample environments and capability of spin-polarimetry.

By commissioning the spin-polarizer, analyzer and resonance spin flipper system for a pulsed neutron beam, we observed MIEZE and NRSE spin-echo signals (Fig 2 and 3). We have started to accept the proposals of General Use in MIEZE spectrometer from 2018. The open use of NRSE spectrometer will follow in 2019.

We will report the details of development of MIEZE and NRSE spectrometer, and recent results obtained at BL06 VIN ROSE.

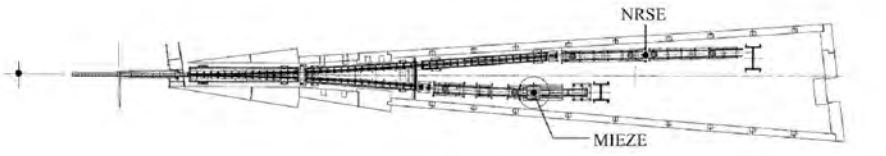

Fig. 1 Top view of BL06 VIN ROSE [Ref. 1]

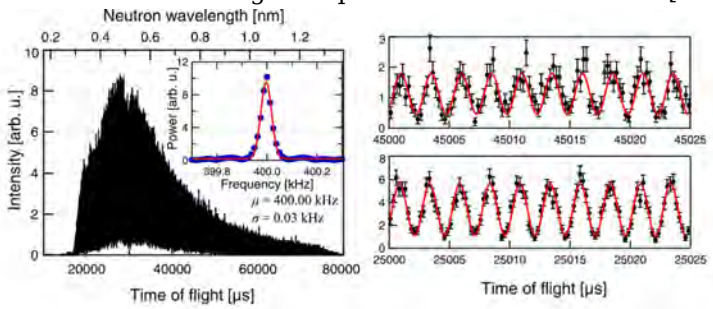

Fig. 2 400-kHz MIEZE signal [Ref. 2]

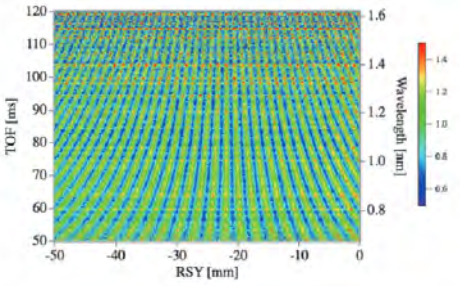

Fig. 3 NRSE signal [Ref. 1]

References:
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Nanosecond dynamics of biopolymers: a comparative neutron spin echo study on folding intermediates of apo-myoglobin

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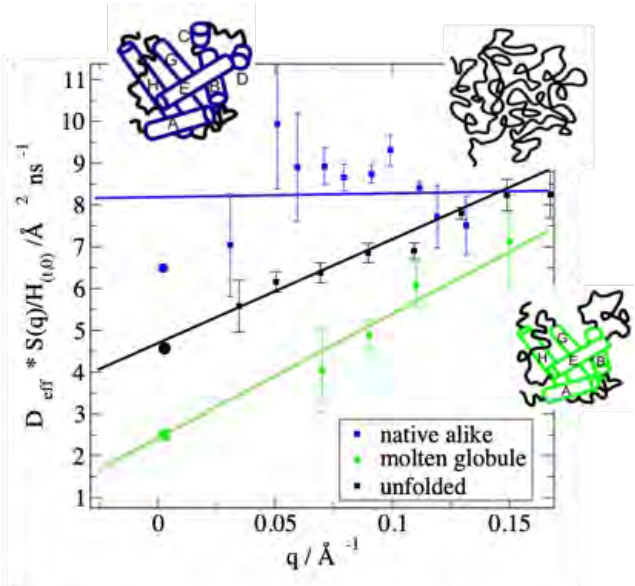
During protein folding different intermediate states occur with varying content of secondary structural elements. To characterize their internal dynamics, we prepared apo-myoglobin in different folded states [1,2]. Its unfolded, folded and partially folded (molten globule) forms were investigated using neutron spin echo spectroscopy (NSE). Information on the form and structure factor was obtained by small angle scattering (SAS). Aggregation state and centre of mass diffusion were monitored in parallel and in particular cases, also in situ, with dynamic light scattering (DLS). The SAS and DLS data account for interparticle and hydrodynamic interactions and were used to "correct" the effective diffusion coefficients measured by NSE [3,4]. Whereas the dynamics of the folded protein is dominated by centre of mass diffusion, the unfolded protein and the molten globule state show a Gaussian polymer-like behaviour. This indicates that powerful polymer models e.g. Zimm and Zimm with internal friction can be used to describe such protein systems.



q- dependency of the corrected effective diffusion coefficient obtained from the initial slope of the NSE spectra investigating for the different folding states. The lines are a guide for the eye.

References: [1] A. Stadler *et al.*, J. Phys. Chem. B 119, 72 (2015) [2] D. Eliezer & P. Wright, J. Mol. Biol. 263, 531 (1995) [3] A. Stadler *et al.*, J. Am. Chem. Soc. 136, 6987 (2014) [4] F. Ameseder *et al.*, J. Phys. Chem. Lett. 9, 2469 (2018)

New Features and upgrades of the Small-Angle Neutron Scattering Instrument SANS-1 at MLZ

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We present the features of the instrument SANS-1 at MLZ, a joint project of Technische Universität München and Helmholtz Zentrum Geesthacht [1]. Measurements of the beam profile, divergence, flux and polarization are given for various positions along the instrument and agree well with simulations. SANS-1 features two interchangeable velocity selectors with 10% and 6% $\Delta\lambda/\lambda$ and a TISANE 14-window double-disc chopper. This combination allows tuning flux, resolution, duty cycle and frame overlap, including time resolved measurements with repetition rates up to 10 kHz. A key feature is the large accessible *Q*-range facilitated by the sideways movement of the detector.

Dedicated to hard matter, materials science and magnetism, SANS-1 features a flexible, spacious sample area with a heavy duty goniometer and unique sample environment like a set of magnets, ovens and a bespoke dilatometer. We show some extreme examples and prospects for future experiments, e.g. to investigate the onset of crystallization in magnetic materials and a future high field magnet project. Finally we present the polarization analysis option that combines a new compensated MEOP and an integrated RF-flipper together with a 2.5 T magnet.

The instrument base of the PIK reactor

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We report on the current status of the construction and commissioning of the instrumental base of the Reactor PIK. The reactor team is actively working on commissioning and the power start-up of the reactor PIK under the project «Modernization of engineering and technical systems». At the same time, the program of the construction and commissioning of the cold neutron source and the neutron guide system, is being implemented. Moreover, a new project on the «Construction of the Instrument Base of the Reactor Complex PIK» is started that will last for the coming 6 years. It envisages the design, construction and commissioning of new 20 neutron instruments those will equip the reactor PIK as a neutron scattering facility satisfying needs of the Russian and foreign scientists.

The following equipment will be built: 20 neutron instruments including neutron diffractometers, neutron spectrometers, small-angle neutron scattering setups and neutron reflectometers. A few stations for the fundamental science with neutrons are under development as well. These instruments are distributed inside three experimental halls: 9 stations are located in the neutron guide hall, 8 stations are in the horizontal channels hall around the reactor and 3 stations are to be built in the hall of inclined channels. In addition we plan to construct 3 neutron moderators, i.e. the hot, cold and ultracold neutron sources. The laboratories and workshops for preparation and certification of the samples are to be built ensuring neutron scattering experiments.

Structure of adsorbed layers and of chains in polymer nanocomposites

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A combined small-angle scattering of neutrons (SANS) and X-rays (SAXS) study of the structure of polymer layers pre-adsorbed on silica nanoparticles (NP) which are subsequently incorporated into polymer nanocomposites (PNCs) is presented. Pre-adsorbed chains are found to promote ideal dispersion, before desorption in the late stages of nanocomposite formation. The microstructure of the interfacial polymer layer is characterized by detailed modeling of X-ray and neutron scattering. Only in ideally well-dispersed systems a static interfacial layer of reduced polymer density over a thickness of ca. 2 nm is evidenced based on the analysis with a form-free density profile optimized using reverse Monte Carlo simulations. This interfacial gradient layer is found to be independent of the thickness and mass of the initially adsorbed polymer, but appears to be generated by out-of-equilibrium packing and folding of the pre-adsorbed layer. The impact of annealing is investigated to study the approach of equilibrium, showing that initially ideally well-dispersed systems adopt a repulsive hard-sphere structure, while the static interfacial layer disappears.

In parallel, SANS and the use of zero average contrast conditions allow the measurement of chain conformation in the PNCs with and without pre-adsorption. Surprisingly, we evidenced the spontaneous formation of thermally-stable adsorbed layers in PNCs containing matrix chains of different mass, whereas a symmetric matrix of identical chain masses does not show this effect.

This study contributes thus to the fundamental understanding of the interplay between effects which are decisive for macroscopic material properties: polymer-mediated interparticle interactions, and particle interfacial effects on surrounding polymer.

SANS/USANS TUNABLE MULTISCALE NANOPARTICLE ORDERING BY POLYMER CRYSTALLIZATION

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Achieving the controlled, multiscale assembly of nanoparticles (NPs), which is known to underpin the unusual mechanical properties of biomaterials such as Nacre, remains a major outstanding challenge in nanoscience. Here we achieve such Nacre-inspired hierarchical NPs ordering by leveraging the kinetics of polymer crystallization. We are presenting a new method to organize the nanoparticles inside a semi-crystalline polymer matrix simply by controlling the temperature of the isothermal crystallization of the polymer. The experimental system is made of silica nanoparticles (radius=14nm, loading 3% vol.) grafted with PMMA (Poly(methyl methacrylate)) chains (M_w=24 kg/mol) which are initially individually dispersed inside a PEO (polyethylene oxide) matrix (M_w=100 kg/mol). From the balance between the attractive and repulsive forces between the crystal front and the NPs, we defined a critical growth rate G_c typically ranged between 0.01 and 1 μm/s for a particle of radius 10 nm and tunable with the temperature of crystallization T_c. When the crystal growth rate is larger than the critical growth rate G_c, all the NPs are engulfed in the crystal and the final NP dispersion is very close to the initial one. Conversely, when the crystal growth rate is lower or very close to the critical growth rate G_c, the NPs are repulsed by the crystal front, aligned along the lamella and aggregated between the fibrils. The process, which yields a multi-length scale structure, spanning lamellae (10 nm), fibrils (~m) and spherulites (~mm), allows us to achieve three distinctly different scales of order: NPs engulfed by the growing crystals, ordered into layers in the inter-lamellar zone [spacing of (10-100 nm)], or assembled into fractal objects at the inter-fibrillar scale, (1-10 m). The relative fraction of NPs in this hierarchy is readily manipulated by the crystallization speed. The crystal growth rate and morphology have been determined by calorimetry and optical microscopy. The organization of the particles at the different length scale have been characterized by TEM and small neutron and x-rays scattering (SANS/SAXS) and ultra-small angle neutrons scattering USANS. The analytical modelling of the scattering enable to determine the volume fraction of the particles in the different population lamella, fibrils and spherulites. The experimental determination have been confirmed with numerical simulations. Adding NPs always increases the Young's modulus of the polymer, but the effects of multiscale ordering are nearly an order of magnitude larger than those for a randomly mixed state: indeed the percolation threshold is typically reached with 10 % vol. for random dispersion ; we obtained here identical percolation modulus with only 1% vol. of aligned particles. Since fracture toughness remains practically unaffected, this assembly strategy allows us to create high strength low weight materials that retain the attractive high toughness and low density of polymers.

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New Horizons for Molecular Deuteration: Diversity in Molecules and Applications

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Until recently the utilisation of deuterated molecules in neutron scattering studies has been limited by the availability of suitable molecules. Common applications included partially deuterated proteins for SANS investigating multi-protein systems, neutron crystallography of perdeuterated proteins, neutron reflectometry of lipid bilayers systems of limited composition, and SANS using saturated lipid vesicles, or detergents amongst others. The development of chemical deuteration for a broader range of molecular classes and a tailoring of deuteration approach to solve specific contrast problems has greatly increased the range of systems that can be fruitfully investigated.

The Australian National Deuteration Facility (NDF) has developed capabilities in both *in vivo* deuteration of biomolecules and chemical deuteration of small organic molecules. Using the latter, lipids, phospholipids (including head or tail or head/tail deuterated mono-unsaturated lipids such as POPC and DOPC), heterocyclics, aromatics, surfactants, ionic liquids, sugars and match-out detergents have been deuterated. This diversity has led to broad applications and a range of case studies will be presented. For example, contrast issues in SANS of self-assembled soft matter can now be more effectively addressed. Self-assembled monolayer-protected nanoparticles are being increasingly used in electronics, drug delivery, catalysis and sensing devices. The composition and structure of the ligands in the shell layer is important because they determine chemical, biological and interfacial behaviour. Tuning ligand molecules allows for the nanoparticles to be tailor made for specific applications. Use of various combinations of immiscible deuterated or hydrogenated Phenylethanethiol (PET) and Dodecanethiol (DDT) enabled MONSA modelling of SANS data to show the Janus and strip like distribution of the ligands on the surface and the effects of nanoparticle core size and ligand ratio on the patterning[1]. Use of matched-out deuterated detergents has vastly improved SANS studies of membrane proteins. Specific deuteration of the hydrophilic head groups and hydrophobic tails of the detergents octyl b-D-glucopyranoside (OG), or alternatively n-dodecyl-b-D-maltopyranoside (DDM), to different predetermined levels in order to precisely contrast match 100% D_2O buffer ensures that intensity from detergents is at the noise-level and this was demonstrated with 5 different proteins[2]. Likewise, in investigating the location of a purely hydrophobic transmembrane peptide in bicontinuous cubic phase liquid crystals suitable for drug delivery, a mixture of deuterated and hydrogenated phytanoyl monoethanolamide was used to perfectly contrast match out either gyroid or diamond phase lipids to pinpoint the peptides location in the latter[3]. In neutron reflectometry studies of thin film triple-layer organic light emitting devices (OLEDS), the use of deuterated and protonated aromatics/heterocyclics has facilitated characterisation of temperature-mediated diffusion across layers - which was effectively controlled by the glass transition temperature (T_g) of the components.[4] Molecular deuteration has also been effective in reducing background from incoherent scattering (from ^1H) in diffraction studies of metal-organic frameworks (MOFs) used for gas-storage and sequestration. Increased resolution enabled observation of a new mechanism of negative thermal expansion when the MOF cages were subjected to heating.

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Low-temperature Dynamical Transition in Concentrated Microgels

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Since long, hydrated protein powders are known to undergo a low-temperature dynamical transition, i.e. the onset of anharmonic atomic flexibility, connected with the activation of biological functionality.

We provide the first observation of a “protein-like” dynamical transition in nonbiological aqueous environments. To this aim, we exploit the popular colloidal system of poly-N-isopropylacrylamide (PNIPAM) microgels, extending their investigation to unprecedentedly high concentrations, in a regime comparable to those of hydrated protein powders. Owing to the heterogeneous architecture of the microgels, water crystallization is avoided in concentrated samples, allowing to monitor atomic dynamics at low temperatures. By elastic incoherent neutron scattering and atomistic molecular dynamics simulations, we find that a dynamical transition occurs at a temperature of about 250 K in all water-containing samples, whereas the transition is smeared out on approaching dry conditions.

The quantitative agreement between experiments and simulations provides evidence that the transition occurs simultaneously for PNIPAM and water dynamics. In addition, the numerical simulations provide a detailed description of the molecular origin of the dynamical transition in these systems, showing how it crucially depends on the water-macromolecule coupling.

The similarity of these results with hydrated protein powders supports the idea that the dynamical transition is a generic feature of complex macromolecular systems, independently from their biological function.

Melts of Single-Chain Polymeric Nano-Particles: Exploring the Impact of Intra-Molecular Cross-Linking by Neutron Scattering, Dielectric Spectroscopy and Rheology.

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Single-Chain Nano-Particles (SCNPs) obtained by intra-molecular cross-linking of linear macromolecules (precursors) are emerging soft nano-objects showing unique and remarkable physicochemical and rheological properties as a result of their locally collapsed structure and ultrasmall size. Sensing capabilities, controlled drug delivery and catalytic applications of SCNPs have been demonstrated in dilute conditions, being thus promising systems in the nano-technology world. From a basic point of view, they can be used to address a fundamental question: what is the impact of purely internal cross-links on the structural and dynamical properties of a polymer melt? This problem has been faced in a combined effort including neutron diffraction, rheology, dielectric spectroscopy and quasielastic incoherent and coherent neutron scattering [1]. The combination of the results from all these techniques has been crucial to elaborate a consistent picture of the effect of intra-molecular cross-links on the properties in a polymer melt. A bulk sample composed by the long linear counterpart chains (precursor macromolecules without crosslinks) has also been investigated as a reference. Neutron scattering demonstrates that the structure and dynamics at local length scales including the inter-molecular distances (in particular, the structural relaxation) are hardly sensitive to chain topology. Its impact, as revealed by this microscopic technique, consists of a slowing down of collective dynamics occurring at larger length scales, associated to emerging structural heterogeneities with a characteristic length of about 1 nm. Macroscopically, a striking practically complete disappearance of the rubbery plateau is witnessed in the internally cross-linked melt.

We suggest that intra-chain loops [2] and their associated relaxation mechanism are key ingredients in the observed phenomenology.

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SANS STUDIES OF STAR-POLYMERS AND STAR-POLYMER GELS EXPOSED TO STRETCH

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One of the major challenges in polymer physics is the fundamentals of the unique visco-elastic properties characterizing soft materials, and their relation to the molecular structure and cross-links. Small-Angle Neutron Scattering is, using the unique H-D substitution, the one and only method to address the molecular conformation and have accordingly been the basis for a number of studies. Still, however, the understanding is only limited. We have recently extended such studies, investigating the effect of very high flow rates, using a filament stretching rheometer [1,2]. We have studied the effect of polydispersity [3], the effect of branched complex polymer architecture[4], and the structural properties when cross-linked into well-defined network structures [5]. The linear chains show typically 2D-SANS pattern with Lozenge shaped contour [1,3], and clear evidence of chain-expansion and subsequent retraction upon relaxation [2]. The three-armed polystyrene star-polymer with short deuterated segments at the end of each arm shows novel, unexpected correlations perpendicular to the flow axis. We show that the form factor of the three-armed star molecules in the relaxed state agrees very well with that of the random phase approximation of Gaussian chains. Upon exposure to large extensional flow conditions, the star polymers change conformation resulting in a highly stretched structure of a fully extended three-armed tube. The cross-linked star-polymers show novel response to strain. While the mechanical properties appear as expected with linear stress-strain relationship, the SANS pattern shows an apparent unchanged structure. The latter is attributed to the local layered star-molecules [5].

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Disentangling polymer network and hydration water dynamics in pHEMA physical and chemical hydrogels

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Hydrogels with optimal release and confining properties for drugs and detergents, such as hydroxyethylmethacrylate (HEMA) based systems, are highly relevant for medical and cultural heritage applications. To optimize their delivery properties, an intimate comprehension of transport phenomena at molecular level is highly desirable. To this aim, we used quasielastic neutron scattering to selectively investigate the dynamics of the polymer network and the transport properties of the water confined into the hydrogel matrix. In particular, we focused onto the effect of crosslinking nature (chemical or physical) and water content.

For the polymer network, a distribution of relaxation processes was observed, mainly related to the side-chains. Water dynamics was found to occur as H-bond governed process with jump diffusion mechanism. The interaction with the polymer matrix considerably slows the water dynamics with respect to water in the bulk and within other confining systems and leads to a fraction of water molecules appearing as immobile. With higher hydration level, the mobility of both the water and polymer network increases. For the same water content, physical gel networks present slower relaxation processes and smaller explored space than their chemical gel equivalents, as a result of side-chains involvement in the formation of the 3D network. The water mobility is sensibly reduced in the chemical gels compared with physical gels in the less hydrated gels, whereas at higher hydration the values are similar but with shorter residence times in the chemical gels.

Quasicrystals from block copolymer micelles

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Quasicrystals in soft matter systems are still a rare occurrence and the underlying principles of formation are not well understood. Recent work from groups either working with block copolymer melts or POSS headed PS chains[1] as well as MD-simulation concluded that the formation of Frank-Kasper and or quasicrystalline phases has to involve the partition of the self-assembly structures into two species with different aggregation numbers. These findings suggest that no true one component system is capable of forming quasicrystals. Here we show with MD-simulations that a true single component system with an isotropic and experimentally proven pair potential can even form an icosahedral type 3D quasicrystal as well as Frank-Kasper and dodecagonal quasicrystalline phases. The well-known purely repulsive logarithmic pair potential of Pinkus and Witten[2] was used to describe the interaction forces between our star shaped micelles at high volume fractions. With the simulations we were able to replicate the phases we found experimentally and also the transition from a fcc crystal to a dodecagonal quasicrystal. Because the pair potential is not limited to a single type of polymer it opens the possibility to produce quasicrystals from a multitude of block-copolymers or composite materials in a systematic way.

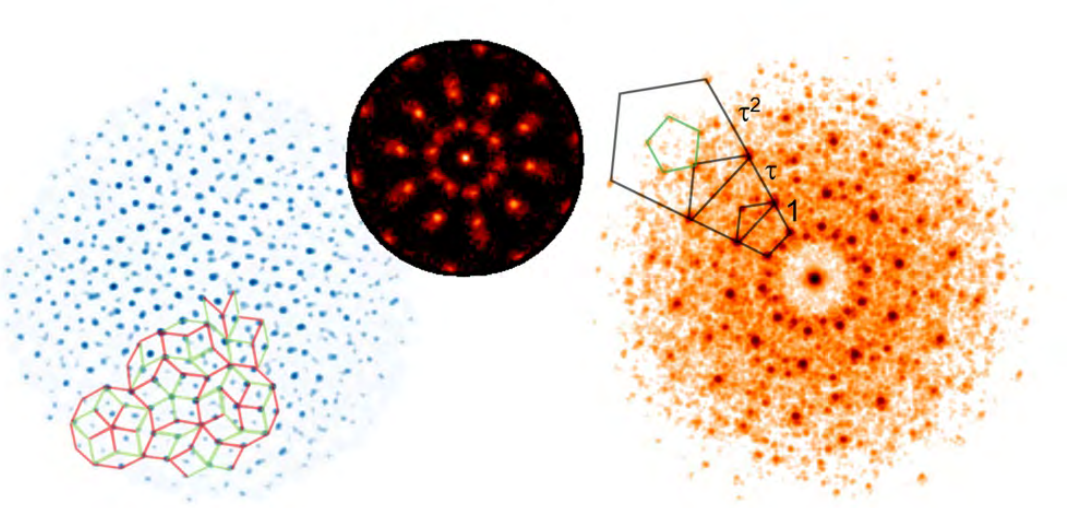

Fig1: Icosahedral Quasicrystal from MD simulation. Projection along the five fold symmetry axis onthe left. Bond order diagram in the middle. Scattering along the 5 fold axis on the right

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SELF-ASSEMBLY IN DEEP EUTECTIC SOLVENTS: FROM SURFACTANT AGGREGATION TO PROTEIN FOLDING

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In recent years many studies into green solvents have been undertaken and deep eutectic solvents (DES) have emerged as environmentally friendly alternatives in many fields, such as separation processes, metal processing, biocatalysis and electrochemistry.[1] DES are solvents obtained through the complexation of organic compounds, where the interaction between the precursors promotes a depression in the melting point that allows the mixture to remain liquid at room temperature. Moreover, through different combinations of precursors the physicochemical properties of the solvent can be tuned for particular applications.

Research into DES has dramatically increased in volume and variety, especially in the last few years, as the advantages of DES in multiple processes becomes clear. Our recent studies have been focused on the ability of DES to sustain self-assembly of amphiphilic molecules. Such alternatives bring the possibility to develop new, sustainable alternatives for surfactant templating, drug delivery and preservation of bioactive molecules.

Here we will explore the behaviour of amphiphilic molecules of different complexity in DES: surfactants, phospholipids and proteins.[2,3]. Our results provide a novel approach for aggregate manipulation in the absence of water through specific and non-specific ion interactions.[4,5] Small-angle neutron and X-ray scattering, in combination with other techniques, have been used to explore the bulk behaviour of these systems, showing that these preserve their activity in DES Aiming to understand the fundamentals of amphiphile behaviour in these solvents, we will present details of self-assembly with varied physicochemical properties of the solvent, amphiphile characteristics and the effects of ion-ion interaction.

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Solid-liquid interfaces: New insights and future opportunities

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Neutrons can penetrate deeply into matter and are sensitive to light elements. If applied under grazing incidence beam geometry (see figure 1) they offer surface sensitivity and the opportunity to address highly relevant scientific challenges on solid-liquid boundaries, like e.g. the hydrodynamic boundary condition. From specular reflectivity the density profile, along the normal of the interfaces, of a liquid close to a solid substrate can be extracted. It turns out that for simple liquids flow anomalies reported from complementary macroscopic measurements can not be explained by density depletion [1]. For polymers this situation changes and the collapse of a grafted polymer brush under shear [2] might be accompanied by a changing hydrodynamic boundary condition, which can be connected to matching length scales of substrate roughness and the liquid structure factor [3].

Lateral correlations, parallel to an interface, are accessible by off-specular (µm) or grazing incidence scattering (nm length scale) [4]. Moreover, by using time of flight (TOF) methods a range of Q (momentum transfers) vectors and related penetration depth can be addressed [5]. In turn the measurements are flux hungry and demanding with respect to brilliance of the source. This in combination with the low absorption of the neutrons in the liquid limits the achievable depth resolution [6]. A combined approach of further improved instrumentation and sample design may allow to overcome this limitations by careful control of the wave amplitude using reference layers and resonators [7].

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Controlling self-assembly with light

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Light responsive materials have gained significant attention in the last years due to their application in photothermal therapy, sensing or as molecular motors. Supramolecular particles of ionic dye molecules and oppositely charged macromolecules have recently been used to create a wide variety of different particle shapes.[1] These assemblies can be controlled by the dye structure, pH, ionic strength but most interestingly by light.[2]

Inspired by these findings we used a cationic azo dye ($AzoC_{10}N_2O_2^{2+}$) and an anionic polyelectrolyte to create well-defined supramolecular structures and study these with small angle neutron-scattering (SANS). The forming structures can be fully disassembled by illumination with UV light (354 nm), which triggers the *trans->cis* isomerization of the dye. Since the trans state is the thermodynamic stable form, *cis->trans* isomerization takes place immediately afterwards. The energy barrier for this process (80 kJ/mol) can be overcome by two mechanisms: collisions with solvent molecules driven by thermal energy or illumination with light at wavelengths larger than 400 nm.

We used time-resolved SANS to follow the thermal *cis->trans* isomerization and the consequent structure formation. This allowed us to study the formation mechanism as well as size, shape and polydispersity of the assemblies. Moreover, we compared the final aggregates at different temperatures and the structure formed when light is used to trigger the *cis->trans* transition. This comparison revealed that the final size of the structures and the rate of *cis->trans* isomerization are strongly correlated. A larger rate of isomerization results in faster structure formation and smaller assemblies.

With the presented system, we can efficiently control the thermodynamics and kinetics of the structure formation in a self-assembling system and elucidate the influence on the resulting assemblies.

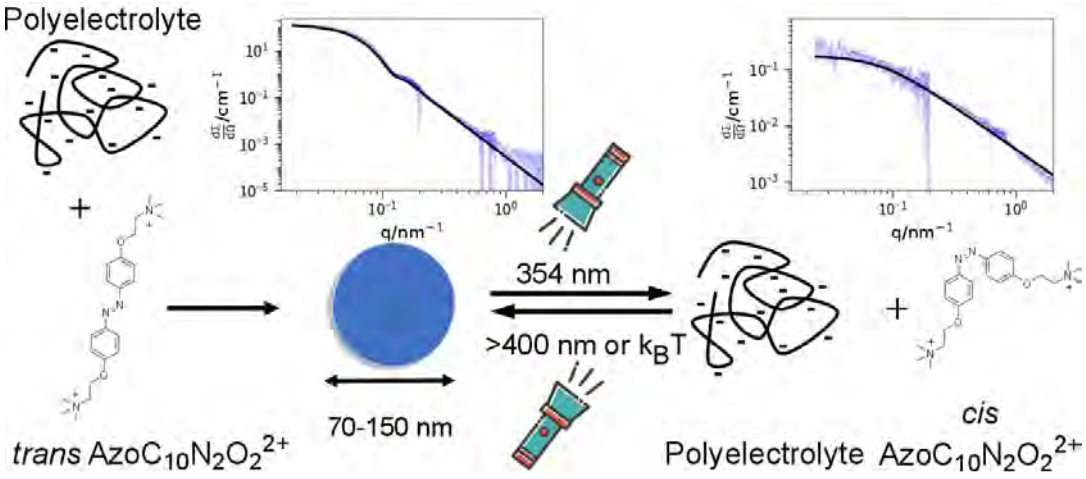

Figure 1: The graphs show SANS curves (D11, ILL), the solid lines are fit with the model of a polydisperse hard sphere and a generalized Gaussian chain (from left to right).

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Self-assembled soft network of hybrid chains

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Wormlike micelles are enormously long flexible cylindrical micelles of a surfactant, which may be formed by long tail surfactant molecules due to balance of hydrophobic interactions of the tails and electrostatic interactions of the heads, controlled by electrolyte concentration [1]. In semidilute regime these long entangled micellear chains impact viscoelastic properties into a solution up to gel-like state. A control of the viscoelastic properties of the wormlike solution is one of the main issue of the field [2]. The wormlike micelles are widely used as thickening agents in food, pains, cosmetics, oilfield industry. In contrast to polymer chains such micellar chains incessantly break and recombine as result of weak hydrophobic interaction between molecules in the micelles. Due to well known interactions of surfactant molecules with number objects likely polymer chains [3], colloidal particles [2], co-surfactants, transformations of the micellar structures easily have been observed in many researches. Thus the other general issue is interactions and self-assembly in surfactant/polymer systems.

Polymer and surfactant self-assembly in aqueous solution attract interest due to influence of the components on a shape and a conformation of each other. In the case of addition of nonsoluble polymer the micellar chains can be transformed into more compact polymer/surfactant complex as we suggest on base of macroscopic rheological investigations, where gel-like state – liquid like state transition was observed. According to literature addition of nonsoluble polymers in a wormlike micelles solution may leads to phase separation or their transformation into short rodlike or spherical micelles. In few works were observed that the polymer/micelles system may form hybrid threadlike micelles that don't break anymore.

SANS results of effect of nonsoluble polymer at small concentrations on the morphology of micellar chains was obtained during last few months with IBR-2 of JINR. Anionic surfactant with long unsaturated hydrophobic tail was used to create wormlike micelles. The scattering density of the surfactants are quite higher that one of the polymers and differ from H_20 D_20 solvent therefore using contrast matching the scattering curve of wormlike micelles and polymer was obtained. SANS allowed to reveal several important effects including shape of surfactant/polymer complex, contour length, cross-section radius, persistent length and mesh size. The results shown flexible cylindrical shape of the scattered objects, that indicates on wormlike micelles covered by polymer chains instead globule-like collapsed polymer chains stabilized by surfactant shell as might be proposed. Other important issue was to study effect of molecular weight of the polymer on the complexes. It allowed to recognize factor of length of polymer chains on the complexes with the surfactant. We demonstrated that in an intermediate concentration range the higher-MW polymer is able to link neighbouring surfactant micelles together, which has never been previously observed.

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Microscopic structure and dynamics of entangled polymers under shear flow - What neutrons can see

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I will present some recent examples of neutron scattering experiments on entangled linear polymer melts and solutions performed under in situ shear deformation. I will start with a combined small angle neutron scattering (SANS) and Neutron Spin Echo (NSE) study of the single chain form and dynamical structure factor of a bulk PDMS melt sheared up to the onset of shear thinning and will explain the potentials and limits of this approach to test single chain theories in out-of-equilibrium conditions [1]. Another example will be a SANS study of the single chain form factor of a semi-dilute Polystyrene solution sheared at high shear rates up to Wi=30 [2]. The last example will be on chemically grafted PS chains in contact with a semi-dilute solution of PS sheared up to Wi=3 examined by neutron reflectometry [3]. All results will be complemented by coarse-grained computer simulations [4].

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Nanocomposites based on Kamagataeibacter xylinus cellulose: Neutron studies

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Nowadays, ones design and synthesize organic-inorganic nanocomposites based on biocompatible polymers including carbohydrates to use them in biomedical applications. One of the tasks is to functionalize them to implicate visualization. Usually, this is achieved by introducing nanoparticles doped with lanthanides or metal-polymer complexes of the latter. Cellulose is a promising polymer in this area because it is an abundant polymer in the Earth. Nano-gel-film (NGF) of cellulose can be extracellularly produced by *Kamagataeibacter xylinus*. Such an NGF can be used to prepare organic-inorganic composites for medical practice because of its unique absorption properties to produce wound covers, bone precursor, and artificial cartilage [1, 2].

Cellulose, being the polymer with a set of functional hydroxyl groups, has complexed supramolecular structure and contains the pores responsible for its sorption properties. Microfibrils of *K. xylinus* cellulose (*Kx*C) were found to have cross-sectional dimensions of 7 × 13 nanometers and aggregate in lamella-like ribbons with a width of 70 – 145 nm [3]. The latter ones form a hydrogen bond network between their hydroxylic groups of anhydroglucose units and water molecules. In the NGF, the water areas (lacunae) can differ in volume [4]. Due to the different mobility of water molecules forming the solvation shells or being in the small-volume lacunae, their freezing temperature can vary. For the time being, revealing the role of the dynamics of confined water in the interaction of supramolecular structure and metal ions in the mesoscopic range is a fundamental problem [5].

This work has been aimed to study the supramolecular structure formation of KxC upon composites forming and different *Kx*C pretreatment, as well as water dynamics at that. The idea was to study interactions of water molecules with the NGF supramolecular arrangement at the mesoscopic level. We used complementary neutron techniques, including SANS (YuMO, IBR-2, JINR, Dubna), ultra-SANS (KWS-3), neutron backscattering (SPHERES, FRM II, MLZ, JCNS, Garching, Germany), and spin-echo-SANS (RID research reactor, TUDelft, The Netherlands). Furthermore, the “zero” level, which presents crystalline ribbons, of NGF of K. xylinus cellulose has been investigated using X-ray diffraction approach.

The supramolecular structure of NGF-nanocomposites happened to have a three-level fractal organization. NGF-nanocomposites impregnated with lanthanide ions in one form or another turned out to luminescence efficiently. Several preliminary experiments have been performed to estimate the nanosecond dynamics of cellulose rearrangement and the presence of different types of confined water.

This work was partially carried out under NFFA-Europe funding (NFFA-Europe ID-700). Aleksandr Bugrov appreciates the Russian Foundation for Basic Research (grant № 16-33-60227) for financial support.

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Magnetic nanoparticles: from self-assembly to drug targeting

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Magnetic nanoparticles are a versatile platform for a large number of technological as well as medical applications.

The magnetic-field-induced assembly of magnetic nanoparticles (NPs) provides a unique and flexible strategy in the design and fabrication of functional nanostructures and devices. We have investigated the field-induced self-assembly of core-shell iron oxide NPs dispersed in toluene by means of small-angle neutron scattering (SANS). The form factor of the core-shell NPs was characterized and analyzed using SANS with polarized neutrons. Large-scale aggregates of iron oxide NPs formed above 0.02 T as indicated by SANS measurements at very small angles. A three-dimensional long-range ordered superlattice of iron oxide NPs was revealed under the application of a moderate magnetic field. The crystal structure of the superlattice has been identified to be face-centered cubic (Fu *et al.*, 2016).

With a suitable coating of NPs by pharmacologically active substances, which provide sufficient binding stability for drug molecules, the drug can be concentrated accordingly and the particles can be accumulated in a certain body region using magnetic field gradient. We performed a complex study of the location of the anti-cancer drug Mitoxantrone (MTO) in the water-based biocompatible system with lauric acid/albumin hybrid coating. The effect of the drug addition on colloidal properties of the system was investigated by means of SANS and SAXS. The application of neutrons and X-rays allowed us to obtain structural information of SPION clusters and find out possible location of MTO by determining the change of interaction between clusters after drug adsorption. Thereby we were able to show that adsorption of the drug to the particles changes colloidal properties of the NPs and partially weakens particle-particle interaction. The drug MTO is most likely adsorbed following electrostatic interaction mechanism, thus potentially reducing interactions of the particles with each other (Zaloga *et al.*, 2018).

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Stabilization of Proteins in Nanopores

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Protein molecules are nature's all-rounders and carry out their specific tasks with great efficiency. For example, some play an important role in converting substances; others are involved in combatting pathogens. As a result, these biological machines are important in technical as well as medical applications. However, proteins tend to clump together irreversibly at high concentrations and thus lose their effectiveness, although this only occurs when they are outside their natural environment of the cell's interior. Spatial restrictions can maintain the activities of concentrated protein solutions. Just why this happens has until now been poorly understood. We demonstrate that despite high concentration levels, proteins do not clump together in nanocavities of porous silicon dioxide, but instead stabilized and behave like a fluid [1]. Crucialreasonsfor such behaviour are on the one hand the interactions between the proteins and the interface, and on the other, the curvature of the nanopores.

Small-angle neutron scattering (SANS) experiment has enabled to directly identify the arrangement of the proteins tested, myoglobin and lysozyme, through the nanostructured materials (SBA-15) [1]. It has been shown that the method enables connections between the characteristics of the pores, the arrangement of the proteins and their activity to be revealed. The knowledge gained can be used for the development of new and better bioinspired applications in biotechnology, medicine and catalytic processes.

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Hybrid solar cells with laser-ablated titania: morphology investigation of the active layer with TOF-GISANS

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In the development of non-conventional solar cells not only the achievements of highest power conversion efficiencies and maximum lifetime of devices is of interest. Also the sustainability of the production process of the devices comes into focus. Following this idea, we developed hybrid solar cells with an active layer based on low temperature processed titania and a water-soluble polythiophene [1]. In our approach titania nanoparticles are produced with laser ablation in liquid (Fig. 1a) in order to initiate a functionalization of titania with the polymer for the active layer. The general layer structure of our hybrid solar cell devices is shown in Fig. 1b. The zoom-in into the active layer emphasizes the importance of the nanostructure of TiO_2 nanoparticles dispersed in the polymer matrix. The devices and the investigated active layers were produced with spray deposition. With the spray deposition technique the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. In order to understand the structure - function relation we investigated the morphology of the spray-deposited active layers with TOF- GISANS.

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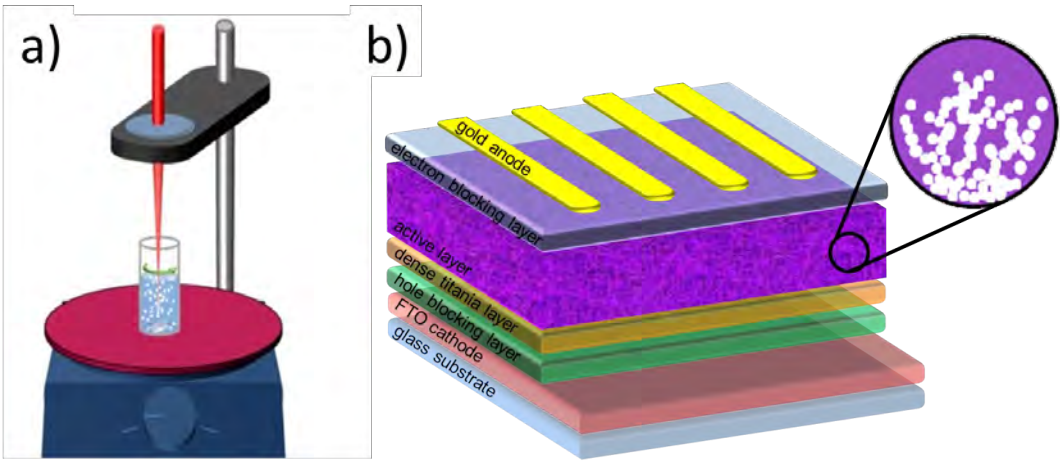

Figure 1. a) Sketch of the laser ablation in liquid process with TiO_2 nanoparticles. b) Layer structure of a hybrid solar cell with an active layer of TiO_2 nanoparticles dispersed in the polymer matrix.

Adsorption and interactions of polymer stabilised lipid nanodiscs with air-liquid and solid-liquid interfaces

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Styrene-maleic acid lipid particles (SMALPs) are self-assembled discoidal structures composed of a polymer belt and a segment of lipid bilayer, which are capable of encapsulating membrane proteins directly from the cell membrane. In recent years a number of different nanodisc forming polymers with varying properties have been developed and characterised [1-6]. For example, Styrene-maleic imide lipid particles (SMILPs) are stable over a different pH range but are still able to solubilize membrane proteins.

Here we will present recent results from a detailed investigation into the interaction of SMALP and SMILP nanodiscs with phospholipids at air-liquid and solid-liquid interfaces. Using Neutron Reflectometry and ATR-FTIR we have examined the kinetics of lipid exchange between nanodiscs and biliayers or monolayers. While lipid exchange is seen in each case, the kinetics and extent to which this occurs are considerably different for each polymer. Further, under certain conditions and highly dependent on the polymer, it is possible to adsorb discs at the solid-liquid interface. This is the first evidence of such adsorption for polymer stabilized nanodiscs and has important implications for future applications that would use SMALP technology to deliver membrane proteins to interfaces.

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Dynamical behaviour of hydration water between lipid bilayers

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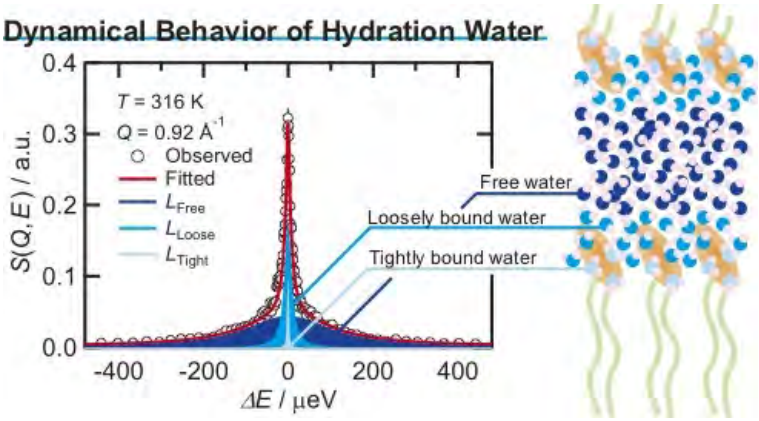
Biological molecules are surrounded by water and their biological functions can only be realized in relation with water. The importance of elucidating the structure and dynamics of water molecules near biological molecules is widely recognized. We investigated the dynamical behavior of hydration water sandwiched between 1,2-dimyristyl-sn-glycero-3-phosphocholine (DMPC) bilayers by quasi-elastic neutron scattering (QENS).

The experiments were carried out at Time-of-Flight near backscattering spectrometer DNA at the Japan Proton Accelerator Research Complex (J-PARC) in Tokai, Japan. Perdeuterated lipid, d_{67}DMPC, was mixed with H_2O in order to investigate the dynamical behaviour of water molecules. These results are compared with that observed for the mixture of DMPC and D_2O.

The results revealed that the hydration water could be categorized into three types: (1) free water, whose dynamical baharior is similar to that of bulk water; (2) loosely bound water, whose dynamical behavior is one order of magnitude slower than that of the free water; and (3) tightly bound water, whose dynamical behavior is comparable with that of DMPC molecules. The number of loosely bound and tightly bound water molecules decreased and increased with decreasing temperature, respectively, and the sum of these water molecules is 14 per DMPC molecule and does not change with temperature. This evidence is consistent with the terahertz spectroscopy measurements. These results indicate that the hydration of lipid molecules changes monotonically with temperature and is independent of the structural transition of lipid bilayers. (Yamada et al., J. Phys. Chem. B, **121**, 8322 (2017).)

Recently we have done further QENS experiments on the mixture of d_{67}DMPC and H_2O with a salt ($CaCl_2$, $FeCl_2$, $ZnCl_2$) to investigate the effect of divalent cations bound to phospholipid headgroups. The results will give important information on the effect of adding salt to the dynamical behavior of hydration water at lipid bilayers.



Rational design of food processing methods with aid of neutron scattering

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Sustainable food production is one of the priorities to prevent further climate change. This requires new processing techniques that with sustainable ingredients yield high quality food. When processing raw materials to final consumer food products, their structures change at length scales from nano-, via meso- to macroscopic sizes. To rationally design food processing routes, insight in these hierarchical structures under dynamic conditions, is a prerequisite. Systems of practical relevance to the food industry are often hard to investigate non-invasively. This is caused by the fact that most food materials are opaque and soft materials. Neutrons make it possible to see the bulk of food materials [1-5]. In the presentation we will show three examples: 1) Fibre formation in casein gels for the production of meat replacements [6]. 2) The effect of processing on the mesostructure of cellulose for food structuring. 3) The mechanism of enzymatic and water degumming on crude oil.

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Localisation of Membrane Components in Lipid Cubic Phases

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By using grazing incidence small angle neutron scattering (GiSANS) on uniaxial orientated thin films where the lipid component, monoolein, is contrast matched out it is possible to confirm that the incorporated membrane components, monopalmitin and cholesterol, sit in the flatter regions of the cubic Pn3m bilayer. As highly ordered nanomaterials, bicontinuous lipid cubic phases are used in a variety of applications, including membrane protein crystallisation[1]. Cubic phases consist of a 3D periodic structure where a lipid bilayer drapes over an infinite periodic minimal surface of either Pn3m, Ia3d, or Im3m symmetry. The surface consists of higher and lower curvature regions and it has been hypothesised that incorporated molecules will localise into these areas. Biologically this means that cubic phases are an excellent tool to study where membrane components will partition within a curved bilayer. Here we show it is possible to predict and confirm the localisation of molecules with in the cubic phase.

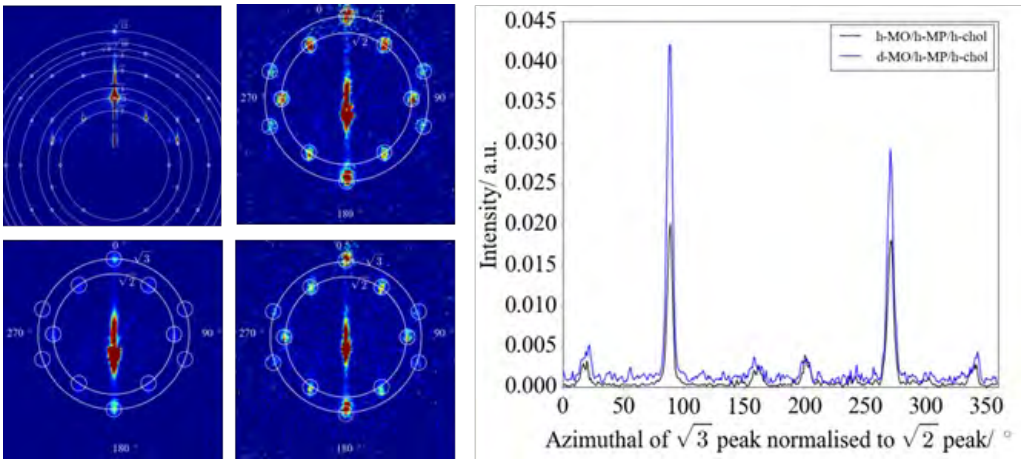

Figure: (top left) GISAXS 2D image of h-monoolein, h-monopalmitin, and h-cholesterol; (***top middle)*** GISANS h-monoolein, h-monopalmitin, and h-cholesterol in D_2O environment, (***bottom left)*** GISANS d-monoolein, h-monopalmitin, and h-cholesterol in D_2O environment, (***bottom middle)*** GISANS d-monoolein, h-monopalmitin, and h-cholesterol in H_2O environment. ***(Right)*** Azimuthal profile of √3 (second row) peaks normalised to the √2 peaks for non-contrast matched (***top middle***)and contrast matched systems (***bottom middle)***

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Protomembranes at the origin of life

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Given the probable extreme environmental conditions at the **origins of life** (high temperature, pressure and pH), the origin and nature of the first cells membranes is still an open question. Due to complex organic carbon limitations, the first membranes were most likely composed of simpler, single chain fatty acids [1], which raises questions as how they could withstand the very variable and extreme surrounding environment [2]. A novel membrane architecture has recently been proposed to explain the stability of contemporary poly-extremophilic archaea, in which apolar alkanes might be present in the lipid bilayer midplane [3], thus shifting the membrane functional domain towards higher pressure and temperature.

Following the same line of argumentation, the current project proposes a similar architecture for **protocell membranes**. Here, the bilayer is made of short **single chain amphiphiles** (e.g. decanoic acid - decanol, hereafter C10mixl), with an **alkane** (e.g. eicosane) inserted in its midplane (Fig. 1 Left). If the functional predictions are proven, this will represent a possible strategy to explain the survival of the first life forms to the early-Earth extreme conditions.

Several techniques have been employed to characterize the model single-chain amphiphiles vesicles varying the alkane presence/amount/type: Light Scattering, to observe **vesicle** appearance, characteristics and **time stability**; Differential Scanning Calorimetry, to study membrane **phase transitions** and temperature stability; Fourier Transform Infrared Spectroscopy, to measure changes in the **vibrational mobility** of the acyl chains vs. T (20 - 90 °C) and p (1 - 1000 bar); Laurdan Fluorescence, to study the **membrane fluidity**. Neutron scattering had a main role to validate and study the protomembrane model. In fact, Neutron Membrane Diffraction and Small Angle Neutron Scattering gave very promising results, with evidences on the **localization** (Fig. 1 Left) and **stiffening effects** (Fig. 1 Right) of the membrane intercalated alkanes. The latest results, obtained with the above mentioned techniques, will be presented.

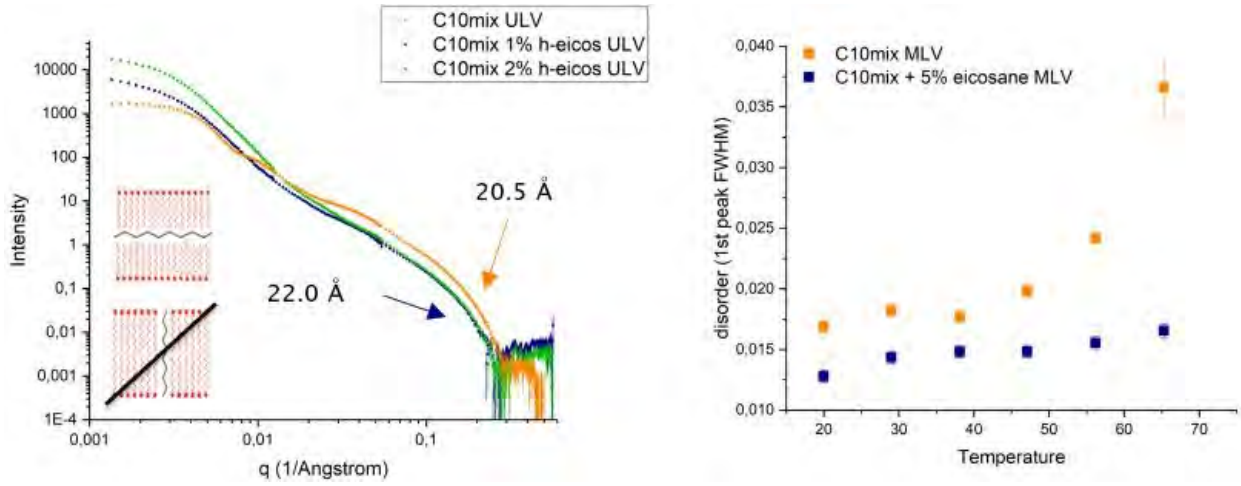

Figure 1: D33 SANS data. Left: vesicle form factors, the alkane causing a membrane thickening. Inset: protomembrane model, a bilayer (red) with alkanes (black), perpendicular to the lipid chains. Right: 1st Bragg FWHM peak of Multilamellar vesicles.

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Protein dynamics and diffusion followed during aggregates formation by time-resolved quasi-elastic neutron scattering

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Most proteins can undergo unfolding and aggregation under particular conditions. The formation of fibrillar aggregates can be associated with neurodegenerative diseases, such as Parkinson's or Alzheimer's (Chiti & Dobson 2006). Treating the inflammation, a consequence of these protein aggregates, has been of limited efficiency so far, therefore, getting a better understanding of aggregation appears necessary to act directly on the cause. Amyloid-fiber formation is characterized by the formation of a cross-beta pattern (Tuttle et al. 2016), leading to a very stable fibrillar structure, from which other super-structures can be formed, such as particulates and spherulites (Vetri & Foderà 2015). The initial monomeric and the final fibrillar states can be isolated and both structural (Fitzpatrick et al. 2017) and dynamical (Fichou et al. 2015; Schirò et al. 2015) information has been obtained. Recently, we suggested that hydration water entropy was increased after fibrillation while protein dynamics remained unchanged (Fichou et al. 2015). However, no information is available about the dynamics of intermediate species, mainly because of their transient and highly unstable nature.

Here, we propose a new approach exploiting the unique capabilities of the backscattering spectrometer IN16B (ILL, Grenoble) to perform fixed-window scans with an acquisition of 15 minutes per time point. We showed in a pilot experiment on a lysozyme solution that aggregation can be triggered inside the spectrometer by raising the temperature and then monitored with a 15-minute time resolution by measuring the backscattering signal at different energy offsets – from 0 to 3 μeV (unpublished). Earlier, it has been shown that center-of-mass diffusion of proteins (Fickian-type diffusion) and internal protein dynamics (deviating strongly from Fickian diffusion) can be observed simultaneously and disentangled (Beck et al. 2018). In the lysozyme pilot experiment, we found that the global diffusion coefficient decreased monotonously during aggregates-formation, while internal protein dynamics remained constant on the accessed energy range. Additional data from simulated unfolded lysozyme provide complementary clues on the oligomerization state.

Combined with a proper deuteration strategy, the method provides a powerful way to follow over time stability or slow phase transition processes for a variety of systems in soft matter and biology.

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Magnetic Order in Topological Insulator Thin Films: Transition Metal and Rare Earth Doping

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Topological insulators (TIs) are one of the most important recent discoveries in condensed matter physics. They have a gapless topological surface state which exhibits robust spin-momentum-locking protected by time-reversal symmetry. If a band gap is introduced by the controlled breaking of TRS in the 2D surface states, interesting quantum phenomena can be observed, such as the quantum anomalous Hall effect. The dissipationless conduction and perfect spin-orbit coupling make TIs particularly suited for thin film device physics relying on spin transport such as spintronics or spin-orbitronics.

However, the nature of ordering in magnetically doped TIs remains poorly understood. In particular, doping inhomogeneity and disorder has been under debate, and various types of magnetic order have been proposed to play a role [1-4].

Here we contrast the microscopic magnetic order in two magnetically doped topological insulator thin films: transition metal doped Cr:Sb2Te3 and rare earth doped Dy:Bi2Te3.

Our combined polarized neutron reflectometry, muon spin spectroscopy and x-ray magnetic circular dichroism studies show that long range magnetic order in Cr:Sb2Te3 [5] is accompanied by significant amounts of inhomogeneity and dynamics – even in films whose magnetic volume fraction tends to 100%. In contrast, Dy:Bi2Te3 [6] does not order ferromagnetically, but instead displays similar, inhomogeneous islands of more static magnetism embedded in a paramagnetic environment [7]. These islands are highly susceptible to moderate magnetic fields. While in Cr:Sb2Te3 ferromagnetic order is mediated by charge carriers [8], this is not the case in Dy:Bi2Te3. We will discuss recent experiments in which we use proximity coupling to try and improve the robustness of magnetic ordering in magnetically doped TIs. For instance, we were able to combine these two materials into heterostructures leading to long range order in the Dy-doped layers as demonstrated using XMCD and polarized neutron reflectometry measurements, shown in Fig. 1 [9].

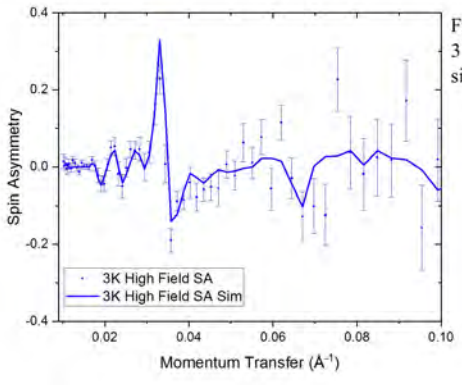

Fig. 1: Spin-asymmetry of a Dy-doped/Cr-doped multilayer at 3 K and 0.7 T. The magnetic response of the Dy-doped layer is significantly changed from that of an equivalent single layer.

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Reflectometry with registration of secondary radiation at total neutron reflection

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Standard neutron reflectometry measures a spatial profile of interaction potential of neutron with medium[1]. Very often it is not enough. For example at study of proximity phenomena at interface of two media or in case of thin layer placed between ones when need to know spatial profiles of two or three elements. Two conditions necessary to realize. Firstly the neutron reflection must be total or close to total. In this case the neutron density in structure is periodical function of coordinate in normal to interfaces direction[2]. Second condition is that need to measure a primary radiation (reflected or(and) refracted neutrons) and secondary one[3]. Secondary radiation appears of nuclei after of capture of neutrons. Types of secondary radiation are charged particles, gamma-quants and nuclear splinters. Special secondary radiation is the spin-flip neutrons which appear in non-collinear magnetic structure or structure with magnetic inhomogeneity. Other special secondary radiation are neutrons which incoherently scattered by nuclei (for example, by vanadium and hydrogen). As result of the intensity dependencies of primary and secondary radiation from neutron wave vector can be defined the spatial profiles of elements-isotopes . In given work a foundation of neutron reflectometry with registration of primary and secondary radiations is fulfilled. The channels of charged particles, gamma-quants and spin-flipped neutrons which created on spectrometer REMUR at IBR-2 pulsed reactor are described [4]. The report presents the result of testing the method with model structures V(10nm)/CoFe(5nm)/^{6}LiF(5nm)/V(5nm)/glass, V(10nm)/ CoFe(5nm)/^{6}LiF(5nm)/V(15nm)/glass, Cu(10nm)V(65nm)/CoFe(5nm)/^{6}LiF(5nm)/V(5nm)/glass и Cu(10nm)/V(55 nm)/CoFe(5 nm)/ ^{6}LiF(5 nm)/V(15 nm)/glass. Glass substrate - neutron reflector had sizes 50mm×70mm. It is showed that sensitivity to changing of layer position and spatial resolution in position of layer ^{6}LiF(FeCo) are 0.1(0.05) nm/hour and 5 nm, correspondently. In the further the atomic spatial resolution 0.4nm can be achieved with supermirror neutron reflector.

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Instabilities of buried polymer layers studied by specular and off-specular neutron reflectometry

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The stability and breakup mechanisms of thin polymer layers are of considerable interest in materials science as polymer coatings have become an integral part of our daily life. They have been subject of intense research in polymer physics during the last few decades. Based on the Hamaker constant alone, the effective interfacial potential suggests that a sufficiently thin film of polystyrene (PS) on silicon substrate, capped with a thick layer of poly methyl methacrylate (PMMA) should undergo spinodal dewetting [1].

In order to elucidate mechanisms of immiscible polymer film decomposition we have investigated a set of dPS/hPMMA (d - deuterated, h - protonated) bilayers on Si substrate. A rather thick (up to 3500 Å) hPMMA cap layer is chosen to minimize possible effects of the free surface on the process of dewetting at the buried interface. We have therefore used specular neutron reflectometry (SR) and off-specular scattering (OSS) [2] in conjunction with selective deuteration to study the buried interface. A combination of these techniques enables us to precisely follow the evolution of the depth density profile (up to the dPS droplet formation, surrounded by hPMMA) in the PS layer and monitor changes in the morphology of the interface [3].

A scope of data collected at the D17 reflectometer at ILL at different annealing times for a set of samples of different thicknesses were quantitatively evaluated employing originally developed software based on the distorted wave Born approximation (DWBA). The model includes not only correlated surface and interfacial roughness, but also correlation lengths across the whole PS layer. The roughness, or intermixing of the two neighbouring polymers increases with thermal annealing along with the increase of two in-plane correlation lengths introduced to fit OSS: one for dPS and the other for hPMMA. It is crucial that SR and OSS are fitted simultaneously and in absolute scale, as OSS is mostly concentrated below the critical edge of total reflection from the deuterated layer, but above that of hPMMA. Within this range neutron waves propagating above the potential of hPMMA layer, tunnelling through the PS layer and constructively interfering with waves totally reflected from the substrate are focused in the PS layer where they are effectively scattered from the layer imperfections in off-specular directions. Similar effect was observed also for a tri-layer system hPS/dPMMA/hPS.

Hence the scattering cross section line shape is not only due to lateral form-factor morphology, but strongly modulated by the interference wave field pattern.

The model describes the evolution of the film breakup from an early stage up to the point when the film totally dewets. The parallel correlation length extracted is of the order of a few μm. In the talk, we will discuss qualitatively and quantitatively the different contributions of the interfaces of interest to the final off-specular neutron scattering pattern and we will point out the potentials and limits of the combination of SR and OSS.

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Phase transition kinetics in a doubly thermo-responsive block copolymer thin film followed with in-situ neutron reflectometry

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Thermo-responsive polymers can show a strong change in volume towards even slight changes of their surrounding temperature. This behavior makes them promising candidates for the implementation in manifold applications such as nano-sensors, artificial pumps and muscles, or optical switches. While the underlying mechanisms of such polymers in solution are well understood, less is known about thermo-responsive polymers in thin film morphology. In our recent work, we follow the phase transition kinetics upon increasing temperature in a doubly thermo-responsive block copolymer (Figure 1a) thin film via in-situ time of flight neutron reflectometry (TOF-NR). The block copolymer consists of a poly(N-isopropylmethacrylamide) (PNIPMAM) block, which shows a lower critical solution temperature (LCST) and a azwitterionic poly(sulfobetaine) (PSPP) block, which exhibits an upper critical solution temperature (UCST) that is lower than the corresponding LCST of the PNIPMAM block. By a combination of spin-coating and solvent vapor annealing thin polymer films in the range of 30 nm to 150 nm with high homogeneity are prepared. At low temperatures, below the UCST, the polymer film is swollen in D_2O atmosphere in order to increase the mobility of the polymer chains. Subsequent, temperature is increased to an intermediate regime (between UCST and LCST) and high regime (above LCST). The kinetic processes (swelling and temperature steps) are followed via TOF-NR with high time resolution (30 seconds). Static TOF-NR measurements (Figure 1b and 1c) and TOF grazing incidence small angle neutron scattering (GISANS) measurements are performed at the beginning and in between the kinetic processes to gain a complete picture of the swelling and temperature-dependent behavior of the polymer thin film. Furthermore, the obtained kinetics are modelled to get a detailed understanding of the underlying mechanisms.

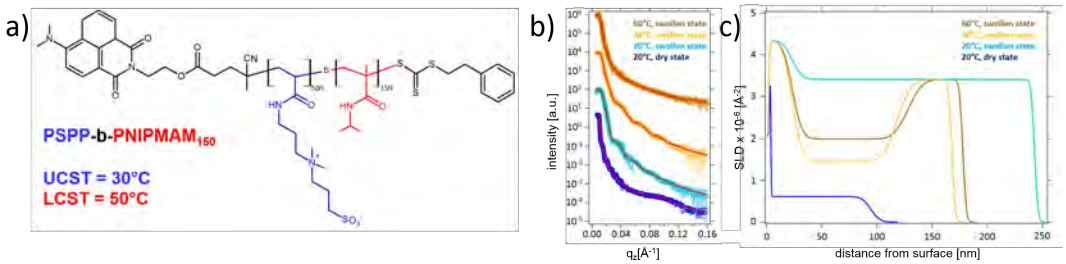

Figure 1: (a) Chemical structure of $PSPP_{500}$-b-$PNIPMAM_{145}$. (b) Static TOF-NR measurements and (c) SLD profiles at 20°C (dry (dark blue) and swollen state (light blue)), 40°C (swollen state, orange) and 60°C (swollen state, brown).

The role of phosphatidylserine lipids in tuning membrane protein domain location in supported membranes

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Membrane proteins are fundamental cellular membrane components as well as relevant targets for selective therapies. Their structure and function are strongly dependent on the surrounding lipid environment, where several specific lipid-protein interactions can take place[1]. Hence, experimental methods able to mimic the protein lipid physiological environment are particularly relevant to investigate membrane proteins. For this purpose, supported membranes (SMs) composed of a planar lipid bilayer are attractive systems as they allow for a detailed structural characterization by surface-sensitive techniques, such as Neutron Reflectometry (NR), Quartz Crystal Microbalance with Dissipation monitoring (QCM-D), and Atomic Force Microscopy (AFM) [2],[3],[4],·

Recently, we have been investigating how the lipid composition of supported membranes might affect their interaction with specific domains of membrane proteins. In particular, we focused on two relevant membrane proteins the Na+/H+ exchanger isoform 1 (NHE1), a ubiquitous membrane protein responsible for the regulation of cellular pH and volume, and Tissue Factor (TF), the membrane protein responsible for the initiation of blood coagulation by forming the protein complex with the activated coagulation factor VIIa (FVIIa). Although structurally and functionally diverse, NHE1 and TF have both been suggested to have specific interactions with anionic phospholipids. In the case of NHE1, a specific lipid interaction domain (LID) was identified as part of the protein intracellular domain protruding outside the cell membrane[5]. Although the affinity of such domain for anionic phospholipid, such as phosphatidylserine (PS) lipids, was recently reported[4], structural information on the NHE1 LID in the proximity of lipid membranes was so far missing. On the other hand, activity assays highlighted that the activity of the protein complex formed by the TF extracellular domain and FVIIa was strongly enhanced if PS lipids were present in the membrane[6]. While atomic structures of the TF extracellular domain alone and as a complex with FVIIa are available, the location of these proteins on a lipid membrane is unknown. Recently, we combined different surface sensitive techniques including Quartz Crystal Microbalance with Dissipation monitoring (QCM-D) and Neutron Reflectometry (NR) to probe the interaction between the NHE1-LID or TF/FVIIa complex and supported membranes with PS lipids. Our results provide relevant structural information on how the presence of the anionic phospholipid strongly affect the location of both the two protein systems with respect to the membrane.

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Artificially Designed Magnetic Domain Patterns Investigated by Neutron Scattering

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Artificially designed domain structures find application in magnetic sensors and logic elements [1]. The stray fields above the thin film surface, emerging at domain boundaries, can be used for positioning and movement of magnetic micro- and nano-objects in liquid environments [2]. In addition, the tailored design of the magnetic pattern allows investigations of lateral interactions of domains and domain walls during the magnetization process [3]. Here, light-ion bombardment of exchanged bias thin films in external magnetic fields has been used to create stripe domain patterns in a head-to-head/tail-to-tail configuration [4].

We report on the structure and magnetizations of the domains and boundaries, resolved in-plane and in depth, using polarized neutron reflectometry and off-specular scattering recorded on the polarized neutron reflectometer D17 at ILL. The specular reflectivity establishes the depth resolved structure and field dependence of the domain magnetizations. Off-specular scattering provides the lateral correlation lengths and domain contrast arising from canting of individual domain magnetizations. Simulations of the magnetic scattering based on the distorted wave Born approximation reveal peculiarities in the scattering arising from asymmetric domain structures, domain wall configurations and magnetic return fields inside the sample structure (Figure 1). We find that the domains do not equally follow the external magnetic field, revealing anisotropy differences created by the light-ion bombardment. Further, domain walls of substantial width and a return field of substantial strength in neighboring layers need to be included in the model to reproduce features of the scattering. Fast measurements, following the hysteresis loop of the magnetization, show the evolution of domains and the persistence of domain scattering well beyond apparent saturation. We will discuss the scattering and resonance features arising from the $IrMn_3$ potential well structure and present a detailed quantitative model of the in-plane and depth resolved magnetic domain structure.

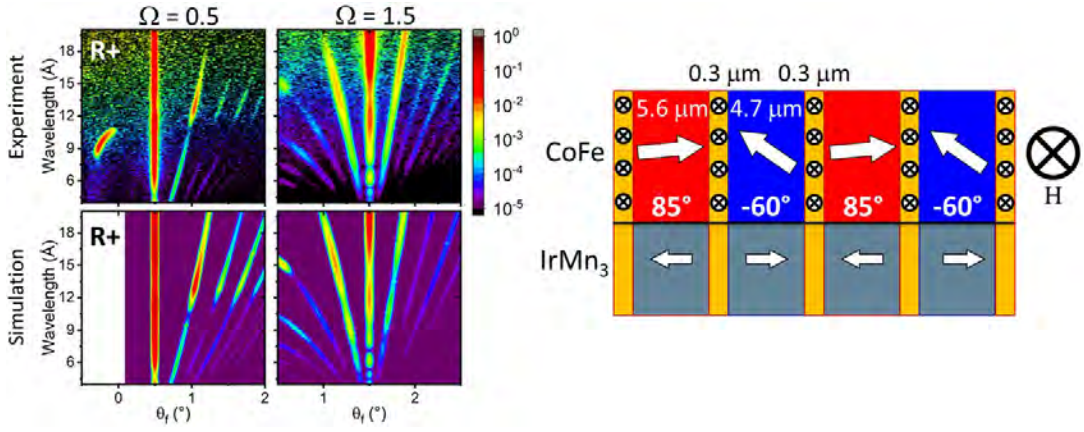

Figure 1: Example scattering from in-plane magnetic domains. Left: Data and preliminary simulation at two angles of incidence for R+ polarization. Right: Model sample structure used in the simulation, including asymmetric domain magnetizations and widths, as well as domain walls and return fields in $IrMn_3$.

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Structured liquids

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Ionic liquids, highly concentrated electrolytes and mono-alcohols are all examples of liquids that show structural correlations on length scales beyond nearest neighbour distance. A signature of these correlations is the presence of a peak in the static structure factor S(Q), e.g. measured by x-ray or neutron diffraction, at momentum transfers in the region 0.1-0.8 $Å^{-1}$, that is below the principle peak in simple liquids typically found around 1.5 $Å^{-1}$. These structures result from either the existence of competing or of highly directional interactions.

For mono-alcohols the presence of hydrogen bonding gives the possibility to form transient clusters of molecules. Apart from the presence of a weak peak at low momentum transfers in S(Q) these structures also lead to dynamics not generally observed in liquids, such as relaxations slower than the structural αrelaxation. In ionic liquids on the other hand the competition between van der Waals and coulombic interactions leads to a very distinct signature in S(Q) corresponding to real space correlations of length scales up to 30-40 Å. This is a result of the typical nature of the constituent ions, in particular the cations which commonly are composed of a charged core and long alkyl side chains. The ionic configuration leads to the formation of long range structures due to the segregation of the alkyl chains and charge ordering of the polar domains.

In this contribution we report on how neutron scattering can be used in combination with complementary techniques and simulations to understand both the structure and dynamics of hydrogen bonded liquids, ionic liquids and highly concentrated electrolytes. The key feature of neutron scattering is that information on both structure and dynamics can directly be obtained on the relevant length scales of these structured liquids. As an example, from neutron diffraction combined with modelling we have shown how the structure of liquid propanol is formed by hydrogen bonded clusters with a relatively wide size distribution [1] and that neutron spin-echo can then be used as one tool to understand the dynamics of these clusters [2]. Similarly the nanostructure of ionic liquids and highly concentrated electrolytes can be characterized by diffraction, but in this case small angle x-ray scattering, revealing how segregation of alkyl chains and charge ordering depends on the constituent ions [3,4] and quasi-elastic neutron scattering reveales the local motion of the ions which we then can correlate to for instance the macroscopic conductivity of the liquid which is of interest for applications.

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Molecular aggregation in binary mixtures of cyclic amines with water: Thermodynamic, SANS and theoretical studies

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Piperidine and *N*-methylpiperidine hydrates aggregate in aqueous solutions due to hydrogen bonds between hydration water molecules. No such effects occur in the mixtures of the amines with methanol, that highlights the active role of water solvent in the aggregation. However, the role of various contributions in thermodynamic functions due to specific interactions, van der Waals forces, and the size and shape of the molecules remains open.

In our study we explore and discuss the family of solutions of pyrrolidine, *N*-methylpyrrolidine, piperidine, and *N*-methylpiperidine in water and methanol, measured by thermodynamic methods and small angle neutron scattering. While in methanolic solutions the trends of the association energies correlate with the thermodynamic data, this is not the case in water. Aqueous solutions required an empirical hydrophobic hydration term to be considered. The hydrogen bonds formation and breaking which accompany the mixtures formation leads to considerable excess volumes, while the size of the solute molecules is manifested in the compressibility of aqueous solutions. Contrary to alcoholic solutions, SANS evidenced that aqueous solutions are microheterogeneous on the nanometer-order length scale, and modelling by various theoretical models are presented.

About the size cut-off effect on small-angle scattering from stochastic mass fractals

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There are several theoretical approaches [1-7] to describe the cut-off effect on small-angle scattering curves from mass fractals because of the finite size of the scattering object (e.g. developed cluster of nanoparticles). The problem [8] is to connect the power-law type scattering, $I(q) = Bq^{-D}$ (corresponding to the fractal dimension D), at high q-values with the Gunier approximation, $I(q) = G\exp(-R_g^2 q^2/3)$, at low q-values. Various empirical or semi-empirical functions are used to cut-off correlations in the direct space with the following Fourier transform to the q-dependence of the scattered intensity. The chosen approach is then tested by comparing the calculated intensity and the model or experimental scattering data. However, up to now no well-proven criterion of correctness was formulated.

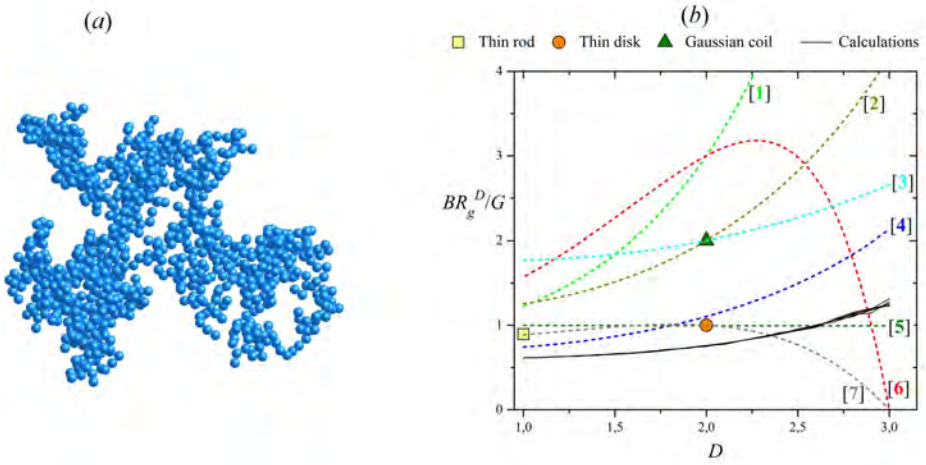

Figure 1: (*a*) Example of generated cluster by algorithm [11]; (*b*) Universal parameter calculated for different models as a function of fractal dimension D.

Here, we employed the fact that the parameters of the two scattering levels are D-dependent, which can be used as an additional test on correctness of the above-mentioned approaches. The analysis of the universal combined parameter BR_g^D/G [9] as a function of D (Fig.1) revealed different behaviors for various models. The true dependence was obtained using the calculations for clusters generated by the algorithm [10, 11], which makes it possible to regulate D. The simulated series of clusters with different sizes and packing densities gave the same predicted [8] universal D-dependence of the combined parameter. The comparison showed that no model data fit the simulations. Either principally different behavior, especially at $D \to 3$, is seen, or some kind of renormalization is required. The given analysis is considered as a step towards understanding of the scattering from multiscale systems at a new level.

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D3 at the ILL: structural studies of hydrogenous liquid and amorphous systems using polarised neutrons

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In diffraction, the structural information of materials is contained in the coherently scattered signal. Unfortunately, the determination of the coherent structure factor of hydrogenous liquid and amorphous systems is very difficult: X-rays are barely sensitive to hydrogen, while neutron results still lack accuracy due to the contamination of the scattering intensities by a huge spin-incoherent signal from ^{1}H, in some cases reaching over 90 % of the total signal.

Using polarised neutrons with polarisation analysis, one can experimentally separate the coherent and incoherent contributions to the scattered intensity, since nuclear coherent scattering does not reverse the neutron spin while 2/3 of the spin-incoherent scattering do reverse it.

The D3 polarised hot neutron diffractometer at ILL, formerly devoted to magnetic studies on single crystals, has been upgraded and now offers a new setup for the studies of liquids over a wide Q-range using polarised neutrons [1]. Within the ILL endurance upgrade program, the capabilities of this new, fully operational, option are currently being enhanced by the implementation of a new detector assembly, including a wide angle ^{3}He spin filter and a multidetector.

We detail the principle of the method, giving special attention multiple scattering, which has a critical impact on the data quality.

Through several examples we demonstrate the power of the method and show the complementarity with what is currently achieved on other dedicated instruments (cold, polarised neutrons, and hot, non-polarised neutrons). Examples include molecular liquids (water, alcohols, sugars in solution) as well amorphous systems of industrial interest (cements, pharmaceutical industry). [2]

The improved accuracy of the data obtained using polarized neutrons will also have a high impact on the assessment of *ab initio* calculations, as shown *e.g.* by recent results in electrolytes.

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Cooperativity Length in a Glass-Forming Liquid Determined by a Combination of Neutron Spin Echo Spectroscopy and Calorimetric Methods

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Although the idea of a 'characteristic' or 'cooperativity' length scale ξ related to the glass transition is now wide-spread, there is much less consensus on whether this length scale can be related to thermodynamic fluctuations and, if yes, one has to consider temperature fluctuations δT. The crucial experiment to this end has to compare values of ξ from 'thermodynamic' formulae to independent values from structural-dynamics experiments.

Recent advances in quasielastic neutron scattering (QENS) by neutron spin echo (NSE) and in AC calorimetry enable an experiment with the aim of determining the cooperativity length ξ in glass forming materials proposed more than a decade ago by E. Donth [1]. The basic idea of this experiment is to assign a length scale to the AC-calorimetric relaxation time using the spatial resolution of QENS. The main problem is to find a range of relaxation times that is accessible by both methods. The problem is aggravated by the fact that in the QENS part one needs to observe the self-correlation which is usually the weaker side of NSE.

Although these kind of studies still face technical difficulties, we can present first results on propylene glycol [2] and poly(ethyl methacrylate). The results indicate a better agreement with a thermodynamic calculation involving temperature fluctuations.

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Proton dynamic behaviour in hydrogen bond networks in oxyhydroxides

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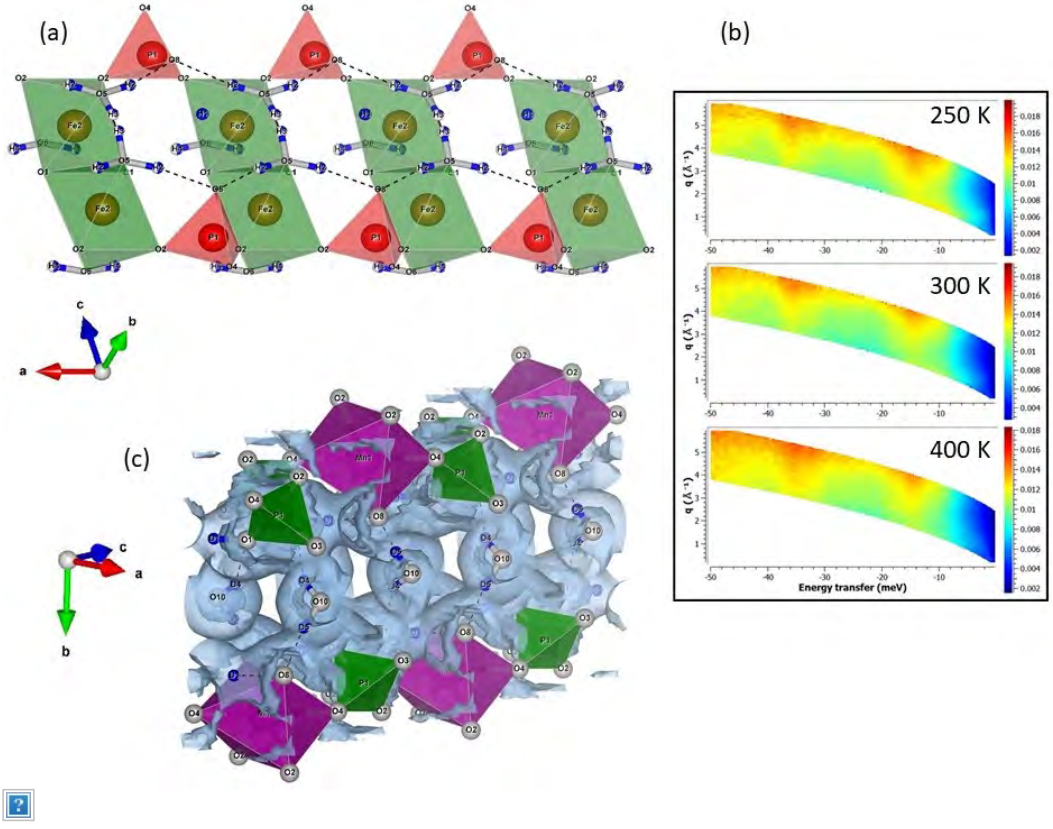
Hydrous phosphates have been taken attention as catalysts and electrolyser for intermediate temperature fuel cells, pseudo-supercapacitors, as well as photocatalyses for water splitting. Phosphatic oxyhydroxide minerals exemplify the critical role of $(OH)^{-1}$ and $(HOH)^{0}$ groups for an extremely wide variety and complexity of their frameworks. Our studies of protonic dynamics in such diverse networks show:

1) proton tunneling in short hydrogen bonds (HB) in $(Mn,Fe)^{2+}AlPO_4(OH)_2(HOH)$; 2) an optimal geometrical condition for protonic conductivity in a honeycomb-like HB Network in $(Fe^{2+}Fe^{3+}_{3.2}(Mn^{2+},Zn)_{0.8}(PO_4)_3(OH)_{4.2}(HOH)_{0.8})$ (Fig a); 3) $(OH)^{-1}$ and $(HOH)^{0}$ groups are site-exchanging between two semi-helical chains of HBs in $(Mn^{2+})_5(PO_4)_2((PO_3(OH))_2(HOH)_4)$ (Fig. c).

A common feature relevant to dynamically disordered protons in these compounds is entourage of lattice dynamics, i.e. collective motions of their mixed framework tetrahedral-octahedral building units (Fig. b). This resembles the so-called vehicle mechanism for superprotonic conductivity. We present at the meeting ECNS 2019 structure-related protonic conductivity, based on results from structural analyses using neutron diffraction in combination with information from quasielastic neutron scattering (QENS) and impedance.

Fig. a) A honeycomb-like H-bond network (dashed line) over which dynamically disordered protons in rockbridgeite are accompanied by rotations of the framework octahedra and tetrahedra; b) Three phonon energies about 15, 35, and 50 meV are resolved from QENS; (b) Bond valence mismatch mapped around H^+ at 0.6 v.u. (in blue) indicates proton dynamics between two semi-helical chains of HBs in Mn-hureaulite (c).



Impact of the external magnetic and electric fields on behavior of ferrofluids at interfaces: neutron reflectometry data

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Ordered arrays of magnetic nanoparticles (MNP) are of current interest due to various potential applications in biomedicine, catalysis, optics and data storage. The effects of self-assembly of nanosized objects are interesting themselves from the fundamental point of view. In this work, this problem is considered for ferrofluids (FF), liquid dispersions of colloidal magnetic nanoparticles coated with various stabilizing agents (surfactants, polymers). The behavior of MNP at interfaces differ from that in bulk as a result of specific adsorption properties, which can be an important factor in applications. A special question for FF concerns the effects of external fields (magnetic, electric or both) on their structure stability at interfaces.

The work was aimed at obtaining structural information about MNP ordering on oxidized silicon substrates contacting FF under different conditions. For this purpose, neutron reflectometry was used to compare structural organization of FF at interfaces with that in bulk (data of small-angle neutron scattering) [1,2]. As a conclusion, both kinds of structure are correlated and determined by the type of magnetic component in MNP regulating the particle interaction, as well as the MNP concentration in FF. The formation of quasi-layers of nanoparticles on silicon surface after application of non-homogeneous magnetic and electric fields was observed [3]. In this connection, the possibility for anchoring MNP from FF on substrates by external magnetic fields is discussed. The studies were accomplished by X-ray reflectometry analysis of the layered structures of MNP formed after evaporation of the liquid carriers from FF under different conditions.

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Structure and Slow Dynamics in Spontelectric Methyl-Formate

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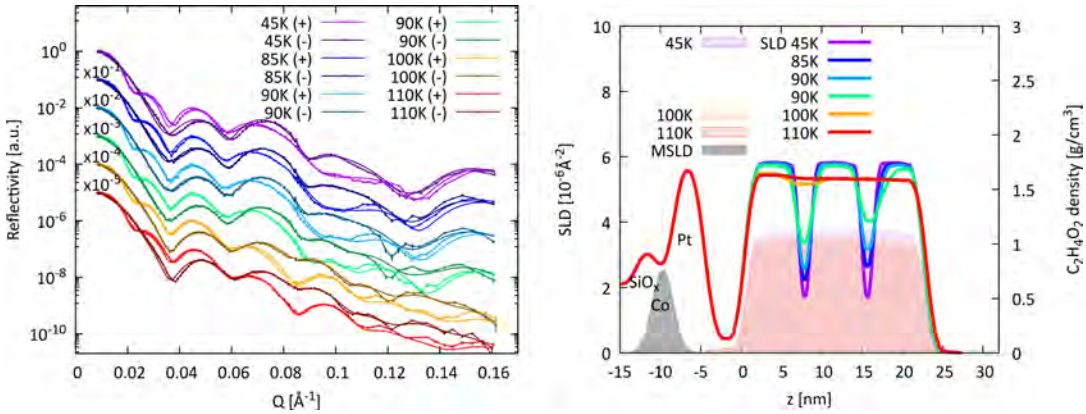
Spontelectrics (SE) are materials that form spontaneous electric polarization when condensing as thin films onto a substrate under high vacuum conditions [1]. The SE forming dipolar molecules orient themselves during the deposition without the need for an external field [2] and show various modifications upon heating films after deposition. These modifications have been interpreted as structural phase transitions [3] and their behavior can depend on the deposition temperature of the films.

Due to the necessary environmental conditions and the thin film nature of the SE it is challenging to access the structure and dynamics in such systems. We have investigated the SE methyl-formate (MF) using polarized neutron reflectometry (PNR) together with a combination of magnetic contrast variation and selective deuteration. We have developed a unique experimental setup for the Magnetism Reflectometer at SNS. With this setup adsorbed films have been grown in-situ and the thickness of the film was controlled via dosing time. In order to get access to the details of the depth structure and the structural modifications we in-situ prepared films via alternating hydrogenated (H-) and deuterated (D-)MF layers during the film deposition, thus labeling the depth via creating buried interfaces between the H-MF and D-MF. The isotope contrast between hydrogen (H) and deuterium (D) generates a scattering length density (SLD) contrast at the interface of two layers thus a high sensitivity to the diffusion process within the MF films is achieved. The MF multilayers of protonated and deuterated molecules were deposited onto a substrate coated with a magnetic reference cobalt layer to amplify the sensitivity with magnetic contrast. We observed the details of the internal modifications of the thin films morphology while heating after deposition. Fitting the PNR data with a single model over a large temperature range we could extract the width of the H/D boundaries and from that extract temperature dependent self-diffusion coefficients for MF films deposited at temperatures of 45K and 65K. The results provided unique information on the structural evolution of the MF system upon heating and show similarities to other glassy systems.



PNR (left) and SLDs (right) for superstructure of MF grown at 45K

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Tuning the high-temperature thermal expansion properties of perovskite-related Co-containing oxides

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Complex perovskite-related cobaltates with Co^{3+}cations exhibit excellent electrocatalytic properties in the oxygen reduction reaction and are considered as prospective cathode materials in intermediate temperature solid oxide fuel cell (IT-SOFC) [1]. However, they suffer from high thermal expansion coefficient (TEC) due to thermally activated transition between low (LS) and high-spin (HS) state of Co^{3+}. In the present work, we discuss influence of this transition on the high-temperature thermal expansion properties of perovskite-related Co-containing oxides.

$Pr_{2-x}Sr_xNi_{1-x}Co_xO_{4-d}$(x = 0.25; 0.5; 0.75) oxides with the tetragonal K_2NiF_4-type structure have been prepared. Room-temperature neutron powder diffraction (NPD) study of x = 0.25 and 0.75 phases together with iodometric titration results have shown the formation of hyperstoichiometric oxide for x=0.25 (d=-0.09(2)) and a stoichiometric one for x=0.75. High-temperature X-ray powder diffraction (HT XRPD) showed substantial anisotropy of the thermal expansion coefficient (TEC) along the a- and c-axis of the crystal structure, which increases with increasing the Co content from TEC(c)/TEC(a) = 2.4 (x= 0.25) to 4.3 (x=0.75). High-temperature NPD (HT NPD) study of the x = 0.75 sample reveals that a very high expansion of the axial (Ni/Co)–O bonds (75.7 ppm K^{-1}in comparison with 9.1 ppm K^{-1} for equatorial ones) is responsible for such behaviour, and is caused by a temperature-induced transition between low- and high-spin states of Co^{3+} [2].

One of the ways to decrease TEC of cobaltates is to stabilize HS Co^{3+}in the ground state. Such compounds can be found among cobaltates with the brownmillerite-type structure. NPD at 2K together with soft X-ray absorption spectroscopy at the Co-$L_{2,3}$ edges studies showed the presence of HS Co^{3+}in the ground state in CoO_6 octahedra of $Sr_2Co_{1.2}Ga_{0.8}O_5$ with the brownmillerite structure [3]. This cobaltate is found to possess as low TEC as 13.1 ppm K^{-1} (298-1073K).

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Lithium diffusion pathways in modern solid state Li conductors

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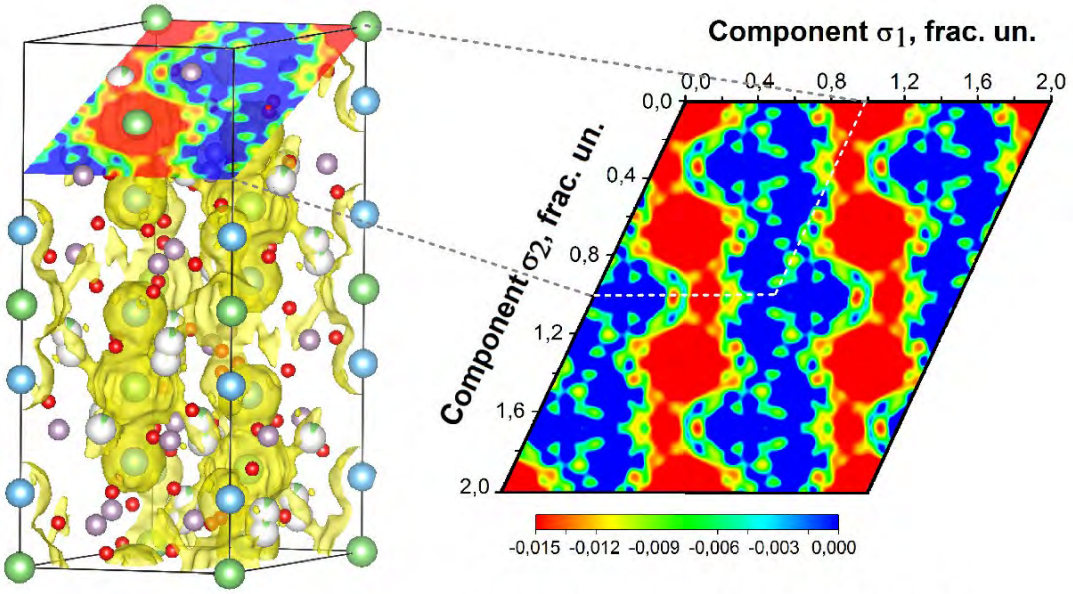
The rapid development of energy storage media permanently requires new electrode and electrolyte materials, which are cheaper, more stable\robust and have better electrochemical performance. To large extent the electrochemical energy storage and energy conversion are diffusion-based processes, where the knowledge about underlying diffusion pathways and mechanisms becomes crucial and indispensable. Unfortunately the information about preferable diffusion pathways of polycrystalline (non-cubic) materials can hardly be obtained by bulk (e.g. resistivity, impedance spectroscopy, quasielastic neutron scattering *etc*) or local measurements. Theoretical methods for prediction of diffusion pathways are often based on molecular dynamics simulations (either force-field or *ab initio*), which creates sufficient computational challenges for the modelling of diffusion properties of new materials.



3D lithium diffusion pathway in LATP - $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ [3]

On the other hand the diffusion processes in a material are determined by its crystal structure, and there are several methods to predict the preferred ion diffusion pathways with high reliability on the basis of the underlying crystal structure or more specifically the corresponding scattering density maps (electron for X-ray and nuclear ones in the case of neutrons). Their analyses in terms of probability density function from anharmonic refinements of diffraction data and/or the reconstruction of electron/nuclear densities by maximum entropy method. The latter approach has been found more robust (better performing) in the case of powder-averaged diffraction data capable to probe weak structural disorder. In the current contribution the application of high-resolution neutron powder diffraction along with the data analysis by maximum entropy method will be reported for the series of promising lithium conductors ($Li_2B_4O_7$ [1], $Li_7La_3Zr_2O_{12}$ [2], $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ [3], $Li_{10}GeP_2S_{12}$ [4], β-Li_3PS_4 [5] etc).

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Magneto-Structural Relationships in 4d and 5d Oxides.

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Oxides containing second and third row transition metals with partially occupied d-orbitals are of interest due to their novel magnetic properties and potential applications. The oxidation state of the cation confers a nominal spin, S, which can be strongly modified by spin-orbit coupling. The ground state is further influenced by the on-site Coulombic interaction (U) and bandwidth (W) both of which are sensitive to the symmetry of the cation. Crystallography, and in particular neutron diffraction, plays a critical role in establishing precise and accurate structures for Ir and Os oxides and in determining their magnetic structures.

Ru, Ir and Os from double perovskites of the type A_2YMO_6, where A = Ba or Sr [1-3]. Structural studies of solid solutions of the type $Ba_{2-x}Sr_xYMO_6$ demonstrate three series exhibit the same sequence of structures with the symmetry lowering from cubic to monoclinic associated with increased tilting of the corner sharing octahedra induced by increasing the amount of the smaller Sr cation present. Magnetic susceptibility measurements between 2 and 300 K for the Ir oxides showed no evidence for long range magnetic ordering, an observation that was supported by neutron diffraction measurements, rather strong spin-orbit coupling results in a Jeff = 0 ground state .

Conversely the Ru and Os oxides are magnetic. Magnetic susceptibility measurements of the Os show a well-defined maximum corresponding to an antiferromagnetic transition for all compositions. The Neel temperature decreases from 74 to 54 K as the Ba content, and hence symmetry, is increased. The observed magnetic moment is insensitive to the precise Ba content but is significantly reduced from that expected a half-filled t^2g^3 electron configuration, from 3.87 to ~ 3.0 μβ due to the combined effects of spin-orbit coupling and covalency.
The structures and magnetic properties of these and related Ru, Ir and Os oxides will be discussed.

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In situ investigation of hydrogenation reactions by neutron powder diffraction

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Time-resolved *in situ* investigations are very useful for unveiling basic steps of hydrogen uptake and release. They are of fundamental importance for many technologically relevant processes, e. g. hydrogen storage, the HDDR process (hydrogenation-decomposition-desorption-recombination) for the production of magnetic materials or hydrogen embrittlement of metals and alloys. For time-resolved solid-gas reactions we constructed a gas pressure cell for elastic neutron diffraction. By proper orientation of a single-crystal sapphire tube as sample holder, Bragg peaks from the container material can be completely avoided, thus yielding high quality powder diffraction data with very clean diffraction background and enabling the extraction of high precision crystal structure data [1]. Gas pressures up to 30 MPa (hydrogen and inert gases) may be applied and heating is provided by a two sided laser heating system. The potential of the gas pressure cell is demonstrated by *in situ studies* of the reaction of solids with hydrogen, which yield detailed models of the reaction pathways. Examples include lithium nitride, Li_3N [2], palladium-rich compounds [1, 3], Zintl phase hydrides [4, 5], and lanthanide based magnetic materials [6].

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Understanding the microscopic origin of oxygen diffusion in ion conductors with complex structure

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Oxygen ionic conductors are materials of fundamental interest for the development of ambient temperature working devices for energy conversion, such as solid oxide fuel cells (SOFC).

Understanding the microscopic conduction mechanism in these materials in relation to their structural characteristics is a key requirement for improving their properties through smart design. Promising materials often adopt complex structures where interconnected polyhedra with different coordination coexist or where partial substitution of cations leads to increased defectivity.

Quasi-elastic neutron scattering experiments, coupled with ab-initio molecular dynamics simulations, give the unique chance to unveil several important parameters of the microscopic mechanism of diffusion, such as the preferred diffusion pathways, the timescale and activation energy of the diffusion process and the possible coexistence of different dynamical phenomena.

This presentation deals with recent results on $Bi_2La_8Ge_6O_{27}$ apatite [1,2], La_2MoO_9 [3] and $Bi_{0.913}V_{0.087}O_{1.587}$ [4] systems, including the observation of oxygen long-range diffusion by QENS on the longest timescales reported to date.

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Recent Advances in Molecular Spectroscopy at the ISIS Pulsed Neutron & Muon Source

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The past few years have been a vibrant period for the *Molecular Spectroscopy Group* at the *ISIS Pulsed Neutron & Muon Source* [1], with an increasing emphasis on the use of neutron spectroscopy across chemistry and industrial R&D [2]. This contribution summarises & illustrates major projects already completed with success or well underway, including: a new guide on TOSCA [3]; upgrades of the secondary spectrometer on OSIRIS [4]; new capabilities on VESUVIO for broadband spectroscopy [5]; the extensive use of computer simulation & high-performance computing [6]; or the development of new equipment for *in-situ* and *operando* studies under realistic conditions [7]. Envisaged developments in the horizon seek further order-of-magnitude gains, and range from a major upgrade of the TOSCA secondary [8]; a boost in flux on OSIRIS [4]; or ETNA, a new station for Epithermal & Thermal Neutron Analysis [9]. All of these have been underpinned by extensive neutronic-characterisation efforts [4,10]. This exercise has provided much-needed insights into the forthcoming upgrade of *Target Station I* at ISIS, new neutronic materials & methodologies [11], or the design of next-generation spectrometers such as VESPA at the ESS [12]. We have also seen a marked increase in the use of direct-geometry spectrometers such as MAPS and MERLIN in new areas of research such as catalysis or archaeometry, with the growing involvement of academic consortia & industry [13]. Our global community [14] has also evolved beyond recognition, as illustrated by a growing number of initiatives [15] or the routine use of more agile access mechanisms [16] and databases [17], all resulting in a substantial & sustained increase in research outputs. As an overarching theme, this presentation also provides an overview of our experience to date in nurturing new communities, including lessons learnt & ways forward [18].

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Neutron Depth profiling at a focused neutron beam: a method of choice to study Li-ion transport in solid state batteries

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In operando observation of Li-ions transport in all-solid-state thin-film batteries during fast dis/charge cycling, as well as the study of mechanisms of battery aging (e.g. formation of interfaces) become possible with *operando* Neutron Depth Profiling (NDP).

For this aim we have recently built and tested a new NDP spectrometer at JCNS. New spectrometer utilizes a focused cold neutron beam of the beamline MARIA (MLZ, Garching) and is equipped with the multi-detector setup for more effective collection of charged particles. This arrangement allows for sufficiently high counting rates necessary for fast, about tens of seconds, measurements of battery samples with the requirement of a fine, of an order of 10 nm, depth resolution. Results of the first test measurements of full and half-cell solid state batteries in “as deposited“ state will be presented.

MAGNETO-STRUCTURAL CORRELATIONS, THERMAL EVOLUTION, IONIC CONDUCTIVITY AND CATALYTICAL ACTIVITY FOR THE PET GLYCOLYSIS OF THE (trimim)[FeCl4] HALOMETALLATE COMPOUND

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Group 8th halometallate compounds based on imidazolium cation display interesting properties, including strong Lewis acidity [1], single-crystal-to-single-crystal transitions [2], paramagnetism with the presence of tridimensional magnetic ordering [3,4] and fascinating applications in relevant catalytic processes [where they are well-represented in reactions of petroleum refining and processing and in the glycolysis of poly(ethylene terephthalate) (PET)] or electrochemistry. [5-7] Among these compounds, we present a novel halometallate compound, based on 1,2,3-trimethylimidazolium (trimim) cation and tetrachlorideferrate(III) anion. It has been characterized by thermal analysis, magnetic susceptibility and ionic conductivity measurements and by X-ray and neutron diffraction techniques.

In this communication, we will present the crystal structure determination, the temperature dependence, the ionic conductivity, the catalytic performance in the glycolysis of PET and the low temperature magnetic structure of the title compound. This material presents three different crystal structures from 2 to 400 K, which were refined by synchrotron X-Ray and neutron powder diffraction. The three of them are built up by layers of cations and anions stacked upon one another in a 3D configuration, with several non-bonding interactions: hydrogen bond, anion-π, and halide-halide. The magnetic susceptibility and heat capacity measurements indicate the existence of long-range antiferromagnetic ordering at approximately 3 K, compatible with the occurrence of a propagation vector **k**=(0, 0, 0). The magnetic structure was solved on the magnetic space group *P21/c*', and suggests that the 3D magnetic ordering takes place via Fe-Cl---Cl-Fe magnetic pathways, displaying a stronger superexchange magnetic interaction between the planes, in agreement with other similar compounds previously studied. [2,3]

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Structure and Dynamics of Intrinsically Disordered and Unfolded Proteins: Insights Gained by Neutron Scattering

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A general property of disordered and unfolded proteins is their structural expansion that results in a high macromolecular flexibility. Structural properties of disordered proteins in solution have been investigated using small-angle neutron scattering (SANS) [1,2]. In particular, SANS data allowed us to determine the underlying chain distribution statistics of the disordered proteins. Dynamics of disordered proteins from the picosecond to several nanoseconds on a local length-scale was investigated using quasielastic incoherent neutron scattering (QENS) [3]. Neutron Spin-Echo spectroscopy (NSE) on the other hand, offers the highest energy resolution in the field of neutron spectroscopy and enables us to study slow collective motions in disordered proteins up to several hundred nanoseconds and in the nanometer length-scale [1,2]. In my presentation, I will summarize recent QENS and NSE results on the dynamics of the intrinsically disordered myelin basic protein (MBP) and the chemically denatured bovine serum albumin (BSA) (1,2,3). Using NSE experiments, we observed a high internal flexibility of the intrinsically disordered MBP and the denatured BSA in addition to centre-of-mass diffusion detected by dynamic light scattering. Internal motions measured by NSE were described using concepts based on polymer theory. The contribution of residue-solvent friction was accounted for using the Zimm model including internal friction (ZIF). Disulphide bonds forming loops of amino acids of the peptide backbone have a major impact on internal dynamics that can be interpreted with a reduced set of Zimm modes.

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Nanostructured lipid carriers for fish oil - A small angle neutron scattering study

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Fortification of foods with essential functional lipids such as omega-3 polyunsaturated fatty acids (PUFAs), beta-carotene and vitamin A are of key importance for health and well-being. omega-3 PUFAs are essential for the human diet to support a good brain and cardiovascular health. Furthermore, they lower the risk of other diseases such as type 2 diabetes and inflammatory disorders. Vitamin A and its precursor beta-carotene are important for growth and development, good vision and immune functions. Integrating such chemically unstable compounds into food products and delivering them into the human body requires encapsulating them into a carrier system. This improves their water-dispersibility and protects them from lipid oxidation.

Recent studies [1-3] show that lipid oxidation of omega-3 PUFAs reduced significantly when incorporated into a solid tristearin matrix, a so called nanostructured lipid carrier, when sufficient amounts of tristearin is added to the samples and lecithin with a high phase transition temperature and bile salts or *Quillaja* saponins are used as emulsifiers. From this observation it is anticipated that during the cooling process the emulsifier molecules at the lipid-water interface promote a co-crystallization of the lecithin chains with the tristearin via heterogeneous interfacial nucleation. The crystallized tristearin limits the mass transport of reactive agents which reduces lipid oxidation of the encapsulated fish oil.

However, the structural composition of such nanostructured lipid carrier particles is still unclear. Does the crystallized tristearin form a shell around a single fish oil core or is the fish oil embedded as smaller islands in the tristearin particle matrix?

To study the morphology of the particles and especially their internal structure small-angle neutron scattering (SANS) was used. Samples with different fish oil : tristearin ratios (60:40, 40:60, 20:80) were studied. Using mixtures of H_2O and D_2O for the dispersion medium and mixtures of tristearin and its fully deuterated analogue, three different neutron scattering contrasts are realized, allowing to highlight the spatial distribution of both fish oil and tristearin alone and as a combination in the lipid particles.

A first analysis of the SANS data showed that it does not match a model of core-shell particles. Thus the particles have either a different inner structure or particles with other structures coexist with the core-shell particles. To facilitate the structural modeling of the SANS data, we recently started to collect cryo-TEM and freeze-fracture TEM images of the samples. So far the TEM data suggests particles with a wider range of inner structures. Besides particles with a potential core-shell structure, also particles with an inverted structure where tristearin crystals are surrounded by fish oil, are present in the samples. In samples with a high fraction of tristearin clusters of tristearin platelets are found as well. The next step and part of the presentation is to analyse the SANS data by a model which combines these differently structured particles.

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Photosynthetic membranes in live cells and organelles studied using SANS

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Photosynthetic cells and organelles contain thylakoid membranes comprised of molecular-scale light harvesting complexes and photosystems. Autotrophs use these for converting sunlight to chemical potential and for storing this harvested energy as carbohydrates. Understanding and harnessing this environmentally benign process has many exciting possibilities including as a 'green' friendly means of splitting water[1], or a means for producing small useful molecules[2]. Advancing our understanding of the molecular structure and mechanistics in the photosynthetic apparatus continues to have broad biotechnological appeal. Small angle neutron scattering (SANS) from actively metabolising cells[3]and organelles provides a unique 'view' of the photosynthetic membrane structures in the live state. A typical SANS experiment samples a large membrane surface and so gives excellent statistics that complement methods like electron microscopy that typically have higher resolution, though see far less membrane volume usually in dead cells. The scattering curves typically feature various peaks or shoulders superimposed on a Porod-like power law function. Here we discuss approaches to optimal SANS data acquisition from photosynthetic membranes and analysis of the scattering curves. The features in the SANS curve may be assigned as repeat structures (Bragg peaks), or membrane form factor scattering. Analysis of the internal structure of photosynthetic cells and organelles using SANS requires a careful integration of real-space (microscopic) information.

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Small angle neutron scattering study of protein-lipid co-assembly

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Alpha synuclein is a 140-amino acid (ca. 14.5 kDa), intrinsically disordered protein that is naturally present in brain cells. Under certain circumstances, alpha synuclein self-assemble into long, insoluble fibrils, which are the main component of so-called Lewy bodies, deposits found in brains of people diagnosed with Parkinson's disease. Together with alpha synuclein fibrils, Lewy bodies also have been found to contain a significant amount of lipids. For this reason, investigation of alpha synuclein-lipid interactions has received significant attention in recent years. In this work, alpha synuclein was allowed to aggregate into fibrils in the presence of lipid bilayers of different lipid content and charge. Experiments were performed at pH=5.5, close to the protein's isoelectric point. At this pH the fibrils are not colloidally stable, but aggregate further into dense clusters, that are characterized by a fractal dimension D=2.5-3. These fibril clusters sediment. Small angle neutron scattering was used to characterize the formed fibrils after re-dispersion, and also after washing with additional buffer. For the different systems studies, data indicate that in the case when lipids do sediment together with the fibrils, they mainly adsorb to the fibril surface and can be washed away.

OBSERVING A CELLULAR PROTEIN UNFOLDING AND DEGRADATION MACHINE AT WORK: A TIME-RESOLVED SMALL-ANGLE NEUTRON SCATTERING STUDY

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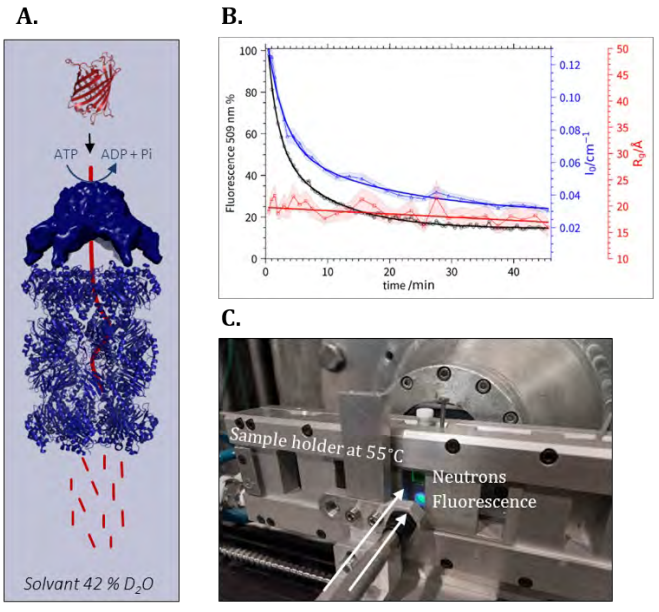
The correct regulation of protein degradation is of major importance for biological cells. A dysfunction of protein degradation can seriously impair cellular function. A key player in the protein degradation process is the proteasome, a large protein complex found in the majority of living organisms (eukarya, bacteria and archaea). In particular, the archaeal proteasome is composed of a catalytic particle, the 20S proteasome, which degrades proteins that are unfolded by a regulatory complex, the Proteasome Activating Nucleotidase (PAN). PAN regulates the access of proteins into the 20S proteasome and controls its activity by unfolding and preparing protein substrates for their translocation and degradation inside the catalytic particle.

Besides its simplicity in terms of subunits, the important thermal and structural stability of this archaeal machinery offer major advantages for the study of the structure-function relationship with biophysical techniques such as Small-Angle Neutron Scattering (SANS). Thus, the archaeal machinery represents a good working model for the study of molecular machines of protein degradation.

Here I will present a novel approach combining SANS, deuterium labelling and contrast variation with online fluorescence spectroscopy in order to obtain insights into the unfolding and degradation process of a model substrate, the Green Fluorescent Protein (GFP) [1]. By using a proteasome from the thermophilic organism M. jannaschii the reaction was thermoactivable at 55°C and the unfolding and degradation process could be tuned and slowed down with respect to the in vivo conditions of 100°C.



Proteolytic machinery as studied by time-resolved SANS coupled with fluorescence measurement

A. *Artist's view of the studied system with deuterated GFP unfolded and subsequently degraded by hydrogenated PAN and 20S catalytic particle in a 42% D_2O solvant.*

B. *Evolution over time of the GFP fluorescence at 509 nm, forward scattering I_0 and radius of gyration R_g of deuterated GFP is in presence of hydrogenated PAN and 20S catalytic particle. The reaction was measured at D22 beamline (ILL).*

C. *Sample environment installed on D22 beamline (ILL).*

The results provide new structural and kinetic insights into the mecanism of molecular machines of protein degradation during the active unfolding and degradation process, at a time resolution of 30 seconds.

Acknowledgements

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Low-pH and desiccating induced reorganizations of thylakoid membranes - as revealed by small-angle neutron scattering

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Small-angle neutron scattering (SANS) is a suitable technique to monitor the structural flexibility of the thylakoid membrane system in oxygenic photosynthetic organisms. These membrane systems, which are assembled into multilamellar layers, accommodate virtually all photosynthetic light reactions. In recent years, SANS measurements have contributed significantly to better understand important regulatory mechanisms in cyanobacteria, algae and vascular plants. Two topic will be presented: (i) reversible membrane desorganizations associated with a novel energy-dissipation mechanism in cyanobacteria, and (ii) the low-pH induced reversible changes in the periodic organization and mosaicity of thylakoid membranes, mimicking the in vivo acidification of the lumenal aqueous phase - activating the photoprotective non-photochemical quenching (NPQ) regulatory mechanism in excess light.

The photosynthesis of the desiccation-tolerant desert cyanobacterium (*Leptolyngbya ohadii*) can be recovered immediately in predawn dew deposition, even though they are in desiccated state most of daytime. The thylakoid system in hydrated cells is multilamellar (one diffraction peak with two additional, higher harmonic peaks in the SANS profile), whereas desiccated cells do not display diffraction peak, only a broad shoulder (Fig. 1). Based on these SANS results and other structural and functional measurements, a novel energy-dissipation mechanism has been proposed, aggregation of the light-harvesting antenna complexes [1].

We have shown that periodic order and lamellar repeat distance of isolated thylakoid membrane exposed to low pH is decreased. At the same time, the mosaicity of the membranes is increased. These reorganizations are largely reversible upon readjusting the pH. It is interesting to note, that these structural changes resemble to a considerable extent to the light-induced changes in intact leaves, upon the build-up of the transmembrane electrochemical potential gradient for protons [2].

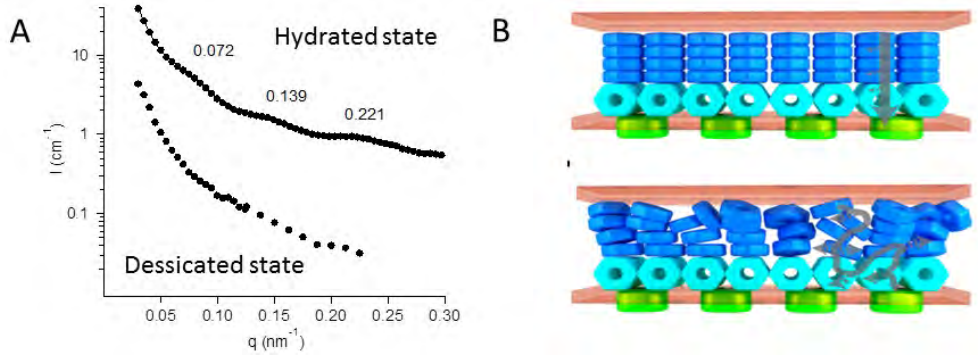

Fig. 1. Radially averaged SANS curves (A) and schematic figure (B) of cyanobacterial thylakoid membranes showing the external light-harvesting antenna proteins, the phycobilisomes in hydrated and desiccated states [1].

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Monitoring food structure during digestion using small-angle scattering and imaging techniques

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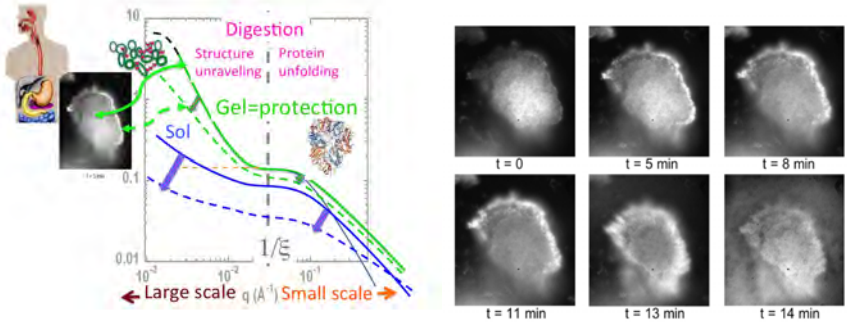

Various studies have shown that food structure has an impact on digestion kinetics. We focus here on the effects of gastric and intestinal enzymes (in-vitro digestion) on two canola seed storage proteins, napin and cruciferin. To monitor structure effect we conducted experiments on gels of these proteins at different pHs, yielding different structures and elastic modulus. What is new is to get information on the mechanisms at the lowest scales, using imaging and radiation scattering at large facilities: Synchrotron fluorescence microscopy, X-Ray scattering, at SOLEIL synchrotron, and Small-Angle Neutron Scattering, at Laboratoire Léon Brillouin reactor. We can identify the mechanisms at each step and in two distinct scale ranges, observed simultaneously, the one of the individual protein scale and the one of the structure connectivity:

- during gelation individual canola proteins are not deeply modified in comparison with their state in solution ; larger scale gel heterogeneity appears due to connectivity or aggregation
- in the gastric step (up to 40 min):
  - o at short scale (large q) we see that the proteins disintegration is much slowed down in gels than in solutions, particularly in the gastric phase;
  - o at larger scales (low q), we see that the gel structure is also self-resistant to the action of the enzyme (pepsin).
- in the intestinal step, such kinetics differences hold until major disintegration after no more than 15 min.

Insights into lipid membrane dynamics from neutron scattering

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Lipid membranes undergo a wide array of dynamic transformations that are essential to cell function. These hierarchical dynamics span several decades in length and time scale, ranging from the rotation and diffusion of individual lipids to undulations of micron-sized patches of the membrane. Accessing the necessary length and time scales to study bilayer fluctuations can be experimentally challenging; however, over the past decade, neutron spin echo spectroscopy (NSE) has proven to be a unique tool for capturing the collective membrane dynamics on the nanometer and nanosecond scales. This talk will highlight new insights into the effects of lipid structure on membrane bending and thickness fluctuations gained from NSE. We will demonstrate how subtle changes in lipid composition, such as mixed tail lengths or charged headgroups, can have significant and unexpected effects on the membrane elastic properties. Together these results illustrate the importance of lipid diversity and composition in tuning the rich structure and dynamics of biological membranes.

Pressure effects on the protein dynamical transition

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The Protein Dynamical Transition (PDT) consists in a steep increase in the temperature dependence of the flexibility of proteins occurring at about 200K. One of the most powerful techniques for its investigation is incoherent neutron scattering, which can give a measure of the Mean Square Displacements (MSD) of the non-exchangeable protein hydrogen atoms, as firstly shown by Doster and co-workers in 1989 [1]. The biological relevance of PDT has been pointed out and its physical origin has raised debates in the literature, still being an open question today [2-6]. Studies of protein structural dynamics in general, and of the PDT in particular, as a function of pressure would be highly desirable both to help clarifying its physical origin and from a more biological point of view, since many biological systems live at high hydrostatic pressure.

Very few studies have addressed the problem of the pressure dependence of protein dynamics as studied with neutron scattering, and most of them have been concerned with samples in solution investigated near room temperature [7,8]. Studies on the pressure dependence of the PDT on protein systems are lacking, probably because of the relevant experimental challenges.

We report here on the temperature dependence of the MSD of Myoglobin (Mb) in an ultraviscous mixture of protein/D8-Glycerol/D_2O [9], in the temperature range 20-300K, and at different pressure values, from ambient pressure to 5 kbar. Data have been analysed within a double well potential model and show a significant reduction of protein dynamics with increasing pressure up to 2 kbar; a sudden MSD increase is observed between 2 and 3 kbar, likely related to protein pressure induced denaturation. However, the pressure effect decreases the MSD amplitude without altering the PDT onset temperature. Implications of these findings to the Mb energy landscape will be discussed.

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Protein Domain Motions as seen by Neutron Spinecho Spectroscopy

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The biological function of proteins is often related to large-scale domain motions, which are induced or suppressed by the binding of a substrate or due to cosolvents. Domain motions can be related to soft hinges, flexible linker regions or -as in the case of intrinsic unfolded proteins- be native to the unfolded protein structure. These large-scale domain motions in solution cannot be observed by X-ray crystallography or NMR spectroscopy. Small angle scattering by X-rays or neutrons in combination with neutron spin echo spectroscopy (NSE) in solution can be used to observe configurational changes and equilibrium dynamics between functional domains on 1-100 nanosecond timescale.

I present here examples for different types of motions related to the structure of proteins and bioconjugates. Phosphoglycerate kinase shows a clear hinge motion between the main domains. PEGylation seems not to influence domain motion but adds additional internal dynamics in the protein-polymer complex. Immunoglobulin 1 (IGG1) presents some strong dynamics due to the short linkers connecting the Fc with the Fab domains.

Relevant forces and friction will be discussed in terms of the Ornstein-Uhlenbeck process.

In-plane dynamics of phospholipid membranes

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We investigated the existence of long-range excitations and correlated structures in phospholipid membranes by means of grazing-incidence neutron spin echo spectroscopy, grazing-incidence small-angle neutron scattering, and corresponding theoretical calculations inspired by smectic-membrane theory. These films serve very well as model systems for biological membranes.

All these methods confirmed the existence of thermal excitations along the surface of the phospholipid membranes. Also, these measurements revealed a temperature dependence of these excitations. These excitations are associated with 100 nm in plane correlations around physiological temperatures and of 75 nm at 16°C. A single excitation has an energy around the µeV-regime. The temperature series revealed a high activity at physiological temperatures and pronounced long-range in-plane structures, which are strongly suppressed at temperatures below 20°C. From the length-scales and energy transfers involved we surmise that these excitations may play a role in several functions of the cell membranes such as stability and energy dispersion along the membrane. From a fundamental point of view, the observed behavior of those excitations is congruent with that of a quasi-particle (surface mode phonon, smomon) that exists in the plane of phospholipid membranes.

In our investigation we could prove the existence of the aforementioned dynamics[1], describe the corresponding structure[2] and back up those measurements with computed results[3]. We therefore understand those in-plane correlations to act on in-plane structures in the length-scales as described above. Here we have to stress that both the structure and dynamics are strictly in-plane and do not have any out-of-plane contributions, which also explains why they have not been reported before, as they usually are averaged out and suppressed by the stronger out-of-plane signal in phospholipid membranes.

The corresponding calculations moreover illustrate that these dynamics, and therefore the resulting structures, are a direct result of the planar structure and mechanical properties of the phospholipid membranes. This also opens up other avenues of research, where the possibility of investigating otherwise inaccessible properties of the phenomena directly, like the in-plane viscosity as well as the behavior at rigid surfaces.

Due to the correlating time and length-scales we can hypothize that these dynamics and structures are contributing to the biological functions of phospholipid membranes. The dynamics transport energies as expected in biological membranes and the length scales are on the scale of micro-organisms or single cells. Thus, the excitations could prove to be a possibility to disperse energy inside the membrane and thereby preventing cells from damage by external mechanical stimuli as opposed to the situation when a localized stimulus is not dissipated and ruptures the membrane. The same could be true for transport along the membrane surface. Another hint at their biological relevance is the high abundance of the excitations and the characteristic structures at physiological temperatures as well as their strong suppression at lower temperatures, which goes analogue with biological activity.

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Compression of flexible chain due to macromolecular and its biological implications.

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The importance of crowding in biology is being increasingly appreciated. In particular, its effect on the conformation of flexible macromolecules has been a subject of numerous studies in the past decade. This subject is a matter of interest experimentally, numerically and theoretically because of the ubiquitous nature of macromolecular crowding in living systems and its influence on flexible molecules is relevant to the understanding biological problems like, for example, protein stability [1], RNA folding [2] or genome compaction [3]. Neutron scattering, with its ability to stain molecules and make their signal visible although at very low concentration with respect to the high concentration of crowder molecules, give the possibility to follow the conformation of molecules as function of crowder concentration that are matched. We have applied this method nearly a decade ago to measure the change of conformation of Gaussian chains when increasing the presence of other molecules and have observed a reduction of the radius of gyration (Rg) of nearly 50% at physiological concentration [4], after extrapolation to zero polymer concentration (Zimm plot) to get ride of a small aggregation. The compression of the flexible molecule has a very strong dependence on the size ratio lbetween the chain and the crowder [5]. This study was questioned by recent study by NMR and neutron scattering [6], motivated by some other papers that predict a limited effect of macromolecular crowding on chain compression when l≈1 [7]. The authors suggest that we are not below the overlap concentration and thus our extrapolation is not valid. We have shown that this claim is not relevant [8].

In this presentation, we will in introduce the importance of the biological problem and will present some new results on flexible molecules change of conformation due to macromolecular crowding.

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Amyloid β-peptides interaction with model membranes: when dynamics matters

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The amyloid β-peptide (Aβ) interacts with membranes of cells in the human brain and is associated with Alzheimer's disease (AD). Hence, the understanding of Aβ influence on the structure [1] and on the dynamical features of model membranes is a crucial molecular challenge [2].

We present the results of a neutron-scattering study on the interaction of large unilamellar vesicles, as cell membrane models, with both freshly dissolved Aβ and early toxic prefibrillar oligomers [3].

By Small Angle Neutron Scattering we compared the structural features of model membranes in presence of Aβ species in different aggregation states, and by Neutron Spin Echo we investigated their dynamical behaviour. In addition, we explored by both the techniques the effect of coincubating the Aβ-peptide with the chaperonin Hsp60, which is known to strongly interact with

it in its aggregation pattern.

Although Small Angle Neutron Scattering spectra did not reveal meaningful structural differences between the investigated samples, Neutron Spin Echo results clearly proved the existence of a noticeable interaction between model membranes and both freshly dissolved and aggregate Aβ species. Membrane stiffness increases after Aβ is released in solution. On the other side, the presence of even very low amounts of Hsp60 maintains unaltered the elastic properties of the membrane bilayer.

These results can be related to the ability of the chaperonin to interfere with Aβ aggregation, by the specific recognition of an Aβ-reactive transient species. In addition, in a freshly dissolved Aβ solution there are species already able to critically modify membrane dynamics.

Hsp60, according to our results, is capable to assist to misfolding events, playing the suitable role of a chaperonine escaping the onset of the aggregation cascade and the consequent insult on the cellular membrane.

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Nanosecond dynamics of biopolymers: a comparative neutron spin echo study on folding intermediates of apo-myoglobin

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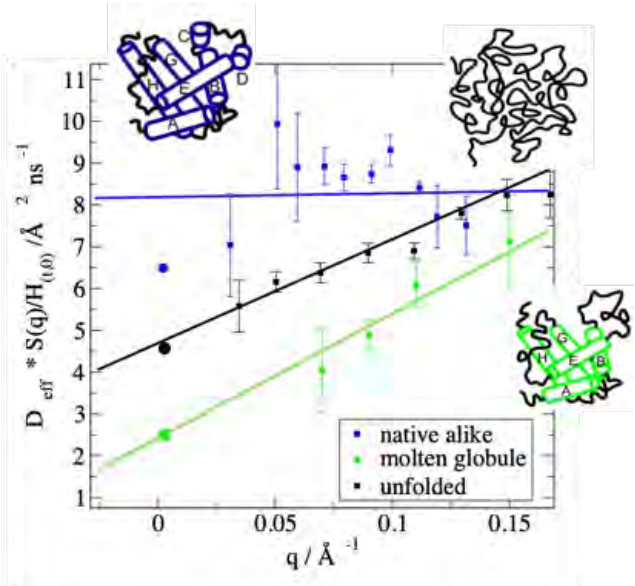
During protein folding different intermediate states occur with varying content of secondary structural elements. To characterize their internal dynamics, we prepared apo-myoglobin in different folded states [1,2]. Its unfolded, folded and partially folded (molten globule) forms were investigated using neutron spin echo spectroscopy (NSE). Information on the form and structure factor was obtained by small angle scattering (SAS). Aggregation state and centre of mass diffusion were monitored in parallel and in particular cases, also in situ, with dynamic light scattering (DLS). The SAS and DLS data account for interparticle and hydrodynamic interactions and were used to "correct" the effective diffusion coefficients measured by NSE [3,4]. Whereas the dynamics of the folded protein is dominated by centre of mass diffusion, the unfolded protein and the molten globule state show a Gaussian polymer-like behaviour. This indicates that powerful polymer models e.g. Zimm and Zimm with internal friction can be used to describe such protein systems.



q- dependency of the corrected effective diffusion coefficient obtained from the initial slope of the NSE spectra investigating for the different folding states. The lines are a guide for the eye.

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High-resolution neutron scattering data reveal the decoupling of proteins and water at the dynamical transition

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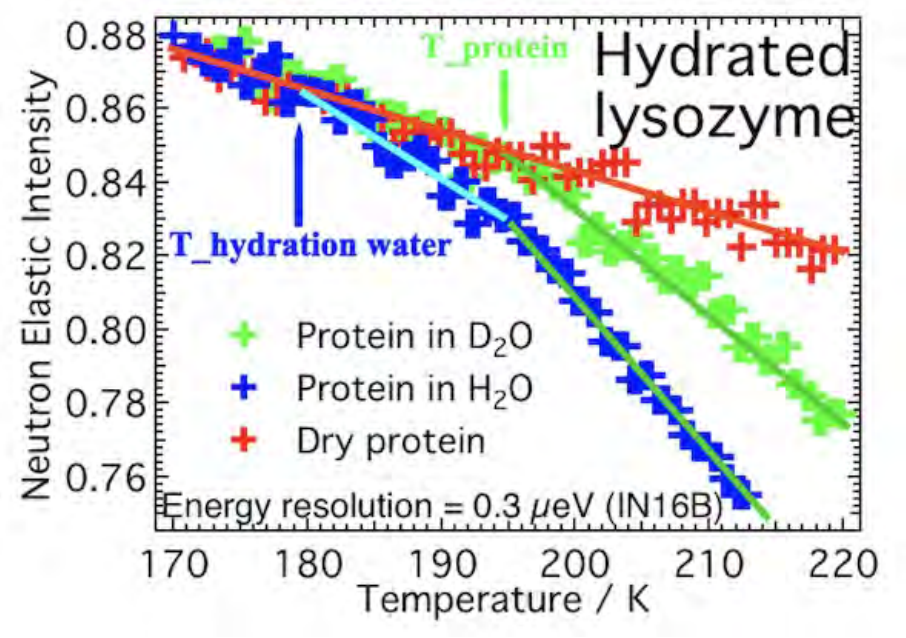
The dynamics of a model protein (Lysozyme) and its hydration water have been investigated by neutron scattering at very high-energy resolutions, up to 3 times better than the best ones used until now (0.3 ueV versus 1 ueV). Because of this improvement, I was able to measure the decoupling between water and protein dynamics in proximity of the protein dynamical transition [1]. This decoupling, never observed before, is a clear sign that the transition in the dynamic of hydration water does not directly drive a corresponding change in the dynamic of proteins. As a result, the scenario generally accepted during the last 30 years has eventually been challenged, and a new theory on the connection between these two dynamics and protein function has to be formulated.



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Neutron scattering application for the characterization of the lipid structure of mammalian stratum corneum and drug delivery systems based on the soybean phospholipids

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The advantages of the neutron diffraction and small angle scattering are reported for the two modern problems of pharmacy: drug penetration through the skin and drug transportation to the cell.

Stratum Corneum (SC) lipid matrix is main skin barrier for drug penetration. Model SC membranes were used for the investigation of the main properties of the SC lipid matrix There is a successful (15 published articles) long term (from 2000) cooperation between the Frank Laboratory of Neutron Physics, JINR, Russia and the Pharmaceutical Paculty of Martin Luther University, Halle -Wittenberg, Germany at the research area of the nanostructure of SC lipid model systems using neutron diffraction. On the basis of obtained results, the main request is formulated for the enhancer of the drug penetration through the skin as development of the multiphase state of the SC membrane to increase the lipophilic pathway of the drug diffusion through the skin.

Nanodrugs, developed in the V.N.Orekhovich Research Institute of Biomedical Chemistry (Moscow) from soybean phosphatidylcholine, were characterized via small-angle neutron scattering (SANS). Five different nanodrugs (phospholipid transport nanosystem, phospholipovit, indolip, doksolip, nanoarbidol) at concentrations in heavy water 5%, 10%, 25% and temperatures 20^{o}C and 37^{o}C have stable vesicular morphology. The concept of the critically small vesicle (maximum therapeutic effect) was formulated as vesicle, which internal radius is equal to the bilayer thickness. It was shown by SANS that application of the soybean phospholipids with trademark S80 (components: phosphatidylcholines 73-79%, phosphatidylethanolamenes 7%, lysophosphatidylcholines 5%) has crucial importance for the formation critically small vesicles. Application of the more purified (and more expensive) soybean phospholipids with trademark S100 (phosphatidylcholines content 95%) does not lead to the formation of the critically small vesicles. Vesicles based on soybean phospholipids with trademark S100 are small vesicles (their internal radius about three times larger relative to the lipid bilayer thickness of the soybean phospholipids).

It is well known that therapeutic effect from nanodrugs application increases at the decrease of the vesicle radius. Critically small vesicles of the nanodrugs have maximum therapeutic effect at the minimal cost.

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Logarithmic fractal structure of the large-scale chromatin organization in the interphase HeLa nuclei

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All information about biological organism is written in the double-helix DNA consequence. Although DNA macromolecules extend up to few meters in unraveled condition, they are packed really tight in the nucleus. One of the most exciting question that scientists are trying to answer is how are meters of DNA packed inside the 1-10-μm diameter nucleus of a cell. Nowadays the concept of the fractal organization of chromatin appears to be one of the most productive hypotheses that, however, is not well established yet. In the present investigation we report on the two-scale fractal structure of the chromatin organization in the nucleus of the HeLa cell. Two neutron scattering methods: small-angle neutron scattering (SANS) and Spin Echo SANS, are used to investigate large scale chromatin architecture. The small-scale fractal level corresponds to the volume fractal with dimension Df = 2.41, while the large-scale fractal level corresponds to logarithmic fractal with correlation function $\gamma(r) \sim \ln(r/\xi)$. The volume fractal is self-similar at different scales, while logarithmic fractal is hierarchically changed upon scaling [1,2]. As a result the logarithmic fractal is more compact than the volume fractal but it still has rather high surface area, which provides accessibility at all length scales. Apparently such bi-fractal chromatin organization is the result of an evolutionary process of optimizing the compactness and accessibility of gene packing. The small-scale volume fractal organization is built to satisfy the necessity of the proteins diffusion. While the large-scale logarithmic fractal is formed under the influence of two factors: proteins diffusion and gene interaction.

The HeLa nuclei tend to agglomerate in time. The long scale logarithmic fractal structure of the large-scale chromatin organization allows HeLa nucleus to penetrate deeply into the adjacent nucleus upon agglomeration process. The interpenetration phenomenon of the HeLa nuclei shows that the chromatin-free space of one nucleus can be occupied not something negligible: it is as big as the volume occupied by the chromatin itself. Free space within nucleus is needed, for example, for a process of the DNA synthesis in order to allows two nuclei to form in the same volume. Interestingly that it is the logarithmic fractal architecture of chromatin that provides comfortable compartment for this most important function of the cell.

The work was supported by the Russian Foundation for Basic Research (grant No.17-02-00313 A).

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Membrane interaction of off-pathway prion oligomers and lipid-induced on-pathway intermediates during prion conversion: a clue for neurotoxicity

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Prion protein (PrP) misfolding is associated with a range of deadly neuropathological diseases - including bovine spongiform encephalopathy and Creutzfeld-Jacob in human - characterized by the accumulation of insoluble proteinaceous aggregates inside the infected tissues [1]. Soluble oligomers of PrP, produced during amyloid aggregation, have emerged as the primary neurotoxic species, instead of the fibrillar end-products. However, whether the membrane is among their direct targets, that mediate the downstream adverse effects, remains a question of debate [2]. Recently, questions arise from the formation of membrane-active oligomeric species generated during the β-aggregation pathway, either in solution, or in lipid environment. In the present study [3], we characterized membrane interaction of off-pathway oligomers from recombinant prion protein generated along the amyloid aggregation and compared to lipid-induced intermediates produced during lipid-accelerated fibrillation. Using calcein-leakage assay, we show that the soluble prion oligomers are the most potent in producing leakage with negatively charged vesicles. The binding affinities and conformational states of the different PrP assemblies were determined by thioflavin T binding-static light scattering experiments on DOPC/DOPS vesicles and FTIR-ATR spectroscopy onto the corresponding supported lipid bilayers. Finally, the modes of interaction of PrP oligomers with supported lipid bilayers were highlighted by specular neutron reflectivity using different contrasts. Our results indicate that the off-pathway PrP oligomers interact with lipid membrane *via* a distinct mechanism, compared to the inserted lipid-induced intermediates (Figure 1). Thus, separate neurotoxic mechanisms could exist following the puzzling intermediates generated in the different cell compartments. These results not only reveal an important regulation of lipid membrane on PrP behavior but may also provide clues for designing stage-specific and prion-targeted therapy.

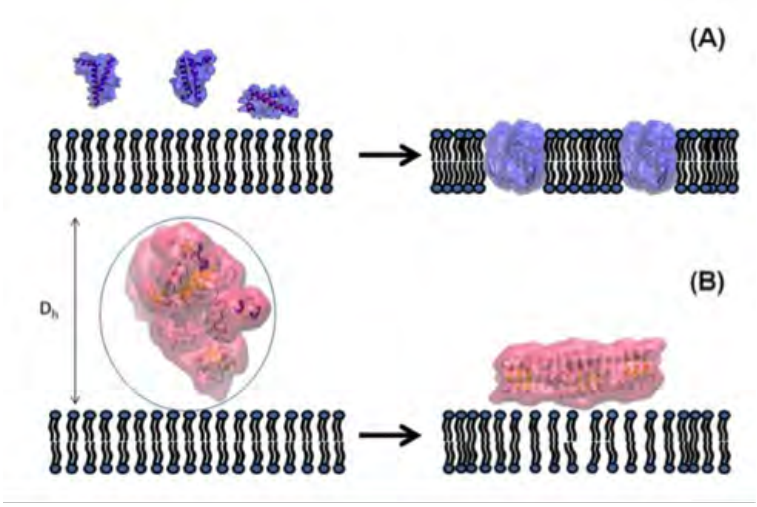

Figure 1. (**A**) Membrane-mediated aggregation of the α- helical monomeric PrP leading to β-sheeted lipid-induced on-pathway oligomers inserted in lipid bilayers and (**B**) interaction of β-sheeted off-pathway oligomers at lipid interface for the purpose of size comparison.

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Structural characterization of rsEGFP2 on-state intermediates using neutron diffraction and time-resolved serial femtosecond crystallography experiments reveal its fluorescent state.

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Fluorescent proteins (FP) have revolutionized life science imaging since the first cloning of the green fluorescent protein in 1992 [1]. Used as genetically encoded markers, they became an invaluable tool to several nanoscopy approaches, allowing for the real-time visualization of *in vivo* biochemical processes such as protein expression, localization and trafficking [2]. Over the last decade, FPs with photo-activation properties have been discovered and optimized to develop new super-resolution light microscopy techniques, among which PALM [3]and RESOLFT [4]are commonly used to dynamically track proteins within living cells. There has been a growing interest for a specific class of photo-activable FPs: the photo reversibly switchable fluorescent proteins (RSFPs)[5]. These proteins have indeed a remarkable peculiarity, as their fluorescence can be toggled back and forth between a fluorescent (on-) and a non-fluorescent (off-) state. This so-called photo-switching needs to be understood in great detail at the molecular level to further improve RSFPs photo-physical properties. Structural investigation performed with X-rays on RSFPs in both their on- and off- states revealed an isomerization of the chromophore upon photo-switching (Figure 1A), and in a recent time-resolved X-ray crystallography at the X-ray free electron laser (XFEL) LCLS (Stanford, USA), we were able to trap the chromophore of the photoswitchable rsEGFP2 protein in an intermediate twisted conformation between its on- and off-states[6]. Using the same technique at LCLS, we also tried to understand the structural and dynamical features of the fluorescent on-state at different time scale from the ps to the ns. We were able to identify different intermediates, which all display a subtle rearrangement of the protein matrix surrounding the chromophore pocket, and inducing a subtle reorganization of the H-bond network. Therefore, in order to fully describe these different intermediates, a precise and detailed map of the H-bond network was needed, and no other tool than neutron crystallography can be used for such purpose. The room-temperature neutron structure of the on-state was solved on the neutron diffractomer LADI-III (ILL, Grenoble) at 2.3 Å and revealed the exact H-bond coordination of the chromophore, from which all intermediates obtained at the XFEL could be precisely described, and in particular one which yields fluorescence. To further validate these results, mutants of rsEGFP2 have been designed to improve its fluorescence properties and are currently under characterization.

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Insights into genetic information storage, repair and translation provided by neutron scattering, synchrotron radiation and molecular dynamics

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Small- and ultra-small angle neutron scattering (SANS and USANS), small-angle X-ray scattering and neutron spin echo together with MD simulations and computer modeling of biological macromolecular systems of different levels of complexity was applied to investigation of the molecular mechanisms of biological function of macromolecular machines responsible for genetic information storage, repair and translation.

Organization of genetic material in eucariotes was investigated by SANS and USANS revealing two-phase fractal organization of chromatin in interphase nuclei of a variety of cell types, as well as changes in both large-scale hierarchy and small-scale nucleosome arrangements of native chromatin induced by molecular crowding agents, thus providing the experimental basis for modeling chromatin organization throughout its structural hierarchy from nucleosome to the whole nucleus.

In the studies of bacterial reparation system the molecular dynamics model of RecX binding to RecA presynaptic complex has been confirmed by SANS experiment. The molecular dynamics model together with neutron spin echo data has revealed marked differences in conformational mobility of RecA self-polymer, the presynaptic filament and its complex with RecX. The use of time-resolved small angle X-ray scattering together with SVD analysis has allowed to describe the structural and kinetic characteristics of the main stages of the presynaptic complex formation process: disassembly of the protein self-polymer, formation of the helical structure on ssDNA, and growth of the presynaptic filament of RecA protein.

Time-resolved small angle X-ray scattering has been applied to investigation of the structural kinetics of bacterial ribosome. We have determined the measurable differences in large-scale conformation between the vacant 70S ribosomes and their functional complexes, including pre- and post-translocation complexes, that were in line with the molecular modeling of the conformational transitions in procariotic ribosome. However, very little changes in the ribosome large-scale conformation were seen during forward and reverse translocation on the tens of milliseconds and longer time scale.

Identifying the correct protonation states of reactive intermediates in urate oxidase catalysis

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Many important enzymes utilize O_2 in their catalytic processes. These commonly contain a metallic centre or organic cofactor to engender organic radicals to react with the O_2, or can activate the molecule directly. However, a branch of enzymes exist that have no co-factor and therefore have very limited chemical tools at their disposal. From the viewpoint of fundamental biocatalysis these enzymes pose many very interesting, and currently unanswered, questions.

Urate oxidase (UOX) is the archetypal co-factor free oxidase enzyme, with therapeutic relevance as treatment in reducing toxic uric acid accumulation. UOX catalyses the O_2-mediated degradation of uric acid (UA) to 5-hydroxyisourate (5-HIU) and recent research has been able to show that the reaction proceeds via a 5-peroxyisourate (5-PIU) intermediate[1]. However, the mechanism of action of UOX is still not fully understood. The answer to this lies in the elusive protonation states of important active site residues before and after O_2 binds to the substrate.

Neutron macromolecular crystallography offers a unique ability to visualise hydrogen positions and bonding networks in reactive intermediates[2]. With perdeuterated UOX (dUOX) complexed with the inhibitor 8-azaxanthine (AZA), we are able to identify the protonation states in the active site environment without O_2. In addition, after structural determination of dUOX complexed with substrate analogue 9-methyl uric acid (MUA), we are able to determine the protonation states of key active site residues with O_2 bound as peroxide. From these two structures we are able to further understand the UOX mechanism of action and give an insight into how these enzymes function.

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Neutron Scattering Experiments of Photoactive Proteins under Illumination

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The structure-dynamics-function relationship in proteins is still a field of great scientific interest. Photoactive proteins form a specific class, whose function can be activated by illumination. Depending on application, samples can be activated by permanent illumination or by light pulses in time-resolved experiments. Subsequently, modulated structure and dynamics can be observed e.g. by small angle and quasielastic neutron scattering (SANS and QENS, respectively). Illumination of samples, with and without time resolution, requires a dedicated setup with light source, focusing optics, optical fiber, and active cooling of the sample in order to prevent efficient back-transfer to the ground state. Time-resolved experiments impose further needs, e.g. temporal synchronization of actinic light pulse and neutron probe as well as selective data storage. We will discuss the example of the Orange Carotenoid Protein, an effector initiating photoprotection in cyanobacterial light-harvesting systems in the case of exposure to excess light energies. We can show that the active state prepared by illumination is characterized by a strongly elongated structure (not available by X-ray diffraction) and by enhanced protein flexibility, which is a prerequisite for the conversion of potentially harmfull excess energy into heat.

Neutron Diffraction in High Magnetic Fields: Application to the heavy fermions systems U(Ru1-xRhx)2Si2

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URu_2Si_2 is undoubtedly one of the most enigmatic strongly correlated electron systems. A consensus about the nature of its hidden-order phase is still absent after more than thirty years of intense investigations [1]. While pressure stabilizes antiferromagnetism with the commensurate wavevector $\mathbf{k}_0$=(1 0 0) (equivalent to (0 0 1)) [2], a high magnetic field applied along **c** induces a cascade of first-order quantum magnetic phase transitions in the narrow field range 35-39 T [3]. In parallel to the hidden-order 'quest', a long-standing challenge has been to determine the magnetic order parameter of the system in such extreme high fields.

From neutron diffraction under intense magnetic fields pulsed up to 40 T, we have shown that URu_2Si_2 is in a spin density wave state characterized by the propagation vector $\mathbf{k}_1$=(0.6 0 0) in fields between 35 and 39 T [4], in contrast to the field-induced phase II of the 4 and 8% Rh-doped compounds which has a squared-modulated ferrimagnetic structure with the wavevector $\mathbf{k}_2$=(2/3 0 0) [5-6]. Recently, this study has been extended to the 2% Rh-doped $U(Ru_{0.98}Rh_{0.02})_2Si_2$ which still exhibits the hidden order and shows three field-induced phases above ≈ 32 T. This work revealed that their magnetic structure is characterized by the incommensurate propagation vector $\mathbf{k}_3$=(0.63 0 δ), with a small transverse component δ. These results may be linked to Fermi surface reconstructions and would suggest that field-induced phases in the 2% Rh-doped system and possibly also in the pure one are of a multi-**k** nature.

High field experiments up to 40 T have been performed thanks to a long-duration (rise time of 23 ms and total duration > 100 ms) pulsed field-cryomagnet developed by the LNCMI-Toulouse, the ILL-Grenoble, and the CEA-Grenoble, and operated on the triple-axis CRG-CEA spectrometer IN22 at the ILL. After an introduction of the experimental setup [7], our neutron diffraction results will be presented and discussed in the light of NMR [8], Fermi surface [9], and magnetic fluctuations [10] studies.

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High-pressure cells for inelastic neutron scattering studies of proton dynamics in materials

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A specific generation of compact high-pressure cells is developed for experiments on inelastic neutron scattering. The cells of a generic “piston-cylinder” type offer a pressure range up to 30 kbar with the sample volumes up to 100 mm^3. The cell body may be composed from different metallic alloys such as Cu-Be, Ti-Zr, Ni-Cr-Al or their combination. The energy of atomic vibrations in these materials does not exceed some 40-45 meV what permits studies of higher energy excitations, including proton vibrations in different compounds, in relatively comfortable experimental background conditions. The cell design is particularly adapted for the neutron spectrometer IN1-Lagrange at ILL with large open solid angle for scattered neutrons. The performance of the first members of this high-pressure cell family is illustrated by the phonon spectra measured at IN1.

Triaxial in situ deformation experiments with pore pressure on a sandstone sample using neutron time-of-flight diffraction at the EPSILON diffractometer

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The mechanical deformation of a rock is coupled to pore fluid pressure. In poro-elastic theory, a change of pore pressure causes a deformation of the porous rock mass and vice versa changes of stress and volume reduction can cause changes in pore pressure if the rocks are undrained. The understanding of the coupling of stress to changes of pore pressure in porous rocks is important for numerous fields in geosciences: 1) circulation of geothermal fluids, 2) stimulation of reservoir sections with low permeability, 3) injection of waste water into aquifers, 4) impoundment of hydropower reservoirs. This is because pressure induced changes of stress can lead to critically stressed faults and thus to fault reactivation. In the case of injection induced pore pressure changes, earthquakes of magnitudes > 5 had been induced.

With the application of neutron time-of-flight diffraction at the EPSILON diffractometer and the triaxial pressure cell TRIXI, *in situ* intracrystalline deformation can be detected for various pressure and stress conditions. The axial loading enables axial stresses up to 150 MPa, the mantle pressure and pore pressure can rise up to 70 MPa in cylindrical saturated porous rock samples. It is also possible to fix the axial displacement and to create a zero axial macroscopic deformation. The cell was designed (mostly 2015/2016), manufactured (2017) and tested (November 2017, January 2018). Due to the long neutron flight path and hence the relative low neutron flux at sample position, the measurement of strain on the rock sample of 60 mm length and 30 mm diameters require a long exposition time. Thus, a deformation experiment with a systematic change of the stress state requires beam time of 8-12 days. Threfore, up to now, we could perform only a few test experiments.

The neutron diffraction enables to detect the intracrystalline microstrains in the bulk sample volume. For increasing axial stress and confining pressure, the microstrains show a nearly linear relationship with respect to the applied loads and confirm that the behavior of the sample is elastic for the chosen stress boundary conditions. Furthermore, this pre-experiment shows that the construction of the triaxial neutron transparent pressure device was successful.

Additionally, we investigated the change of microstrains for increasing pore pressures while keeping the confining stress and the axial stress constant. According to the classical effective stress approach of Terzaghi (1943) the microstrain should be reduced significantly since part of the external loads (axial stress ad confining stress) which have not been changed but carried partly by the pore pressure. Under the assumption of poroelasticity with coupling of pore pressure and stress, the microstrains should be significantly less reduced. Our first experiments with TRIXI favour the poro-elastic approach and would be the first really *in situ* neutron diffraction observation of pore pressure / stress coupling.

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High-pressure neutron diffraction: state-of-the-art at the SNS and near future opportunities at the ESS

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High pressure provides a powerful tool to manipulate the structure of matter. Even modest pressures can produce large changes in density affecting changes in the bonding and properties of matter and inducing a rich variety of exotic phenomena. As a result, studies of properties at high pressure can provides fundamental and deep insight into structure-property relationships. However, the necessarily small sample volumes have traditionally prevented accurate neutron diffraction studies above pressures of 20-30 GPa achieved in the early 1990's as a result of the development of the Paris-Edinburgh press.

In the last few years, the combination of intensely-bright, next-generation sources and new designs of large-volume, diamond-anvil cells (DACs) developed at the SNS is revolutionising what is possible. In addition to ultra high-pressure capability, the low mass of the new cells offers new opportunities for ultra-low T studies: unlocking parameteric studies of magnetism and quasi-particles with neutrons. Furthermore, the optical access provided by diamond windows enables the possibility of laser heating, which could greatly impact geoscience studies using neutrons.

The technique of neutron diffraction with diamond anvils cells is particularly well suited to the intense beams of the ESS. And, in collaboration with the University of Edinburgh, UK and the SNS, USA, the ESS is working to interface these new capabilities with the initial suite of diffractometers and spectrometers to generate early science in the earliest phases of hot-commissioning. In the longer term, we believe that the true potential of these devices can only be realised with a dedicated diffractometer at the ESS and will present our proposal for: the Extreme Sample PRESsure Spallation Observatory (ESPRESSO).

TO THE PROBLEM OF GRANITE MONUMENTS DESINTEGRATION: STRUCTURAL, TEXTURE, ULTRASONIC AND PERMEABILITY MEASUREMENTS

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The mineralogical composition of granites and the mechanism of their formation in the thermodynamic conditions of the Earth crust ultimately determine the durability and integrity of granites as building stones. Rapakivi granite is a special type of granite. It is very common in construction and decorative stone. It was used in the Isaac Cathedral and in the Alexander Column in St.Petersburg, Russia. However, it has been reported [1] about accelerating Rapakivi deterioration in Alexander Column, which has already more than 20 open fractures. It is possible to interpret these deterioration events by frost weathering, because the St.Petersburg area climate conditions include subfreezing temperature variations and relatively high degree of precipitation and humidity. The purpose of this study is to investigate the relationships between petrographical, physical and mechanical properties of Rapakivi granite (Viborg, Russia). We applied different experimental methods for rock characterization: determination of crystallographic textures by neutron diffraction, permeability measurements and ultrasonic P-wave sounding of rock sphere at different confining pressures. The modal composition of granite sample is 25% plagioclase, 28% quartz, 47% alkali K-feldspar, as obtained by X-ray powder diffraction. This sample is coarse-grained rock with a typical K-feldspar ovoids (crystals of about 1 cm in diameter), that are entirely mantled by quartz-plagioclase. The texture measurements were performed by the SKAT time-of-flight texture diffractometer at the Frank Laboratory of Neutron Physics at JINR (Dubna, Russia) [2]. Diffraction spectra were analyzed with the Rietveld method, which relies on a full diffraction pattern and provides information about modal composition and preferred orientation of minerals, specifically pole figures. Neutron diffraction measurements revealed weakly pronounced textures with low density values of crystallographic preferred orientations (CPOs) for all major minerals (K-feldspar, plagioclase and quartz). Ultrasonic sounding of spherical sample was carried out using high pressure vessel of the Institute of Geology, Czech Academy of Sciences (Prague) by the pulse transmission method. Measured 3D velocity distributions on spherical sample show that Rapakivi granite has a moderate anisotropy (A = 14%) at atmospheric pressure. The increase of confining pressure up to 50 MPa makes the decrease of anisotropy to about 8%. We applied the effective media modeling of elastic properties of Rapakivi rock sample at atmospheric pressure based on two-phase model: mineral texturized matrix and empty penny-shaped inclusions imitating microcracks. Evidently, that these microcracks control the elastic anisotropy of Rapakivi sample substantially and their evolution under the specific climate condition refer to the distinctive weathering behavior of disintegrated or crumbly granite.

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Neutron sounding of Mars from orbit with FREND instrument

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Neutron sounding is a technique widely used in planetary science to locate hydrogen-bearing materials in the regolith of celestial bodies with no or thin atmosphere. Similar techniques are used on Earth in geology and oil industry. In space, neutrons are a by-product of bombardment of planets by Galactic Cosmic Rays. Their quantities and spectra, as seen from orbit, is very sensitive to the presence of hydrogen, the latter being an excellent moderator. In this talk we will present more details of this technique and its applications in space, as well as provide latest results of FREND instrument as an example application.

Fine Resolution Epithermal Neutron Detector (FREND) is a neutron telescope installed onboard Trace Gas Orbiter (TGO). Its collimator is another characteristic of the instrument, defines an unprecedented field of view allowing for a spatial resolution of up to 60 km. Currently, TGO reached its science orbit in April 2018 and continues successful mapping of the planet's epithermal neutron flux.

FREND is a statistical instrument, meaning that the more it observes the planet the more significant its maps become. In this talk we will present how hydrogen maps evolved during the first year of measurements, revealing new features of the subsurface hydrogen that were not known before.

Determination of the planetary soil composition by means of neutron and gamma detectors

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Neutron and gamma-ray detectors were installed on the spacecrafts from the very beginning of the space era. Thus, the first data on the geochemical composition of the moon were obtained from the measurements of gamma radiation from its surface by the Soviet mission Luna-10 and the American Apollo-15 and Apollo 16. During the past 25 years, a number of spacecrafts, both orbital and rovers, were equipped with neutron and gamma-ray detectors to determine the elemental and isotopic composition of the soil of celestial bodies.

The principles of operation of complex instruments designed to register neutron and gamma radiation in a wide spectral range, as well as the methods for determining the elemental and isotopic composition of the planetary soil will be described using as examples several devices created by the authors for orbital spacecrafts and rovers.

Keywords: neutron detector; gamma detector; neutron spectra unfolding;

Neutron lifetime measuring experiments with UCN magnetic storage

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Precision measurements of the neutron lifetime provide stringent tests of the standard electroweak model [1] as well as crucial inputs for Big-Bang nucleosynthesis calculations [2]. When combined with measurements of other neutron beta decay correlation coefficients [1], the neutron lifetime enables the determination of the Vud element of the Cabbibo-Kobayashi-Maskawa quark mixing matrix, providing a complementary unitarity test to that obtained from superallowed nuclear beta decay [3]. The neutron lifetime is also one of the key parameters for the determination of yields of light elements in BBN since the ratio between the free neutron and proton abundances drives the extent of fusion reactions during the first few minutes of the Universe [2].

Magnetic trapping of ultracold neutrons (UCN) permits to control neutron losses during neutron lifetime measuring. To realize this advantage of UCN magnetic storage is possible only using of magnetic shutter. Without this unique opportunity, experiments with magnetic storage are indistinguishable from experiments with storage in material traps. Systematics in neutron lifetime measuring experiments using UCN magnetic storage is discussed.

Measurement of the neutron lifetime using ultracold neutrons stored in a magneto-gravitational trap made of permanent magnets is discussed. Neutrons surviving in the trap after fixed storage times have been counted and the trap losses have continuously been monitored during storage by detecting neutrons leaking from the trap. The value of the neutron lifetime resulting from this measurement is $\tau_n = (878.3 \pm 1.6_{stat} \pm 1.0_{syst})$ s. A unique feature of this experiment is the monitoring of leaking neutrons providing a robust control of the main systematic loss.

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Crystal-diffraction gain of the Stern-Gerlach effect

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The gain factor of the spatial beam displacement of Laue diffracted neutrons in a transverse gradient of a magnetic field was directly measured (see Fig. 1). This factor can reach values up to 10^6 in comparison with the free neutron. The amplification can be associated with two phenomena:

1. The reduction of the effective neutron "mass" in Laue diffraction [1].
2. An increase of the time for which the neutron stays in a crystal for Bragg angles close to 90° [2].

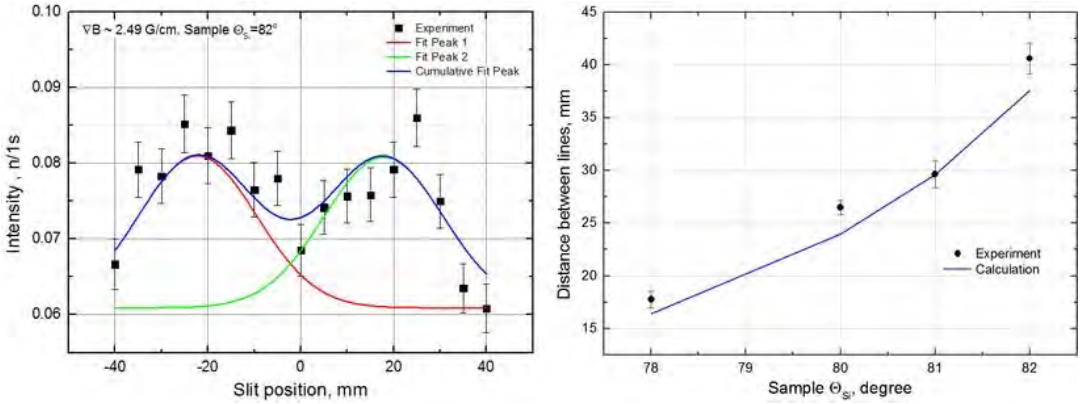

Fig. 1. The left hand plot shows the splitting of the beam in two components for the magnetic field gradient of about 2.5 G/cm in the case of Laue diffracted neutron at the (220) plane of silicon. The right hand plot shows the dependence of beam splitting on the Bragg angle

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A new approach to search for free neutron-antineutron oscillations based on coherent neutron and antineutron reflections

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An observation of neutron-antineutron oscillations, which violate both B and B-L conservation, would constitute a scientific discovery of fundamental importance to physics and cosmology. A stringent upper bound on its transition rate would make an important contribution to our understanding of the baryon asymmetry of the universe by eliminating the post-sphaleron baryogenesis scenario in the light quark sector. We show that one can design an experiment using slow neutrons that in principle can reach the required sensitivity of 10^{10} s in the oscillation time, an improvement of 10^4 in the oscillation probability relative to the existing limit for free neutrons. This can be achieved by allowing both the neutron and antineutron components of the developing superposition state to coherently reflect from mirrors. We present a quantitative analysis of this scenario and show that, for sufficiently small transverse momenta of neutrons/antineutrons and for certain choices of nuclei for the neutron/antineutron guide material, the relative phase shift of the neutron and antineutron components upon reflection and the antineutron annihilation rate can be small. While the reflection of antineutrons from surface looks exotic and counterintuitive and seems to contradict to the common sense, in fact it is fully analogous to the reflection of neutrons from surface. The later phenomenon is well known and used in neutron research from its first years.

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Search for new internucleon short-range interaction in neutron scattering

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There are 4 known types of interaction in nature, but nowadays the existence of a new force mediated by new unknown bosons is widely discussed in the literature [1], [2]. This work deals with the application of neutron scattering technique for the search for a new short-range interaction and for setting constrains on the coupling constant of such interaction.

The main idea is to perform an experiment of neutron scattering on the powder of silicon (powder diffraction) and to get the information on scattering amplitude dependence on scattering angle. Within this work the calculations showing the possibility of the idea were made. The coupling constant constrains were obtained using the data of silicon powder diffraction from the FRM II reactor, Munich, Germany. It is shown that a new constrain is competitive to the existing one.

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Interaction of ultracold neutrons with a neutron interference filter oscillating in space

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The work presents the results of the study dedicated to the problem of the interaction of ultracold neutrons with a neutron interference filter oscillating in space – Fabry-Perot interferometer. The numerical solution of the non-stationary Schrödinger equation was found by splitting the evolution operator. The spectra of transmitted and reflected states are obtained, depending on the parameters of the interferometer motion.

For the most part, the calculation results correspond to the expectations. The transmitted state is modulated in amplitude, and the state spectrum has a discrete form. At the same time, the essential details of the obtained picture differ from the predictions based on semi-classical ideas. Probably the most significant of the discovered effects is the shift of transmission maxima of the system with increasing frequency followed by the merging of neighboring peaks. As a result, the apparent frequency of intensity modulation is halved. Such behavior of the transmission state cannot be explained on the basis of simple considerations on the temporal intensity modulation due to the variable speed of the interferometer. Apparently, the finite time of state formation in the resonant system represented by a Fabry-Perot interferometer and completely unaccounted effects of its acceleration plays a significant role.

The obtained results are based on the assumption that the description of the interaction of neutrons with matter by means of the effective potential is valid. At the same time, in the case of a medium moving with great acceleration, the validity of such an assumption is not obvious. Therefore, it is very important to conduct an experiment in which it would be possible to verify the theoretical results. Preparations for this experiment are underway.

Oral

Weak Measurements and Which-Way Measurements studied in Neutron Optics

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Weak measurements [1], introduced more than 30 years ago, underwent a metamorphosis from a theoretical curiosity to a powerful resource for exploring foundations of quantum mechanics, as well as a practical laboratory tool. However, unlike in the original textbook experiment, where an experiment with massive particles is proposed, experimental applications are realized applying photonic systems. We have overcome this gap by developing a new method to weakly measure a massive particle's spin component. Our neutron optical approach is realized by utilizing neutron interferometry, where the neutron's spin is coupled weakly to its spatial degree of freedom [1]. This scheme was then applied to study a new counter-intuitive phenomenon, the so-called quantum Cheshire Cat: If a quantum system is subject to a certain pre- and post-selection, it can behave as if a particle and its property are spatially separated, which is demonstrated in an experimental test [2,3]. State tomography, the usual approach to reconstruct a quantum state, involves a lot of computational post-processing. So in 2011 a novel more direct method was established using weak measurements. Because of this weakness the information gain is very low for each experimental run, so the measurements have to be repeated many times. Our procedure is based on the method established in 2011, without the need of computational post processing, but at the same time uses strong measurements, which makes it possible to determine the quantum state with higher precision and accuracy. We performed a neutron interferometric [4] experiment, but our results are not limited to neutrons, but are in fact completely general. In our latest neutron interferometric experiment [5], a which-way measurement is applied to investigate the paths taken by neutrons in a three-beam interferometer. In each paths of the interferometer, the total energy of the neutrons is partially shifted such that the faint traces are left along the beam path. By ascertaining an operational meaning to "the particle's path," which-path information is extracted from these faint traces with minimal perturbation measurements.

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Oral

On ray and wave optics description in neutron planar waveguides

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Ray optics approach can be applied to describe neutron beam trajectories in macroscopic objects, for example, beam propagation along the channel in neutron guides or refraction in a semi-infinite medium. In our report we demonstrate that this ray optics description in microscopic waveguides is limited by diffraction effects. Planar waveguides [1] are tri-layer films with a well-like neutron optical potential. Neutron beam of the width about 0.1 mm falls on the sample surface under a small grazing angle, tunnels through the upper thin layer, is reflected from the bottom thick layer, propagates along the middle layer as in a channel and goes out from the end face as a microbeam of the initial width about 0.1 μm and the angular divergence about 0.15°. In [1] the far-field angular distribution of the microbeam intensity was measured and compared with theory for fixed neutron wavelength and the width of the channel. The microbeam intensity is described by Fourier-transform of the neutron wavefunction density inside the waveguiding channel. Recently [2,3] we measured directly the angular divergence of the neutron microbeam from the waveguides $Ni_{67}Cu_{33}$(20 nm)/Cu(d)/$Ni_{67}Cu_{33}$(50)//Si(substrate) where d = 80, 100, 120, 150 and 180 nm as a function of the channel width and the neutron wavelength. The microbeam divergence is described by Fraunhofer diffraction on a narrow slit and does not depend on the grazing angle of the beam refracted in the guiding layer. As a result, this experimental fact confirms the far-field Fraunhofer diffraction phenomenon.

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Ancient arms and armour production technologies revealed through neutron imaging and neutron diffraction

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The history of metallurgy represented for several centuries the history of the main technological features reached by civilizations. Among metal objects production, arms and armour are some of the most interesting objects in archaeometallurgy and historical metallurgy because they were manufactured, over the ages, using the highest quality materials and the most advanced technology and skill [1-2]. The compositional and microstructural characterization of these artifacts can hence allow us to learn about the technological skills reached by different civilizations. The use of non-invasive techniques allows for the study of museum objects in excellent conservation conditions, thus giving a clear view of their characteristics. Neutron imaging and neutron diffraction are, to the author's knowledge, among the best methods to quantify phase composition and microstructure, study morphology, identifying non-metallic inclusions, cracks and defects [3-6]. Thanks to the use of advanced techniques such as energy selective imaging, the microstructural features and the distribution of the different phases in metal complex artifacts can be determined [7-10], so gaining important information about composition and manufacturing treatments (both thermal and mechanical). Following this path, we have performed a number of experiments using neutron imaging and neutron diffraction to reveal the characteristics of many artifacts from different civilizations, of which the production procedures are not yet fully clear. The results obtained and presented in this work, allow us to identify unique features that can shed new light on the manufacturing methods, thus increasing the level of our knowledge about the technological skills of such civilizations.

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Neutron and synchrotron imaging study of metal artefacts from Chernaya Mogila burial mound ("Black Grave") from State Historical Museum

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In the study of objects of cultural heritage, one of the main tasks is to determine their preservation. This is especially true for metal artifacts that have been exposed to factors such as fire and moisture, leading to a significant chemical transformation of the material.

The present work describes the results of experiments on neutron and synchrotron imaging of iron objects from the collections of the State Historical Museum. Comprehensive study of unknown-purpose artifacts from the archaeological monument of Old Rus' of the end of the 10th century — the Chernaya Mogila mound (Chernigov, present-day Ukraine) is carried out. According to the results of the imaging, reconstruction of the probable appearance of the objects is performed.

It is shown that in the projections obtained on a monochromatic neutron beam, the metal manifests itself in diffraction on grains, so that it is possible to determine the areas of its preservation. Examples of inhomogeneous corrosion of archaeological objects detected using neutron and synchrotron tomography are also considered.

New studies have led to the discovery of a previously unknown category of artefacts which may be interpreted as power insignia ('barbarian scepters').

This work was performed using the equipment of Research reactor IR-8 and Kurchatov Synchrotron Radiation Source.

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Neutron diffraction for archaeometry: results obtained on ancient Sardianian bronzes using the Italian Neutron Experimental Station INES

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The Italian Neutron Experimental Station INES, located at the pulsed neutron source ISIS (UK), is a general-purpose powder diffractometer built to focus its use on material science and in particular cultural heritage studies. Thanks to the high penetration power of thermal neutrons, archaeometric measurements performed through neutron diffraction allow for quantitative determination of bulk properties of the sample in a non-destructive way, in particular regarding composition and microstructure. This opens up the possibility of scientific investigation on objects otherwise unsuitable, due to their cultural and/or historical importance. Here, we describe INES and present the results of some recent measurements on bronze objects from Sardinia.

Sardinian bronze metallurgy represents an important example concerning the study of the development of Bronze technology in an insular area located in the centre of Mediterranean sea, isolated but with important links with the surrounding lands.

Three bronze swords of the so-called "Monte Sa Idda" type, and a nuragic boat model from Vetulonia, presenting a detailed representation of animals on the body, were studied through neutron diffraction. The obtained results show a very specific procedure for sword forging: the bronze composition, the presence of dendritic segregation and the microstructure are very peculiar. A comparison with micro-structural characteristics of contemporary swords produced in the other areas of the Mediterranean, in particular the Iberian peninsula, adds important details about the exchange of knowledge and artifacts in this geographic area. We could also add important information about the composition, casting technique and conservation status of the boat model.

Imaging investigation of Chinese bimetallic sword fragment from 2nd-1st century BCE

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Archaeometric studies have played a major role in the field of archaeology, especially with regard to materials transformed through human activity. Metals are generally investigated through metallography and SEM, which require sampling or surface preparation. Neutron techniques instead can provide the bulk properties of metals non-invasively.

Here we present a neutron imaging study of a Chinese bimetallic sword fragment from 2nd-1st century BCE. White beam Neutron Tomography (NT) and Neutron Resonance Transmission Analysis (NRTA) have been applied, using the IMAT and INES beamlines of the ISIS neutron source in the UK, respectively.

The earliest example of bimetallic weapons in China dates as early as the Shang Dynasty (1600–1100 BCE), where meteoric iron and bronze were combined to forge weapons. With the discovery of iron smelting technology during the Spring and Autumn Period (770–473 BCE), bimetallic swords with bloomery iron and bronze became more common [1]. They have been found in many parts of central China.

The sword fragment investigated has an iron blade mounted on a studded bronze grip (probably for a twine binding) and a ricasso with three long spikes protruding on each side. The object resembles two published examples with similar form of hilts [2] listed as originating from burials investigated in the mountainous regions of Longpaozhai, in the Min River Valley, dating from the 2nd or 1st century BCE. Similar swords are found further north and may have been introduced from further west.

NT allowed us to study the inner morphology of the sword, revealing details of its conservation status and the forging and/or casting of the different components. NRTA provided a 2D map of the elemental composition of the artefact, indicating the nature of the bronze alloy of the grip (whether tin bronze, leaded tin bronze, or arsenical tin bronze) and of the iron blade.

The study presented was complemented by Neutron Diffraction, and Neutron Resonance Capture Analysis, providing a characterisation of the object in terms of alloy composition, microstructural characterisation and elemental information, non-destructively.

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Neutron tomography reveals lead cores in Late Bronze Age palstaves at ISIS Pulsed Neutron and Muon Source

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Bronze artefacts were buried in large quantities in isolated hoards in the Atlantic façade of Europe, between the Bronze Age and the beginning of Iron Age. This practice was particularly intense, and despite many years of research, even today we do not understand what motivated such disparate and widespread communities to express themselves in this way (Armada and Martinón-Torres, 2016; Montero Ruiz et al, 2015).

This presentation is focused on the totally non-invasive characterisation of leaded bronze unused (as-cast) axes from NW Iberia through neutron tomography (NT), radiography and prompt gamma activation analysis (PGAA). Our main focus is to unveil the presence and distribution of high quantities of lead in the axes cores, which raises interesting questions about their manufacture as well as challenges for conventional x-ray based analytical techniques (Harrison et al. 1981; Gutierrez Neira et al, 2011). The samples include a variety of compositions and states of preservation, as well as an enigmatic palstave that has a hidden thick lead core as well as a large lead ball inside the casting sprue. Our specific objectives are (1) study the manufacturing processes of these axes; (2) study the inner morphology; (3) quantify their bulk chemical composition without analytical biases derived from sampling uncertainty.

The experiments were performed at ISIS pulsed neutron and muon source in Oxfordshire UK at the IMAT beamline where ad hoc instrumentation has been installed to allow the simultaneous acquisition of NT and PGAA spectra. Neutrons are a unique probe for the investigation of metal objects because of their weak interaction with matter and high penetration power allowing the study of hidden features in the bulk of the artefacts in a non-destructive and non-invasive way (Festa et al, 2018).

Results from the NT study unveil the inner morphology of the axes, allowing the segmentation of their various inner parts and materials, leading to new hypotheses about their manufacturing techniques. The presence of a sphere of pure lead in the core of one of the axes opens multiple scenarios on the manufacturing processes of this object, suggesting the presence of a double casting or the occurrence of a massive lead segregation. Through prompt gamma activation analysis, it is possible to perform a thorough chemical characterisation in the bulk of the objects.

The effects of manufacturing processes on historical ceramic morphology studied by Small Angle Neutron Scattering

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The study of ancient archaeological ceramics is challenging: samples have a considerable physical complexity which originates from the coexistence of several phases including amorphous ones; and, at the same time, porosity and clay/inclusion strongly depends on the geological sources of raw materials and on the production techniques.

Analytical techniques applied to art and archaeological objects can give the opportunity of gaining information about their composition and, therefore, to answer questions regarding where, when or by whom such artefacts were made. Additionally, these studies can help us to understand the manufacturing processes and technology, providing clues for interpreting the social, political, economic and cultural context of the civilizations involved. Such investigations are also valuable and, in some cases, fundamental for conservation, restoration and authentication projects [1].

In this work, we present a SANS study performed on historical ceramics fragments [1], in order to correlate the characteristics (porosity and pore dimensions) of the ceramics found in several sites with specific production techniques. In cooperation with the Landesamt für Archäologie Sachsen in Dresden, ceramic samples (16^{th}, 17^{th} century) have been collected from the region of Central and Eastern Germany, which were in the past and still nowadays important stoneware production sites. From Italy, ceramic shards were collected in Torcello, first inhabited island in Venice Lagoon, which had its greatest period of prosperity in the Middle Age related to commercial navigation (samples from 7^{th} to 10^{th} century). From SANS measurements over several orders of magnitude of Q on D11 at ILL, we evaluated the Porod's invariant [2], which allows us to assess the relative porosity. The results are very promising, evidencing that samples coming from different geographical regions and produced by different technologies are in two well-separated groups, allowing us to distinguish samples with different origin and manufacturing.

Laboratory-made samples with different clays and firing conditions were also characterized in order to compare them with the ancient ceramics and to study the evolution of porosity by temperature of firing. Total porosity is necessary in order to completely describe the morphological changes occurring during the firing process. In literature, specific studies on total porosity calculation are lacking and neutrons are a unique techniques that may open new insights in considering the trend of total porosity influenced by the closed porosity. That parameter needs to be studied for a complete awareness of the ceramic material features.

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Neutron Sources and Facilities

ID	Participant	Organization	Title
NS&F - 1	Alsaidan Shaykhah	King Saud University, Saudi Arabia	Simulation of a Neutron Source at the KFSH&RC CS-30 Cyclotron
NS&F - 2	Bulavin Maksim	Joint Institute for Nuclear Research, Russia	New data of upgrade of basic system of the pelletized cold moderator of the IBR-2 reactor
NS&F - 3	Deledda Stefano	Institute for Energy Technology, Norway	New instrumentation in the JEEP II reactor at IFE, Kjeller: Norwegian Center for Neutron Research – NcNeutron
NS&F - 4	Eshraqi Mohammad	European Spallation Source, Sweden	The ESS Linac
NS&F - 5	Georgii Robert	Heinz Maier-Leibnitz Zentrum and Physik-Department E21, Technische Universitat Munchen, Germany	Study of magnetic and quantum phenomena at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany
NS&F - 6	Jamalipour Mostafa	University of Milano-Bicocca, Italy	Implementation of neutron reflection with Nano-dispersed media in Geant4
NS&F - 7	Javorsky Pavel	Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Czech Republic	Materials Growth and Measurement Laboratory
NS&F - 8	Jullien David	Institut Laue Langevin, France	Polarized 3He recent developement at ILL
NS&F - 9	Kirilov Andrey	Joint Institute for Nuclear Research, Russia	Instruments control software at the IBR-2 reactor: features and prospects
NS&F - 10	Kuchugura Mariia	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	The diffraction study of low-dimensional spin frustrated $CoSb_2O_6$
NS&F - 11	Kulevoy Timur	NRC "Kurchatov institute" - ITEP, Russia	Compact linac for neutron generation as a part of BELA project

NS&F - 12	Lyamkin Vitaliy	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	A powerful UCN source at PNPI based on superfluid helium
NS&F - 13	Mikhailov Yury	The Federal State Unitary Enterprise “All-Russia Research Institute of Automatics named after N.L. Dukhov” (VNIIA), Russia	Modeling of the neutron radiation spectrum of plasma focus chambers
NS&F - 14	Mityukhlyaev Victor	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Cold Neutron Sources Historical Review
NS&F - 15	Mukhin Konstantin	Joint Institute for Nuclear Research, Russia	Combined pelletized neutron moderator for IBR-2 reactor
NS&F - 16	Ronnow Henrik	EPFL, Switzerland	Single shot neutron diffraction and spectroscopy at 100 T magnetic field?
NS&F - 17	Sitnikov Alexey	NRC "Kurchatov Institute" - ITEP, Russia	The proton linac for DARIA compact neutron source
NS&F - 18	Tartaglione Aureliano	CONICET-CNEA-LAHN, Argentina	Update in the design of ASTOR: A cold neutron imaging instrument for the future argentine multipurpose reactor RA-10
NS&F - 19	Ulyanov Vladimir	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	First measurements of neutron spectrum at horizontal experimental channel of reactor PIK
NS&F - 20	Willendrup Peter	Physics Department, Technical University of Denmark and ESS DMSC, Denmark	New developments in the McStas neutron ray-trace simulation package
NS&F - 21	Zakalek Paul	Julich Centre for Neutron Science, Forschungszentrum Julich GmbH, Germany	Tuning of target / moderator / reflector unit for optimized instrumentation at compact accelerator driven neutron sources
NS&F - 22	Golosov Oleg		Structure and phase studies of highly irradiated dispersed u-mo/al fuel by the neutron diffraction method
NS&F - 23	Sitnikov Alexey	NRC "Kurchatov Institute"- ITEP	The proton linac for DARIA compact neutron source

Magnetism, Multiferroics, Skyrmions, Superconductivity

ID	Participant	Organization	Title
M&S - 2	Boehm Martin	Institut Max von Laue - Paul Langevin, France	Magnetic field dependence of spin stripe in highly under doped LSCO superconductors
M&S - 3	Bykov Alexey	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Magnetic phase diagram of the uniaxial helimagnet Cr1/3NbS2: evidence from small angle neutron scattering
M&S - 5	Chang Lieh-Jeng	Department of Physics, National Cheng Kung University, Taiwan	Low temperature magnetism of the quantum spin ice candidate $Nd_2Ru_2O_7$
M&S - 6	Deriglazov Vladimir	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Phase separation in half-doped manganites with isovalent substitution of rare-earth cations exemplified by $Sm_{0.32}Pr_{0.18}Sr_{0.5}MnO_3$
M&S - 7	Dubitskiy Ilya	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Emergence of the perpendicular to the magnetic field magnetization in nickel inverse opals studied by SQIUD, MFM and micromagnetic modelling
M&S - 8	Elmekawy Ahmed	Saint Petersburg State University, Russia	Study of the magnetic properties of arrays of iron-based nanowires by FORC and SANS.
M&S - 10	Fernandez Barquin Luis	CITIMAC, Facultad de Ciencias, Universidad de Cantabria, Spain	Size and lattice distortions as driving agents of long-range magnetic correlation and crystal field excitations of $TbCu_2$ nanoparticles
M&S - 11	Fogh Ellen	Department of Physics, Technical University of Denmark, Denmark; Institute of Physics, Ecole Polytechnique Federale de Lausanne, Switzerland	Magnetism and magnetoelectricity in mixed-anisotropy magnets
M&S - 12	Franz Christian	Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitat Munchen, Germany	MIEZE neutron spin-echo spectroscopy of strongly correlated electron systems
M&S - 13	Giansiracusa Marcus	School of Chemistry, The University of Manchester, UK	Measuring the phonon spectra of single-molecule magnets with inelastic neutron scattering
M&S - 14	Golosova Natalia	Frank Laboratory of Neutron Physics, JINR, Russia	Structural and magnetic properties of the Fe-doped layered perovskite $TbBaCo_{1.91}Fe_{0.09}O_{5.5}$ at high pressure

M&S - 15	Grigoriev Sergey	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Measurements of the spin wave stiffness in helimagnets by small-angle polarized neutron scattering
M&S - 16	Gubkin Andrei	M.N. Mikheev Institute of Metal Physics UB RAS, Russia	Magnetic structure of the ternary $GdMn_2Si_2$ compound
M&S - 17	Hansen Ursula Bengaard	The Niels Bohr Institute, University of Copenhagen, Denmark	Magnetic triplon excitations in the alternating chain system $(VO)_2P_2O_7$
M&S - 18	Hernandez-Velasco Jorge	Instituto de Ciencia de Materiales de Madrid (ICMM) CSIC, Spain	From Nuclear SRO and Incommensurate Magnetic LRO in $SbVO_4$ Catalyst to non-magnetic ground state in SbV_9O_{20}
M&S - 19	Jochum Johanna	Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitat Munchen, Germany	Magnetic characterization of oblique angle deposited Co/CoO on gold Nanoparticles
M&S - 20	Klicpera Milan	Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Czech Republic	Magnetic structures of $RCuAl_3$ (R = Ce - Nd) compounds
M&S - 21	Kremer Reinhard	Max Planck Institute for Solid State Research, Germany	Magnetic Ordering in the 2-dim Quantum Antiferromagnet alpha-CuV_2O_6
M&S - 22	Krezhov Kiril	Institute for Nuclear Research and Nuclear Energy, Russia	Half Replacement of Bismuth by Neodymium in Half-Hole Doped Bismuth-Based Manganites $Bi_{0.25}Nd_{0.25}X_{0.5}MnO_3$ (X=Sr, Ca): A Neutron Diffraction Study
M&S - 23	Kurbakov Alexander	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Complementary Neutron Diffraction and OjSR Studies of the Static and Dynamic Magnetic Properties of New Spin-frustrated Chiral Magnet $MnSnTeO_6$
M&S - 25	Lvov Dmitrii	NRC «Kurchatov Institute» – ITEP, Russia	Theory of Multiple Small-Angle Neutron Scattering in Ferromagnets
M&S - 26	Magnitskaya Maria	Institute for High Pressure Physics RAS, Russia	Doping evolution of the gap structure and spin-fluctuation pairing in $Ba(Fe_{1-x}Co_x)_2As_2$ superconductors
M&S - 27	Matsuo Masashi	National Institute for Materials Science (NIMS), Japan	Neutron diffraction study in magnetic fields of the antiferromagnetic spin-1/2 trimerized chain compound $Cu_3(P_2O_6OD)_2$

M&S - 28	Matsuo Yukari	Department of Advanced Sciences, Hosei University, Japan	A Possible Magnetic Structure of the Hexamer-Based Haldane Compound $K_2Cu_3O(SO_4)_3$
M&S - 29	Matveeva Anna	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Some aspects of the magnetism in $Dy_{1-x}Ho_xMnO_3$
M&S - 30	Neetika Sharma	Max Planck Institute for Solid State Research, Germany	Cr and Ce magnetic ordering in $CeCrO_3$: revisited
M&S - 31	Ovsyanikov Alexandr	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Spin waves in a rare-earth orthoferrite $HoFeO_3$
M&S - 32	Pirogov Aleksandr	Institute of Metal Physics of UB RAS, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia	Magnetic structures of the $La_{1-x}Tb_xMn_2Si_2$ compounds
M&S - 33	Potashnikov Daniel	Faculty of physics, Technion-Israeli Institute of Technology, Israel	Neutron diffraction of nano-laminated rare earth containing i-MAX phases
M&S - 34	Przenioslo Radoslaw	Faculty of Physics, University of Warsaw, Poland	Monoclinic super-space group description of the magnetic modulations in bulk BiFeO3 at ambient conditions
M&S - 35	Pshenichnyi Kirill	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Spin-wave stiffness of Dzyaloshinskii-Moriya helimagnets $Fe_{1-x}Co_xSi$ studied by small-angle neutron scattering
M&S - 36	Quintero Castro Diana Lucia	University of Stavanger, Norway	1D Magnetism in the Russian Mineral Pauflerite
M&S - 37	Ray Pia J.	Niels Bohr Institute, University of Copenhagen, Denmark	Mapping complex superstructures in the co-doped high-temperature superconductor family $La_{(2-x)}Sr_{(x)}CuO_{(4+y)}$
M&S - 38	Sadykov Ravil	Institute for Nuclear Research, Institute for High Pressure Physics, Russia	Magnetic spiral in $ZnCr_2Se_4$ under pressure up to 56kbar
M&S - 39	Savchenkov Pavel	National Research Nuclear University MEPhI, Russia	Analysis of the intermediate valence of Eu and Sm in SmB_6 and $EuCu_2Si_2$ compounds
M&S - 40	Semkin Mikhail	Institute of Natural Sciences of the Ural Federal University, Russia	Magnetic structures of Li-Ni/Co-P-O
M&S - 41	Shaginyan Vasily	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Optical conductivity of quantum spin liquids

M&S - 42	Shen Junying	Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institute, Switzerland	Stability of the Q-phase of $CeCoIn_5$ in the presents of localized magnetic impurities
M&S - 43	Sikolenko Vadim	Joint Institute for Nuclear Research, Russia	High pressure neutron diffraction study of magnetic and structural transitions in anion deficient cobaltites
M&S - 44	Skanchenko Daria	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Investigation of the magnetic structure of $Rh_{1-x}Fe_xGe$ by small-angle neutron diffraction
M&S - 45	Sukhanov Aleksandr	MPI CPfS Dresden, Germany	Magnon-polaron excitations in the noncollinear antiferromagnet Mn_3Ge
M&S - 46	Susloparova Anna	St. Petersburg University, Russia	Crystal and magnetic structure of layered orthorhombic Li_2MnGeO_4
M&S - 47	Testa Luc	Laboratory for Quantum Magnetism, Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland	$Ba(TiO)Cu_4(PO_4)_4$ - a neutron scattering journey towards the understanding of a chiral magnet family
M&S - 48	Titov Ivan	University of Luxembourg, Luxembourg	Effect of grain-boundary diffusion process on the geometry of the grain microstructure of Nd−Fe−B nanocrystalline magnets
M&S - 49	Tutueanu Ana Elena	Institute Max von Laue Paul Langevin, France	Non-destructive determination of critical temperature distribution in LSCO superconductor by means of polarized neutron imaging
M&S - 50	Urusova Natalia	Institute of Solid State Chemistry of the Ural Branch of the RAS, Russia	Features of magnetic phase transitions in lithium-nickel orthophosphate
M&S - 51	van Well Natalija	Laboratory of Crystallography, University of Bayreuth, Germany; Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland	Magnetic phases in the $Cs_2CuCl_{4-x}Br_x$ mixed system
M&S - 52	Vaulin Artyom	M.N. Mikheev Institute of Metal Physics UB RAS, Russia	Incommensurate magnetic structure of Ho_7Rh_3
M&S - 53	Waliszewski Janusz	Faculty of Physics, University of Bialystok, Poland	Magnetization distribution in noncollinear systems
M&S - 54	Wan Wenjie	Department of Physics, Technical University of Denmark, Denmark	Persistence of the roton minimum into the disordered state of a square-lattice antiferromagnet

M&S - 55	White Jonathan	Paul Scherrer Institute, Switzerland	Disordered skyrmion phase stabilized by magnetic frustration in a chiral magnet $Co_7Zn_7Mn_6$
M&S - 56	Zhu Fengfeng	Julich Centre for Neutron Science (JCNS), Forschungszentrum Julich GmbH at Heinz Mair-Leibnitz Zentrum (MLZ), Germany	Magnetic structure of 2D Dirac fermion antiferromagnet $EuMnBi_2$
M&S - 57	Zhu Tao	Institute of Physics, Chinese Academy of Sciences, China	Polarized neutron reflectometry in China spallation neutron source

Functional Materials

ID	Participant	Organization	Title
FM - 1	Almasy Laszlo	University of Messina, Italy	Branched polyethyleneimine/TEMPO-oxidized cellulose nanofibers xerogels for water remediation: a Small Angle Neutron Scattering (SANS) study
FM - 2	Borisova Polina	National Research Center «Kurchatov Institute», Russia	Interaction of Fe-Ni alloy with amorphous fullerene C60 in sintering
FM - 3	Chtchelkatchev Nikolay	Landau Institute for Theoretical Physics RAS, Russia	Ab initio study of lattice dynamics of rear-earth borides
FM - 4	Doan Huan	University of Bristol, UK	Defective hierarchical porous copper-based metal-organic frameworks synthesised via facile acid etching strategy
FM - 5	Eliovich Ian	National Research Center «Kurchatov Institute», Russia	New possibilities of time resolved X-Ray studies of defect structure of crystals
FM - 6	Embs Jan	Laboratory for neutron Scattering & Imaging, Paul Scherrer Institute, Switzerland	QENS studies of Reorientational Hydrogen Dynamics in Complex Hydrides
FM - 7	Fabian Margit	MTA Centre for Energy Research, Hungary	Structure of oxy-halide glasses for solid state batteries
FM - 8	Fruhner Lisa Sarah	Julich Centre for Neutron Science (JCNS-1) and Institute for Complex Systems (ICS-1), Forschungszentrum Julich GmbH, Germany	Self-assembly of iron oxide nanoparticles in magnetic field studied by Small-Angle Neutron Scattering
FM - 9	Iuzviuk Mariia	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	In situ synchrotron study of layered double hydroxides loaded with chloride and sulfate anions
FM - 10	Ivankina Tatiana I.	Joint Institute for Nuckear Research, Russia	Effect of crystallographic textures on the functional properties of TiNi shape memory alloy
FM - 11	Kiani Sajad	Energy Safety Research Institute (ESRI), Swansea University, UK	A New Class of Low Surface Energy Anionic Surfactant for Enhanced Oil Recovery (EOR)

FM - 13	Kopitsa Gennady	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Supercritical vs subcritical drying of silica aerogels: Structural considerations
FM - 14	Lohstroh Wiebke	Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitat Munchen, Germany	A quasi-elastic and inelastic neutron scattering study of alkaline and alkaline-earth borohydrides $LiBH_4$ and $Mg(BH_4)_2$
FM - 16	Marchenkov Nikita	National Research Centre "Kurchatov Institute", Russia	Time-Resolved X-Ray Diffraction for Investigation of Effects Induced in Non-Centrosymmetric Crystals by External Electric Field
FM - 18	Paul Neelima	Heinz Maier-Leibnitz Zentrum, Technische Universitat Munchen, Germany	Investigating the SEI in silicon-based anodes with contrast-matched SANS
FM - 19	Perez Gabriel	Department of Chemical and Biological Engineering, University of Sheffield, UK	Determination of the morphology modification of zwitterion doped PEDOT: PSS with neutron scattering techniques
FM - 20	Pesach Asaf	Physics Department, Nuclear Research Centre-Negev, Israel	Microstructure Study of Ti-6Al-4V Additively Manufactured using Neutron Diffraction
FM - 21	Porcher Florence	Laboratoire Leon Brillouin, France	Microporous (guest-host) systems: from (micro-)structure to optical properties
FM - 22	Runov Vladimir	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Highly sensitive estimation correlation scale of magnetic impurities or phase in functional materials by means of SANS of polarized neutrons
FM - 23	Ryzhov Vyacheslav	Petersburg Nuclear Physics Institute of NRC "Kurchatov Institute", Russia	Magnetic phase separation and unusual scenario of its temperature evolution in porous carbon-based nanomaterials doped with Au and Co
FM - 24	Seidlmayer Stefan	Heinz Maier-Leibnitz Zentrum (MLZ), TU Munchen, Germany	Operando neutron diffraction improves understanding of lithiation dynamics in graphite anodes
FM - 25	Shekunova Taisiya	Kurnakov Institute of General and Inorganic Chemistry of the RAS, Russia	Cerium (IV) hydrogen phosphate ultralight aerogels

FM - 26	Soerensen Daniel	University of Southern Denmark, Denmark	A New Measuring Cell for Operando Neutron Diffraction on Li-Ion Battery Cathode Materials
FM - 27	Sumnikov Sergey	Joint Institute for Nuclear Research, Russia	Lattice parameter changes under ordering in Fe-Al(Cr) and Fe-Ga alloys
FM - 28	Targonskiy Anton	NRC "Kurchatov Institute", Russia; FSRC "Crystalloraphy & photonics" RAS, Russia	Adaptive X-ray optical elements based on combination of longitudinal and transverse acoustic waves in the kHz and MHz frequency ranges
FM - 29	Tsvigun Natalia	FSRC “Crystallography and Photonics” RAS, Moscow, Russia	The morphology of the structure of calcium carbonate $CaCO_3$, obtained in the process of biomineralization
FM - 30	Tyulyusov Anton	National Research Center «Kurchatov Institute» — Institute for Theoretical and Experimental Physics named by A.I. Alikhanov, Russia	Multiple ultra-small-angle neutron scattering on materials obtained by selective laser melting: theory and experiment
FM - 31	Vasin Roman	Joint Institute for Nuclear Research, Russia	Martensitic transformation in NiTi(Hf,Zr) shape memory alloys studied by TOF neutron diffraction
FM - 32	Wardecki Dariusz	Chalmers University of Technology, Sweden	A determination of CO_2 molecule sites in $K_{2x/3}Cu[Fe(CN)_6]_{2/3}$ with x = 0 and 1 at various temperatures and CO_2 gas pressures
FM - 33	Yoskamtorn Tatchamapan	Wolfson Catalysis Centre, Department of Chemistry, University of Oxford, UK	Elucidation of the structural geometries and the ammonia-responsive behaviors of Zr-based metal-organic frameworks
FM - 34	Zhang Yifei	Division of Applied Surface Chemistry, Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Sweden	Structure of quaternary type-I clathrate $Ba_8(Al_xGa_{1-x})_{16}Ge_{30}$

Engineering Applications

ID	Participant	Organization	Title
EA - 1	Coppola Roberto	ENEA-Casaccia, FSN-SICNUC, Italy	Stress distributions in P91 martensitic steel and in AISI 316LN steel welds for Gen IV nuclear applications
EA - 2	Dovzhenko Gleb	Helmholtz-Zentrum Geesthacht, Germany	Residual Stresses and Temperature Fields in AA6082 Friction Surfacing
EA - 3	Gan Weimin	GEMS at MLZ, Helmholtz-Zentrum Geesthacht, Germany	In-situ neutron diffraction study of engineering materials under thermo-mechanical treatment at STRESS-SPEC
EA - 4	Hoelzel Markus	TU Munich, FRM II / MLZ, Germany	Diffraction based determination of single-crystal elastic constants on polycrystalline titanium alloys
EA - 5	Huang Yuanding	MagIC, Helmholtz-Zentrum Geesthacht, Germany	In-situ neutron diffraction study on compressive behavior of solution heat-treated Mg-Ca alloys at room and elevated temperature
EA - 6	Isakova Natalia	National Research Centre "Kurchatov Institute", Russia	Two-directional stress-free comb sample for neutron stress diffractometry
EA - 7	Karpov Ivan	National Research Centre "Kurchatov Institute", Russia	Neutron diffraction research of residual stress in thin 410 steel plate, deposited on rigid substrate by DLMD method
EA - 8	Kononikhina Victoria	Helmholtz-Zentrum Geestacht, Germany	The order/disorder transformation of OI phase in binary and ternary Oi TiAl based alloys studied by synchrotron and neutron diffraction
EA - 9	Kucerakova Monika	Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic	Investigation of textures of alpha zirconium and zirconium-alloy by neutron and X-ray diffraction

EA - 10	Makhmudov Khairullo	Ioffe Institute, Russia	A study of the acoustic properties of rock massif and concrete lining under natural conditions
EA - 11	Michtchenko Alexandre	Instituto Politecnico Nacional, SEPI-ESIME-Zacatenco, Mexico	Printed technologies for supercondensators - one of the applications of graphen-like materials
EA - 12	Mikhail Egorov	Saint-Petersburg State University of Aerospace Instrumentation, Russia	Efficiency upgrade of separator-superheaters in NPP with pressurized water and boiling water reactors by physical-modeling based modernization
EA - 13	Murashev Mikhail	National Research Centre "Kurchatov Institute", Russia	The method for neutron imaging of components with lattice structure, produced by additive manufacturing
EA - 14	Noguera Crespo Pedro	AVS	New small-angle scattering beamlines for MAX IV and SIRIUS synchrotrons
EA - 15	Ohl Michael	Forschungszentrum Julich, Jllich Centre for Neutron Science, Germany	Boosting charge transport in Poly(ethylene-oxide) comb polymers for applications in Li-ion batteries
EA - 16	Protsenko Andrey	National Research Centre "Kurchatov Institute", FSRC "Crystallography and Photonics" RAS, Russia	QEXAFS methods development using X-ray adaptive bending piezo-actuator
EA - 17	Romanelli Giovanni	ISIS Facility, Rutherford Appleton Laboratory, UK	Visualisation of the catalysed nuclear-spin conversion of molecular hydrogen using energy-selective neutron imaging
EA - 18	Rylov Sergey	National Research Centre "Kurchatov Institute", Russia	Residual stress investigation by neutron diffraction in a 7.4 mm thick Inconel 625 plate produced by direct metal laser deposition (DLMD) on rigid substrate
EA - 20	Soria Sergio	Forschungs-Neutronenquelle FRM II, Technische Universitat Munchen, Germany	Quantification of phases by strain-induced martensitic transformation in Austempered Ductile Iron (ADI) using neutron transmission

EA - 21	Strunz Pavel	Nuclear Physics Institute of the CAS, Czech Republic	Evaluation of anisotropic small-angle neutron scattering data from metastable OI-Ti alloy
EA - 22	Strunz Pavel	Nuclear Physics Institute of the CAS, Czech Republic	Neutron diffraction study of Ti-Zr alloy microstructure evolution during annealing after severe plastic deformation
EA - 23	Tsapatsaris Nikolaos	European Spallation Source, Sweden	Correlation of Microstructural Damage o Functional Properties of Irradiated Carbon Fibre Based Composites Used in Neutron Chopper Discs
EA - 24	Lychagina Tatiana	Joint Institute for Nuclear Research	The comparison of neutron pole figure extraction methods
EA - 25	Yang Bin	Collaborative Innovation Center of Steel Technology, University of Science and Technology Beijing	Enhanced radiation and corrosion resistance of 316LN stainless steel with high densities of dislocations and twins

Neutron Instrumentation

ID	Participant	Organization	Title
NI - 1	Alba Venero Diego	Isis neutron and muon source, Rutherford Appleton Laboratory, UK	Zoom, a polarised small angle neutron scattering diffractometer at ISIS target station II
NI - 2	Appavou Marie-Sousai	Juelich Centre for Neutron Science at Maier Leibnitz Zentrum, Germany	Cryo-TEM – A Complementary Technique for Neutron Scattering
NI - 3	Backis Alexander	European Spallation Source (ESS), Sweden	Characterization of the boron-based Multi-Grid detector on the thermal neutron spectrometer SEQUOIA at the SNS
NI - 4	Beddrich Lukas	Heinz Maier-Leibnitz Zentrum, Germany	In-situ, bellow-driven pressure cell for neutron scattering investigations in hydrostatic conditions
NI - 5	Belushkin Alexander	JINR, Institute of Physics, Kazan Federal University, Dubna State University, Russia	Study of $LiInSe_2$ single crystals for the thermal neutron detection
NI - 6	Bergback Knudsen Erik	DTU Physics, Denmark	Latest Developments in McStas for Polarized Neutron Experiment Simulation
NI - 7	Bertelsen Mads	European Spallation Source ESS ERIC, Sweden	McStas Union components and python interface
NI - 9	Blostein Juan Jeronimo	CONICET - Instituto Balseiro, Argentina	Neutron detection by using Water Cherenkov Detectors
NI - 10	Bobrikov Ivan	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	High-resolution Fourier diffractometer at the IBR-2 pulsed neutron source
NI - 11	Bokuchava Gizo	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	Fourier diffractometer FSS at the IBR-2 pulsed reactor
NI - 12	Boyd Hannah	Malmö University, Sweden	Development of a sample environment for the study of mechanically confined and sheared geometries

NI - 13	Buffer Jean-Claude	Institut Laue Langevin, France	3He linear PSD for SANS, reflectometry, and TOF instruments: Two decades of development at the ILL
NI - 14	Chetverikov Yuriy	PNPI, Russia	Study of periodic density modulation in holographic diffraction gratings
NI - 15	Chudoba Dorota	FP AMU, Poland, FLNP JINR, Russia, SPBU, Russia	New TOF INS spectrometer at FLNP JINR
NI - 16	Deen Petronella Pascale	Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany, European Spallation Source ESS ERIC, Sweden	CSPEC: Development of the cold chopper spectrometer of the ESS
NI - 17	Desert Sylvain	Laboratoire Leon Brillouin, France	International Society of Neutron Instrument Engineers (ISNIE)
NI - 18	Dewhurst Charles	Institut Laue-Langevin, Grenoble, France	ILL Modernisation Programme: Endurance. The ambitious renewal of the H15 cold neutron guide and instrumentation
NI - 19	Dian Eszter	Hungarian Academy of Sciences, Centre for Energy Research, Hungary	Complex Geant4 Simulation Study for Background Suppression in the Multi-Grid Detector
NI - 20	Doege Stefan	Technical University of Munich, Germany	New Aspects of Ultracold Neutron Scattering in Condensed Deuterium and on Material Surfaces
NI - 21	Durniak Celine	Data Management and Software Centre, The European Spallation Source ERIC, Denmark	Universal library of models for Quasi Elastic Neutron Scattering
NI - 22	Dzheparov Fridrikh	NRC "Kurchatov Institute" - ITEP, Russia	Correction of the Fermi pseudopotential conception in the theory of dynamic scattering of thermal neutrons
NI - 23	Em Viacheslav	National Research Center «Kurchatov Institute», Russia	Study of through-thickness stress distribution in steel double-V butt weld

NI - 24	Erhan Raul Victor	Institute for Energy Technology, Norway	FREYJA – a new multipurpose time-of-flight neutron reflectometer at the JEEP II reactor in Norway
NI - 25	Fabrykiewicz Piotr	Faculty of Physics, University of Warsaw, Poland	Studies of the d-spacing distribution in powder alpha-Fe_2O_3 and $CaCO_3$ by Larmor diffraction
NI - 26	Fenske Jochen	Helmholtz-Zentrum Geesthacht, Germany	Design and features of the Engineering Diffractometer BEER at ESS
NI - 27	Formisano Ferdinando	IOM-CNR Italy, Operative Group in Grenoble (OGG), c/o Institut Laue Langevin, France	The project of the spectrometer BRISPX
NI - 28	Funama Fumiaki	Department of Nuclear Engineering, Kyoto University, Japan	Observation of TOF-MIEZE signals with focusing mirrors at BL06 at J-PARC MLF
NI - 29	Fuzi Janos	MTA Wigner RCP Budapest, Neutron Spectroscopy Department, Hungary	Neutron Beam Tests of ESS Test Beamline Components
NI - 30	Gabold Henrik	Technical University Munich, Germany	Development of a Miniture Polarisation Analysis Device
NI - 32	Gordienko Ekaterina	National Research Center «Kurchatov Institute», Russia	Gd-loaded scintillation ceramics - a flexible detector material for neutrons
NI - 33	Gorkov Dmytro	Institute of Physics II, University of Cologne / FRMII, Germany	KOMPASS – the polarized cold neutron triple-axis spectrometer at the FRM II
NI - 34	Granada Rolando	Argentine Atomic Energy Commission (CNEA), Argentina	Scattering kernel and neutron transport properties of nanodiamond at cold and thermal energies
NI - 35	Gunther Gerrit	Helmholtz-Zentrum Berlin, Germany	Implementation of polarized neutron spectroscopy on TOF spectrometer NEAT at Helmholtz-Zentrum Berlin
NI - 36	Gutfreund Philipp	Institut Laue-Langevin, France	Neutron Reflectometry at ILL on D17 and FIGARO: Recent Developments

NI - 38	Hino Masahiro	Institute for Integrated Radiation and Nuclear Science, Kyoto University, Japan	Recent development of multilayer neutron mirror at KURNS
NI - 39	Holmes Alexander	European Spallation Source ERIC, Sweden	Huginn: peltier-based temperature controlled sample platforms for neutron scattering
NI - 40	Ionita Ion	Institute for Nuclear Research, Valahia University Targoviste, Romania	Developping a High Resolution Focussing Configuration for the Pitesti TRIGA Reactor Neutron Diffractometer
NI - 41	Ivanov Alexandre	Institut Laue-Langevin, France	From IN8 to THERMES - development of the thermal three-axis spectrometer at ILL
NI - 42	Jaksch Sebastian	Juelich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Germany	The SoNDe high-flux neutron detector
NI - 43	Juranyi Fanni	Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Switzerland	Design of the new guide for the time-of-flight spectrometer Focus at SINQ
NI - 44	Kai Tetsuya	Japan Atomic Energy Agency, Japan	Visualization of the boron distribution in simulated melted core material by neutron energy resolving method
NI - 45	Kalyukanov Andrew	National Research Center «Kurchatov Institute», Russia	New control system for single crystal diffractometer MOND at reactor IR-8
NI - 46	Karpati Peter	Neutron Spectroscopy Department, Wigner Research Centre for Physics, Hungary	Large Phase Space Extraction with High Time Resolution at ESS
NI - 48	Kireenko Yurii	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Unconventional neutron guides for horizontal sample reflectometers
NI - 49	Kittelmann Thomas	European Spallation Source ERIC, Sweden	NCrystal: a library for thermal neutron transport

NI - 50	Klenke Jens	Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Germany	The MEPHISTO beam port for nuclear and particle physics at FRM II
NI - 51	Klepp Juergen	University of Vienna, Austria	Observation of Slow-Neutron Diffraction from Holographic Nanodiamond Composite Gratings
NI - 52	Klinkby Esben	DTU Nutech,Technical University of Denmark, Denmark	Interfacing multiple simulations using Monte Carlo Particle Lists, MCPL
NI - 53	Kocharyan Vahan	National Research Tomsk Polytechnic University, Russia	Control of thermal neutron and hard X-ray beam parameters under external influences
NI - 54	Koehli Markus	Physikalisches Institut, Heidelberg University, Germany	URANOS - a voxel engine Neutron Transport Monte Carlo Simulation
NI - 55	Kolevatov Rodion	Dept. for Neutron Materials Characterization, Institute for Energy Technology, Norway	Prompt gamma shielding of neutron guides from ray-tracing Monte-Carlo simulations
NI - 56	Kraan Wicher	TU Delft (retired), Netherlands	Progress in simulating realisation SESANS at the reactor PIK
NI - 57	Kreuzpaintner Wolfgang	Materials Science and Engineering Program Guangdong Technion-Israel Institute of Technology	In situ Thin Film Growth Capabilities for Polarized Neutron Reflectometry
NI - 58	Kruglov Vladimir	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	Development of a new wide-aperture backscattering detector (BSD) for the HRFD diffractometer on IBR-2 facility
NI - 59	Lee Jeong Soo	Korea Atomic Energy Research Institute, South Korea	Current status of neutron reflectometer at HANARO
NI - 60	Leemreize Hanna	DTU Physics, Danish Technological Institute, Denmark	Full field neutron microscopy based on refractive optics
NI - 61	Litvin Vasily	Institute for Nuclear Research RAS, Russia	Neutron reflectometry at spallation neutron source IN-06 of INR RAS

NI - 62	Litvinenko Elena	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	Comparative study of the characteristics of the data acquisition systems for position-sensitive detectors with a delay line on the neutron instruments of the IBR-2 reactor
NI - 63	Lupberger Michael	University of Bonn, Germany	The Scalable Readout System: A generic readout system for next generation detectors
NI - 65	Magerl Andreas	University Erlangen-Nürnberg, Germany	GaAs-extension on IN16B for improved energy resolution in backscattering
NI - 66	Mangiapia Gaetano	German Engineering Material Science Centre am Maier-Leibnitz Zentrum, Germany	REFSANS: The horizontal time-of-flight reflectometer with GISANS option at the Heinz Maier-Leibnitz Zentrum
NI - 67	Marais Deon	Necsa SOC Ltd, Research and Technology Development, South Africa	Implementation of attenuation correction procedures for position resolved neutron powder diffraction studies
NI - 68	Marko Marton	Wigner Research Centre for Physics, Hungary	Generalization of Bewley splitter: Application for fast pulse shaping
NI - 69	Matveev Pavel	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Software project for the texture diffractometer (TEX) as an element of the instrumental base of the PIK reactor
NI - 70	Maulerova Vendula	European Spallation Source ERIC, Sweden	Beam Monitors at ESS
NI - 71	Mauri Giacomo	European Spallation Source ERIC, Sweden	Neutron reflectometry with the Multi-Blade detector, correlation between detector performance and scientific output
NI - 72	Meven Martin	RWTH Aachen University, Institute of Crystallography, Germany	Single Crystal Diffraction Experiments under Extreme Conditions with Hot Neutrons on HEiDi
NI - 73	Mikula Pavol	Nuclear Physics Institute ASCR, Czech Republic	High resolution analysis with bent perfect crystal (BPC) in powder diffraction - I

NI - 74	Mikula Pavol	Nuclear Physics Institute ASCR, Czech Republic	High resolution analysis with bent perfect crystal (BPC) in powder diffraction - II
NI - 75	Moore Michael	Department of Nuclear Engineering, University of Tennessee, USA	Microstructured multicore SCIntillating FIber (SCIFI) for high resolution thermal neutron radiography
NI - 76	Morgano Manuel	Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen PSI, Switzerland	The ODIN instrument at ESS
NI - 77	Morkovnikov Ivan	Joint Institute for Nuclear Research, Russia	Service for storage of measurement results from the spectrometers of the IBR-2 reactor
NI - 78	Moskvin Evgeny	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Novel sputtering facility at NRC KI - PNPI
NI - 79	Niedermayer Christof	Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland	Technical design and performance of the novel multiplexing spectrometer CAMEA
NI - 80	Noferini Daria	Forschungszentrum Jülich GmbH, JCNS at MLZ, Germany	Upgrades at the high-resolution backscattering spectrometer SPHERES
NI - 81	Nowak Gregor	Helmholtz-Zentrum Geesthacht, Germany	Design study of a new 1m2-Multi-Wire-Proportional-Chamber Neutron detector
NI - 82	Orban Janos	Wigner Research Centre for Physics, Hungary	Evaulation of beam diagnostic apparatus
NI - 83	Perelli Cippo Enrico	Istituto di Fisica del Plasma - CNR, Italy	Development of a GEM-based neutron transmission detector for 2D-resolved TOF measurements
NI - 84	Perrichon Adrien	Department of Physics and Astronomy, Uppsala University, Sweden	Neutron ray-tracing simulations for the upgrade of the OSIRIS spectrometer

NI - 85	Ponsonby Joel	ISIS, STFC, Rutherford Appleton Laboratory, UK	In-situ calorimetry with Quasi-Elastic Neutron Spectroscopy: current developments realising a complimentary dynamic and thermodynamic sample description
NI - 86	Quan Yifan	Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institute, Switzerland	A novel transportable neutron spin filter based on dynamically polarized protons
NI - 89	Rofors Emil	Lund University, Sweden	Response of a Li-glass/multi-anode photomultiplier detector to O±-particles from Am-241
NI - 90	Sadilov Valentin	State University of Dubna, Russia	First experimental test of the time-gradient magnetic field SESANS prototype
NI - 91	Sadykov Ravil	Institute for Nuclear Research, Russia	Hemispherical high-pressure cells for inelastic neutron scattering studies of proton dynamics in materials
NI - 92	Salhi Zahir	Julich Centre for Neutron Science at the Heinz Maier-Leibnitz Zentrum, Germany	High performance in-situ 3He-NSF polarizer for Thermal neutrons and analyzer for cold neutrons
NI - 93	Saroun Jan	Nuclear Physics Institute of the CAS, Czech Republic	Neutron ray tracing: from modelling of instruments to analysis of experimental data
NI - 94	Scheffzuek Christian	Frank Laboratory of Neutron Physics, JINR, Russia; Institute of Applied Geosciences, Karlsruhe Institute of Technology, Germany	The neutron time-of-flight strain/stress diffractometer EPSILON with extended sample environment for investigations in material and geoscience
NI - 95	Scionti Giuseppe	University della Calabria, Italy	Neutronic calculations for shielding designing of the VESPA instrument at the European Spallation Source
NI - 96	Seki Yoshichika	J-PARC Center, Japan Atomic Energy Agency, Japan	Phase imaging using pulsed polarized neutrons with Talbot-Lau interferometer

NI - 97	Shushunov Mikhail	National Research Center «Kurchatov Institute», Russia	Creation of a facility for radiography and tomography on channel 7B of the IR-8 reactor of the NRC “Kurchatov Institute”
NI - 98	Skoro Goran	ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, UK Research and Innovation, STFC, UK	Neutronics and everyday life at a neutron source
NI - 99	Skoulatos Markos	Heinz Maier-Leibnitz Zentrum (MLZ) and Physics Department E21, Technical University Munich, Germany	Relocation of the cold triple axis spectrometer FLEXX to MLZ, Munich: Larmor diffraction and more
NI - 100	Steffens Paul	Institut Laue-Langevin, France	MARMOT - New generation multiplexed analyser unit for cold Triple Axis Spectroscopy
NI - 101	Sumbatian Armen	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Hardware project for the texture diffractometer (TEX) as an element of the instrumental base of the PIK reactor
NI - 102	Syromyatnikov Vladislav	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Using a new type of chopper in neutron reflectometry
NI - 103	Thijs Michel	Delft University of Technology, Netherlands	SEMSANS with RF flippers: calculation and realisation
NI - 104	Tovar Michael	Helmholtz-Zentrum Berlin fur Materialien und Energie, Germany	Capabilities of applying neutron Laue diffraction
NI - 105	Trunov Dmitry	National Research Center «Kurchatov Institute», Russia	Multichannel scintillation neutron detector for microsample research under high-pressure
NI - 106	Vicente Alvarez Miguel	Neutron Physics Department/LAHN Project, Centro Atómico Bariloche, CNEA, Argentina	Present status of the ANDES, a multi-purpose neutron diffractometer for LAHN
NI - 107	Stepanova Angelina	Petersburg Nuclear Physics Institute of National Research Center “Kurchatov Institute”, Russia	Compact neutron supermirror transmission polarizer for SANS

NI - 108	Ward Simon	Data Management and Software Centre; European Spallation Source, Denmark	Using the LSWT engine SpinW in an experimental workflow.
NI - 109	Widmann Tobias	Technische Universitat Munchen, Physik-Department, Lehrstuhl für Funktionelle Materialien, Germany	3D printed humidity chamber for neutron scattering experiments
NI - 110	Willendrup Peter	Department of Physics, Technical University of Denmark, Denmark	Progress in simulation software, shielding methods and compact Larmor devices: A status report from SINE2020 WP8
NI - 111	Wolf Marcell	Technical University of Munich, Germany	Time-of-flight spectrometer TOFTOF at FRM2
NI - 112	Wuttke Joachim	Forschungszentrum Jülich, JCNS-MLZ, Germany	Multiple Bragg reflection by mosaic crystals
NI - 113	Yamada Masako	Research with Neutrons and Muons, Paul Scherrer Institute, Switzerland	Neutron field spectrometry at high energy neutron facilities with extended range Bonner Sphere Spectrometer system
NI - 114	Yano Shin-ichiro	National Synchrotron Radiation Research Center, Taiwan	Recent Issues from Taiwan’s cold triple axis spectrometer SIKA at ANSTO
NI - 115	Ye Jingfan	Technische Universität München, Physik-Department, Germany	Setup for in situ Neutron Reflectometry on Magnetic Thin Films
NI - 116	Yokoo Tetsuya	J-PARC Center and KEK, Japan	Suite of the Neutron Spectrometers in J-PARC
NI - 117	Zimnik Samantha	Karlsruhe Institute of Technology, Institute for Applied Materials - Energy Storage, Germany	
NI - 118	Zobel Mirijam	University Bayreuth, Germany	Free-Film SANS - Container-free in-situ sample environment for neutron scattering

Soft Condensed Matter

ID	Participant	Organization	Title
SCM - 1	Akiyama Tomoko	Uppsala University, Sweden	Topological Interactions In Polymers Under Shear
SCM - 2	Almasy Laszlo	Wigner Research Centre for Physics, Hungary	Microscopic origin of the scattering in aqueous amine mixtures: X-ray and neutron experiments versus simulations
SCM - 3	Anghel Lilia	Institute of Chemistry, Republic of Moldova	Glucose oxidase from Aspargellius niger studied by small angle neutron scattering
SCM - 4	Balasoiu Maria	Horia Hulubei National Institute for Physics and Nuclear Engineering, Romania	Structure organization of silicone-rubber based magnetic and magnetorheological elastomers reveled by means SANS and neutron depolarization methods
SCM - 5	Brok Erik	Niels Bohr Institute, University of Copenhagen, Denmark	Small-angle scattering of interpenetrating polymer networks (IPNs) as medical devices with reduced risk of infection
SCM - 6	Bryant Gary	Centre for Molecular and Nanoscale Physics, School of Science, RMIT University, Australia	Elucidating the mechanisms of small molecule cryoprotection using Neutron Membrane Diffraction
SCM - 8	Cristiglio Viviana	Institut Laue Langevin, France	Influence of freezing conditions on the protein stability during freeze-drying and long-term storage of biopharmaceuticals
SCM - 9	De Francesco Alessio	CNR IOM c/o OGG, France	Model free description of polymer coated gold nanoparticle dynamics in aqueous solutions obtained by Bayesian analysis of neutron spin echo data
SCM - 10	Dudas Zoltan	Neutron Spectroscopy Department, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary	SANS study of organically modified silicas obtained by sol-gel technique

SCM - 11	Dudas Zoltan	Neutron Spectroscopy Department, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary	Structural modification induced by different doping concentration of Ce^{3+} in silica gels. A SANS study
SCM - 12	Ermakova Elena	Joint Institute for Nuclear Research, Russia & Faculty of Pharmacy, Comenius University, Bratislava, Slovakia	Influence of divalent cations of essential metals on the structure of lipid membranes: SAND study
SCM - 14	Gorshkova Yulia	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	Supramolecular gels based on lithocholic acid and its derivatives: Small-angle neutron scattering vs. atomic force microscopy
SCM - 15	Grzimek Veronika	Helmholtz-Zentrum Berlin fur Materialien und Energie, Germany	Nanoscale mechanics and energy storage in porous materials: neutron scattering insight
SCM - 16	Hori Koichiro	Sumitomo Rubber Industries, Ltd., Japan	Dynamics of Rubbery Dead Layers Bound on Carbon Surfaces
SCM - 17	Houston Judith	European Spallation Source, Sweden	Small-angle neutron scattering and in situ UV/Vis absorption spectroscopy of photosurfactant worm-like micelles
SCM - 18	Sergey Grigoriev	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Classification of fractal objects by SANS: case of the logarithmic fractal
SCM - 19	Jestin Jacques	Laboratoire Leon Brillouin, France	Dynamical exchange lifetime of the bound layer on silica nanoparticles in nanocomposites
SCM - 20	Kopitsa Gennady	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Structure of the monolithic nanostructured aluminium oxohydroxide (NOA): small angle scattering studies
SCM - 21	Krauss Sebastian	University Bayreuth, Germany	SANS investigations on ligand shells during CdS nanoparticle formation
SCM - 23	Kruteva Margarita	Julich Centre for Neutron Science, Germany	Stabilization of Proteins in Nanopores

SCM - 24	Kucerka Norbert	Frank Laboratory of Neutron Physics at Joint Institute for Nuclear Research, Russia	Hydration Interactions in Model Membranes Studied by Neutrons
SCM - 25	Kulvelis Yuri	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Structure studies of detonation nanodiamonds complexes with metal ions and poly(vinylpyrrolidone) by small-angle neutron scattering
SCM - 26	Lebedev Vasily	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Ordering mixtures of diamagnetic and paramagnetic fullerenols in aqueous solutions in magnetic fields
SCM - 27	Len Adel	MTA Centre for Energy Research, Nuclear Analysis and Radiography Department, Hungary	SANS measurements on new Rh(III) chromonic-like coordination complexes
SCM - 28	Lind Tania	Biofilms Research Center for Biointerfaces, Dept. of Biomedical Science, Faculty of Health and Society, Malmo University, Sweden	Formation and characterisation of supported lipid bilayers composed of POPE and POPG by vesicle fusion - a simple but relevant model for bacterial membranes
SCM - 29	Liu Pengfei	Queen Mary University of London, UK	Interaction of Stimuli Responsive Nanogels with Proteins at the Interface: a Neutron Reflectivity Study
SCM - 31	Metwalli Ezzeldin	Institute for Crystallography and Structural Physics, Friedrich-Alexander-Universitat Erlangen-Nurnberg, Germany	A portable SAXS system for simultaneous SANS/SAXS measurements at ILL
SCM - 32	Michalska Joanna	Julich Centre for Neutron Science, Forschungszentrum Julich GmbH, Germany	Collapse-kinetics of block copolymer PS-PNIPAM and PnBA-PNIPAM micelles
SCM - 33	Mora Cardozo Juan Francisco	Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland	Equilibrium structure, hydrogen bonding and proton conductivity in half-neutralised diamine ionic liquids
SCM - 34	Motlaq Vahid	Uppsala University, Sweden	Amphiphilic properties of drug molecules and their self-assembly in presence of phospholipids

SCM - 35	Naidjonoka Polina	Lund University, Physical Chemistry, Sweden	On the interaction of softwood hemicellulose with cellulose surfaces in relation to molecular structure and physicochemical properties of hemicellulose
SCM - 36	Nemoto Fumiya	IMSS / J-PARC Center, High Energy Accelerator Research Organization (KEK), Japan	Neutron reflectivity studies on crystal growth of cocoa butter at the solid substrate
SCM - 37	Patel Vijaykumar	J. N. M. Patel Science College, India	Investigations on surface active ionic liquid micelles modulated by bile salts: A SANS study
SCM - 39	Saini Apurve	Uppsala University, Sweden	Macroscopic Alignment of Micellar Crystals with Magnetic Micro-Shearing
SCM - 40	Saini Apurve	Uppsala University, Sweden	Structural ordering of Magnetic Nanoparticles in a Ferrofluid on Silicon Surfaces
SCM - 41	Schoenhals Andreas	Bundesanstalt fuer Materialforschung und в-pruefung, Germany	Vibrational density of states and molecular mobility in a polymer with intrinsic microporosity PIM-1 as revealed by inelastic neutron scattering
SCM - 42	Schweins Ralf	Institut Laue - Langevin, France	Elucidating the self-assembly of dendrimers and oppositely charged dyes using small-angle neutron scattering and itsothermal titration calorimetry
SCM - 43	Skoi Vadim	Joint Institute for Nuclear Research, Russia	Changes in the structural parameters of model membranes of DMPC phospholipid under high pressure by the SANS method
SCM - 44	Tian Bei	Delft University of Technology, Netherlands	Size and structure of fibres in meat analogues studied by neutron scattering
SCM - 47	Zajac Wojciech	Institute of Nuclear Physics Polish Academy of Sciences, Poland	Towards understanding of glass-forming by some isomers of globular alcohols. A QENS approach
SCM - 47	Velichko Evgenii	Delft University of Technology	Combining rheology and small-angle scattering of neutrons and X-rays for dynamic assessment of microfibrillated cellulose under shear

Thin Films and Interfaces

ID	Participant	Organization	Title
TF&I - 1	Arakelian Vladimir	Vladimir State University, Russia	Controllable electrophysical and optical properties of granulated thin films: the 4D-laser-induced topological nanoclusters
TF&I - 2	Guasco Laura	Max-Planck Institute for Solid State Research, Germany	Exchange interactions at the manganite/manganite interface of FM/AFM type
TF&I - 3	Gubanova Nadezhda	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Institute of Silicate Chemistry of the Russian Academy of Sciences, Russia	Thin silica films containing bimetallic Pt/Pd nanoparticles
TF&I - 4	Kilbride Rachel	Department of Physics and Astronomy, The University of Sheffield, UK	Investigating the Effect of Processing Conditions on the Vertical Profile of Non-Fullerene Organic Bulk Heterojuntion Thin Films
TF&I - 6	Maranloo Zahra	Technical University of Munich, Germany	Skyrmions in multilayers Fe/Gd: Investigation of the morphology
TF&I - 7	Matveev Vasilii	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Combination of neutron and X-ray reflectometry for the investigation of thin metal films and multilayers
TF&I - 8	Paul Amitesh	Technical University Munich, Germany	Grain boundary self-diffusion in $^{56}Fe/^{57}Fe$ multilayers by in situ neutron reflectometry
TF&I - 10	Trunk Markus	TU Munchen, Physik-Department, Elementarteilchen bei niedrigen Energien, Germany	The Neutron Depth Profiling Instrument N4DP at the Heinz Maier-Leibnitz Zentrum in Garching, Germany
TF&I - 11	Veres Tamas	Wigner Research Centre for Physics, Hungary	Depth Profile of Replicated Interface Roughness Correlation in NiTi Supermirrors by GISANS

TF&I - 12	Zhaketov Vladimir	Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia	Relaxation of magnetization in the ferromagnetic-superconducting structure V/Fe70%V30%/V/Fe70%V30%/Nb, measured by real-time neutron reflectometry
TF&I - 13	Nikova Ekaterina	Institute of Metal Physics UB RAS	Development of reference layer method in resonant neutron reflectometry
TF&I - 14	Grigoryeva Natalia	Saint-Petersburg State University	Structure and magnetic properties of the SiO_2(Co)/GaAs and SiO_2(Co)/Si interfaces

Disordered Systems and Liquids

ID	Participant	Organization	Title
DS&L - 1	Almasy Laszlo	University of Messina, Italy	Micelle growth in cationic and anionic surfactant solutions
DS&L - 2	Azarova Liubov	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Saint-Petersburg State University, Russia	The model of crystallization in a fractal structure under conditions of a substance shortage: experimental study in case of zirconium dioxide
DS&L - 3	Borisova Polina	Moscow Technological University (MIREA), Russia	Effect of deuterium on phase transformations in amorphous phases of fullerenes at high temperatures (HT) and high pressures (HP)
DS&L - 4	De Panfilis Simone	Istituto Italiano di Tecnologia, Italy	Dynamics in water-methanol mixtures
DS&L - 5	Hansen Henriette Wase	Institut Laue-Langevin, Roskilde University, Chalmers Technical University, France, Germany, Sweden	High-pressure study on an ionic liquid with simultaneous dielectric and neutron spectroscopy
DS&L - 6	Kirillov Andrey	Institute for Physics of Mining Processes NAS, Ukraine	Investigation of tectonically disturbed zones of coal seams of the Kuznetsk coal basin using SANS
DS&L - 7	Lundin Filippa	Chalmers University of Technology, Department of Physics, Sweden	Local structure and dynamics in ionic liquids
DS&L - 9	Monet Geoffrey	LPS, University Paris Saclay – CNRS, France	Specific water structure in a geo-inspired nanotube and interrelated dynamics
DS&L - 10	Pustovoit Polina	Saint Petersburg State University, NRC "Kurchatov Institute" - Petersburg Nuclear Physics Institute	Classification of the fractal and non-fractal objects in two - dimensional space
DS&L - 11	Sharapova Tatyana	Dimitrovgrad Engineering and Technological Institute of the National Research Nuclear University MEPHI, Russia	The use of fractal analysis to assess the characteristics of the spread of radioactive substances in geological environments

DS&L - 12	Stefanopoulos Konstantinos	Institute of Nanoscience & Nanotechnology, NCSR "Demokritos", Greece	An In Situ Neutron Scattering Study upon Cooling Confined CO_2 on a Carbon Material below the Bulk Triple Point
DS&L - 13	Stoliarov Andrei	Institute for Nuclear Research RAS, Russia	Momentum distribution of nickel and niobium in the $Ni_{44}Nb_{56}$ metallic glass by neutron Compton scattering: isotopic substitution in action

Solid State Chemistry

ID	Participant	Organization	Title
SSC - 1	Nowicka-Scheibe Joanna	Joint Institute for Nuclear Research, Russia; West Pomeranian University of Technology, Poland	New organic compounds as materials with nonlinear optic properties
SSC - 2	Parshin Petr	National Research Center «Kurchatov Institute», Russia	Dependence of the phonon spectrum of narrow-gap semiconductor FeSi from atomic volume
SSC - 3	Rivin Oleg	Physics Department, Nuclear Research Centre - Negev, Israel	A Tungsten-based nano-laminated ternary carbide: $(W,Ti)_4C_{4-x}$
SSC - 4	Vottero Eleonora	Institut Laue-Langevin, France	How do the graphenic domains terminate in activated carbons? An INS & DFT study
SSC - 5	Yatoo Mudasir	Imperial College London, UK	Correlation of Local Structure and Oxygen Transport in Oxide Ion Conductors

Life Sciences

ID	Participant	Organization	Title
LS - 1	Blakeley Matthew	Institut Laue-Langevin, France	Visualizing hydrogen atoms and protons in proteins
LS - 2	Bode Kinga	Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, HAS, Hungary	Structural flexibility of thylakoid membranes revealed by small-angle neutron scattering
LS - 3	Combet Sophie	Laboratoire Leon-Brillouin, France	Human dystrophin structural changes upon binding to anionic membrane lipid
LS - 4	Doster Wolfgang	Technical University Munich, Germany	Are proteins dynamcially heterogeneous? A rotation-translation model combining elastic, time domain and multiple neutron scattering
LS - 5	Egorov Vladimir	Petersburg Nuclear Physics Institute of NRC "Kurchatov Institute", Smorodintsev Research Institute of Influenza, RMH; Federal State Budgetary Scientific Institution "Institute of Experimental Medicine", Russia	Chromatin Structural Organization And Protein-Oleic Acid Complexes
LS - 6	Fisher Zoe	European Spallation Source, Sweden	DEMAX: The Deuteration and Macromolecular Crystallization Support labs for the European Spallation Source
LS - 7	Gorshkova Yulia	Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Russia	Biohybrid entities with potential applications in biomedical field
LS - 8	Kuklin Alexander	Research center for molecular mechanisms of aging and age-related diseases, Moscow Institute of Physics and Technology, Russia	Complementarity of SAXS and SANS investigations of large protein complexes: SAXS/SANS EID and SEC-SAXS methods

LS - 9	Lattanzi Veronica	Division of Biochemistry and Structural Biology, Lund University, Sweden	Structural determinants for secondary nucleation pathway in Amyloid-beta fibrils formation by contrast variation SANS
LS - 10	Longo Marialucia	Julich Center for Neutron Science, Germany	Novel crystallization device for large protein crystal growth.
LS - 11	Mothander Karolina	Lund University, Physical Chemistry, Sweden	Lipid bilayer covered nanoweiers studied with GISANS
LS - 12	Nagy Gergely	Wigner Research Centre for Physics HAS, European Spallation Source ERIC, Sweden; Institute of Plant Biology, Biological Research Center HAS, Hungary	Effects of Stressors on the Macroorganisation of Thylakoid Membranes
LS - 13	Ostermann Andreas	Heinz Maier-Leibnitz Zentrum, Technische Universitat Munchen, Germany	Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum MLZ
LS - 14	Ramos Joao	Institute Laue Langevin, France	Protein and water dynamics at the atomic level: realistic atomic displacement parameters using neutron crystallography
LS - 15	Rudic Svemir	ISIS Facility, Rutherford Appleton Laboratory, UK	Inelastic neutron scattering study of gallic acid and its monohydrate
LS - 16	Ryzhykau Yury	Research center for molecular mechanism of aging and age-related diseases, Moscow Institute of Physics and Technology, Dolgoprudny, Russia	SANS study of the NpSRII/NpHtrII complex
LS - 17	Schmidt Alexander	Petersburg Nuclear Physics Institute of NRC "Kurchatov Institute", Russia	Small angle scattering study of Aspergillus awamori glucoamylase
LS - 18	Shvetsov Alexey	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Peter the Great St.Petersburg Polytechnic University, Russia,	A new method for calculating the SANS spectra including H_2O/D_2O contrast contribution estimation directly using all-atom molecular dynamics trajectories

LS - 19	Telling Mark	Science and Technology Facilities Council, UK	Probing structure and mobility of proteins in the amorphous state at low hydration
LS - 20	Usmanov Oleg	Petersburg Nuclear Physics Institute of NRC "Kurchatov Institute"	The enhancement of the proton therapy efficiency with PBCT
LS - 21	Vazina Alvina	Institute of Theoretical and Experimental Biophysics, RAS, Russia	Small-angle diffraction study of proteoglycan structures of mucins and extracellular matrix of biological tissues
LS - 22	Vlasov Aleksey	Research center for molecular mechanism of aging and age-related diseases, Moscow Institute of Physics and Technology, Russia	High-Throughput SANS characterization of lipidic in meso phases

Planetary Sciences and Extreme Conditions

ID	Participant	Organization	Title
PS&EC - 1	Litvak Maxim	Space Research Institute, Russia	Neutron component of radiation background at Mars
PS&EC - 2	Mitrofanov Igor	Institute for Space Research, Russia	Active neutron sensing of the Mars subsurface onboard the NASA's Marsrover Curiosity

Fundamental Science

ID	Participant	Organization	Title
FS - 1	Fedorov Valery	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Neutron spin rotation at Laue diffraction in a transparent weakly deformed noncentrosymmetric crystal
FS - 2	Kovalev Anatoliy	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Russia	Spontaneous breaking of time-reversal invariance at magnetic phase transitions
FS - 3	Pismak Yury	Department of elementary particles and high energy physics, Saint-Petersburg State University, Russia	Interaction of Dirac particles with two-dimensional materials in models of quantum electrodynamics with a singular background.
FS - 4	Semenikhin Sergey	Petersburg Nuclear Physics Institute of NRC «Kurchatov Institute», Peter the Great St.Petersburg Polytechnic University, Russia	Test of a new technique for ultra-precise neutron spectrometry

Cultural Heritage and Archaeometry

ID	Participant	Organization	Title
CH&A - 2	Di Martino Daniela	University of Milano-Bicocca, Italy	A multidisciplinary non-destructive study of historical pipe organ fragments
CH&A - 3	Kovalenko Ekaterina	National Research Center «Kurchatov Institute», Russia	Neutron imaging study of preservation of metal in the cultural heritage artefacts
CH&A - 4	Len Adel	MTA Centre for Energy Research, Nuclear Analysis and Radiography Department, Hungary	Small Angle Neutron Scattering analysis of early medieval pottery wares
CH&A - 5	Murashev Mikhail	National Research Center «Kurchatov Institute», Russia	Complex neutron studies of the cross-enkolpion of the XVI century from the Novodevichy Convent
CH&A - 6	Podurets Konstantin	National Research Center «Kurchatov Institute», Russia	Study of artifacts from the Chernaya Mogila burial mound (X CE) by neutron tomography and complementary methods
CH&A - 7	Rosta Laszlo	Budapest Neutron Centre, Hungary	Neutron methods for Heritage Science
CH&A - 8	Talmațchi Cristina	Museum of National History and Archaeology	Scientific Investigations regarding Ancient and Byzantine ceramics in Dobrudja, Romania
CH&A - 9	Ina Reiche	PSL, ENSCP, Institut de recherche de Chimie Paris-Centre de recherche et de restauration des musées de France	Trace elemental composition of Palaeolithic mammoth ivory as a valuable record of ancient human behaviour

Simulation of a Neutron Source at the KFSH&RC CS-30 Cyclotron

Shaykhah Alsaidan[1], Hanan Akhdar[2], Faisal Alrumayan[3], Khalid Kezzar[1]

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The aim of this work is to optimize the parameters of the neutron source of the CS-30 cyclotron at King Faisal Specialist Hospital & Research Center (KFSH&RC). The CS-30 cyclotron is a positive ion machine capable of accelerating protons with internal and extracted beam current up to 200μA and 60μA, respectively. Geant4 simulation package based on Monte Carlo methods with FTFP_BERT module physics list was used to study, and compare the energy spectra and angular distributions of the neutrons resulting from a 26.5 MeV proton beam on a 0.5 cm thick Beryllium-9 and Lithium-7 targets with Copper-63 back stop.

New data of upgrade of basic system of the pelletized cold moderator of the IBR-2 reactor

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The pelletized cold moderator of the IBR-2 reactor has been successfully operating for physical experiments since 2012. It has worked over 3500 hours since then. Due to the stable operation of the cold moderator, a large number of experiments with cold neutrons have been carried out at the IBR-2 spectrometers which show significantly improved results compared to a standard moderator based on room-temperature water. At the same time, the regular operation of the moderator would not be possible without modernization of its technological control system. Progress of the main moderator units, implemented in the course of its operation, is presented in the current paper.

New instrumentation in the JEEP II reactor at IFE, Kjeller: Norwegian Center for Neutron Research – NcNeutron

Stefano Deledda[1], Christoph Frommen[1], Geir Helgesen[1], Kenneth D. Knudsen[1], Isabel Llamas-Jansa[1], Magnus H. Sørby[1], Bjørn C. Hauback[1]

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The 2 MW JEEP II reactor at IFE in Kjeller, Norway has been in operation since 1967. Currently, a significant upgrade of the neutron scattering and imaging instrumentation is ongoing in the framework of a research infrastructure grant from the Research Council of Norway. The total investment to achieve a state-of-the-art instrumentation is approximately 10 mill. euro.

The current operating instrumentation includes: our upgraded SANS instrument (with cold neutrons), the powder diffractometer PUS, the amorphous materials diffractometer DIFF and the ESS test beamline R2D2.

The upgrade will include a new state-of-the-art time-of-flight neutron reflectometer FREYJA (with cold neutrons), a neutron radiography and tomography instrument NIMRA, a residual stress diffractometer NEST as well as a new cold moderator. This upgrade will be completed in 2020. With the NcNeutron research infrastructure the JEEP II reactor will become the regional neutron scattering and imaging facility in the northern Europe both before and from 2023 when the user program at the ESS in Lund, Sweden starts. This presentation will give an overview of NcNeutron with examples and possibilities for neutron scattering and imaging at the JEEP II reactor. The Research Council of Norway is acknowledged for financial support.

The ESS Linac

Mohammad Eshraqi[1], Mats Lindroos[1], Natalia Milas[1], Ciprian Plostinar[1], Björn Gålnander[1], YuanShuai Qin[1], Emelie Nilsson[1], Yngve Levinsen[1], Ryoichi Miyamoto[1]

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The European Spallation Source (ESS), currently under construction in Lund, Sweden, will be the world's most powerful linear accelerator driving a neutron spallation source, with an average power of 5 MW at 2.0 GeV. The linac accelerates a proton beam of 62.5 mA peak current at 4 % duty cycle (2.86 ms at 14 Hz). The accelerator uses a normal conducting front-end bringing the beam energy to 90 MeV, beyond that the acceleration up to 2 GeV is performed using superconducting structures. The first protons were accelerated at the ESS site during the commissioning of the ion source and low energy beam transport**,** that started earlier this year and will continue to the next stage of the commissioning up to 21 MeV later this year. This paper gives an overview of the status of the ESS accelerator and the commissioning of the ion source and the low energy beam transport.

Study of magnetic and quantum phenomena at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

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The suite of neutron instruments at the MLZ, located at the research reactor FRM II in Garching, provides a unique opportunity to study emerging properties of strongly correlated electron materials. The MLZ provides beam time for scientific use at its instruments, according to the decision of the review panel and under the condition of publishing the results.

In this poster presentation, we will introduce:

- the diffuse scattering neutron time of flight spectrometer with polarization analysis **DNS**,
- the universal cold three axis spectrometer **MIRA**,
- the small angle scattering diffractometers **KWS-1**, **KWS-3** and **SANS-1**,
- the magnetic reflectometer **MARIA**,
- the three axis spectrometers **PANDA** (cold) and **PUMA** (thermal),
- the polarized cold three axis spectrometer **KOMPASS,**
- resonance spin echo spectrometer **RESEDA**,
- and the spin echo three axis spectrometer **TRISP**.

Our recent highlights cover a broad variety of scientific fields such as frustrated magnetism (e.g. bilayer perovskite $Sr_3Fe_2O_7$ or lifetime of spin waves in 2D and 3D systems), magnetic excitations in insulators (e.g. in cobalt oxides), quantum phase transitions (e.g. absolute zero vibrations in superfluid helium or Higgs mechanism in quantum spin ice), superconductivity (e.g. nematic correlations in high temperature superconductors) or novel magnetic states (e.g. helimagnons, skyrmions, spiral spin-liquids), as well as magnetic nanoparticle ordering in bulk and self-assembly at interfaces.

Implementation of neutron reflection with Nano-dispersed media in Geant4

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A study has been carried out in order to see the feasibility of Nanodiamond Particles (NDP) application as a reflector for Cold Neutrons (CN), Very Cold Neutrons (VCN) and Ultra Cold Neutrons (UCN) in Geant4. NDP have a large scattering angle probability against VCN and UCN compared to the other materials due their high optical potential. This unique feature makes this powder a prominent candidate to be used as a reflector for VCN and UCN. Moreover, they can also be implemented for quasi-specular reflection of CN at small incidence angle due to multiple small-angle scattering of neutrons from nano-sized inhomogenities in the scattering potential. A new process has been prepared in order to add NDP cross sections to the predefined processes. The Three-Dimensional geometry of previous experiments carried out in order to observe the NDP reflection has been developed in Geant4, in order to validate the implementation. The results show that there is a good agreement between the new method implemented in Geant4 and the experimental data.

Materials Growth and Measurement Laboratory

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The Materials Growth and Measurement Laboratory (MGML; www.mgml.eu) is a Research Infrastructure operated by the Faculty of Mathematics and Physics, Charles University in cooperation with Institute of Physics of Czech Academy of Sciences. The main mission of MGML is to provide the broad scientific community unique possibilities for comprehensive experimental investigation of Condensed Matter Physic and Materials R&D. The MGML offers access to: i) broad range of top-class instrument suite for metals purification, novel materials synthesis and high-quality single-crystal growth finalized by structure and composition characterization and ii) large portfolio of physical characterization techniques focusing on measurements of material properties (thermodynamic, cohesive, magnetic, electrical and thermal transport, etc.) as a function of a wide range of external conditions (temperature, magnetic field, electric field, hydrostatic pressure, uniaxial stress).

Here we introduce the facility to users of neutron facilities which can use MGML for sample synthesis, characterization and measurement of physical properties needed to be done prior to neutron scattering experiments. The facility is closely connected with Czech neutron community and has a rich experience in growth and characterization of the samples for further neutron investigation.

The facilities are available in open access mode to all users from the scientific community. Researchers interested in using the MGML instrumentation are invited to submit experimental proposals via the User Portal (www.mgml.eu). The proposals will be evaluated by the MGML Panel according to their scientic excellence.

Polarized 3He recent developement at ILL

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Polarized 3He station TYREX at ILL is successfully used for neutron experiments since 2002, and provided 77% polarization routinely. The total amount per year increased from 30 to 200 bar.liters/year. To satisfy increasing request in future, ILL decided to upgrade the station. The production rate will be doubled to 2.5 bar.liter/hour and polarization will be push to 80%. We present the details of the project and recent development in the field.

Instruments control software at the IBR-2 reactor: features and prospects

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The Sonix package [1] is the main instrument control software at the IBR-2 reactor. It was originated in the beginning of 1990s for the Neutron Spectrometer with High Resolution (beam 6a of IBR-2). Later the complex was transferred to other instruments, including those located outside FLNP. A little bit less than 20 installations are in operation now. When developing the complex, we were guided both by world trends [2] as well as by the specifics of our laboratory. Many important requirements were formulated by our users, therefore they can be considered as real co-authors of the project.

Besides an instrument control itself, the complex also includes remote measurement supervising subsystem (WebSonix service) and the central repository for measurement results.

The presentation will review the main features and components of the complex, as well as plans for its future development.

[1] https://sonix.jinr.ru/wiki/doku.php?id=en:index
[2] https://www.nobugsconference.org/

The diffraction study of low-dimensional spin frustrated $CoSb_2O_6$

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In the quasi-two-dimensional magnets with acentric (chiral) crystal structure and a triangular lattice of magnetic atoms in a layer, the competition between exchange interactions, frustrations and anisotropy can revolutionary affect the fundamental mechanisms of spin ordering and the corresponding phase transitions. Low-dimensional spin frustrated systems assume noncollinear incommensurate spin orderings in order to reduce the degree of their spin frustration. It is inherent in $MnSb_2O_6$, a magnet with a chiral crystal and a cycloidal magnetic structure, a multiferroic with a unique ferroelectric switching mechanism [1,2].

We have discovered and synthesized a new rosiaite-type (s.g. *P-31m*) form of $MnSb_2O_6$ that is isostructural with $MnAs_2O_6$ and differs from the known form of $MnSb_2O_6$ (s.g. *P321*).

We also have synthesized and studied $CoSb_2O_6$ [3]. The $CoSb_2O_6$ sample was characterized by Rietveld analysis of the neutron powder diffraction patterns, magnetic susceptibility and specific heat temperature dependence measurements.

The appearance of additional reflections related to the antiferromagnetic ordering organization of the $CoSb_2O_6$ sample below T_N=13.5 K is clearly visible on the low-temperature neutron powder diffraction patterns measurement by the SPODI neutron powder diffractometer at Munich, Germany.

Magnetic structure is described by the propagation vecto **k** = (1/3, 1/3, 1/6). The carried out analysis of the spin interactions of resulting magnetic structure indicates that spin exchange interactions is not determining factor leading to the superstructure. At the same time the magnetic dipole-dipole interactions play important role in forming the magnetic superstructure.

The reported study was funded by RFBR according to the research project № 18-32-00297.

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Compact linac for neutron generation as a part of BELA project

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BELA (Based on ECR ion source Linear Accelerator) project is under design in NRC «Kurchatov Institute» – ITEP. The proton cw-linac is a key part of the project. The high intensity linac includes the 1.5 MeV RFQ and a set of DTL with step-by-step increasing of ion beam energy. Starting from 2.5 MeV the linac will be used as the neutron generator (with lithium target) for a set of practical applications such as boron neutron capture therapy, neutron activation analysis and many others. The accelerator technologies elaborated in framework of the BELA project will be a base for the project DARIA - neutron source Dedicated to Applied Research and Industrial Applications (S.-Petersburg State University) directed to the development of compact neutron generators for Universities, Scientific Centers and Industry. The current status of the project is presented.

A powerful UCN source at PNPI based on superfluid helium

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The WWR-M and PIK reactors at PNPI is planned to be equipped with a high-flux source for ultracold neutrons (UCNs). The method of UCN production is based on neutron conversion in superfluid helium, exploiting the particular qualities of that quantum liquid. As a result of optimizing the source parameters, we expect a UCN density up to 1.3×10^4 cm^{-3} in a neutron electric dipole moment (EDM) spectrometer. The expected flux densities of cold neutrons (with wavelengths in the range 2-20 Å) and very cold neutrons (50-100 Å) at the output of a neutron guide with a cross section of 30×200 mm^2 are 8.6×10^7 $cm^{-2}s^{-1}$ and 7.4×10^5 $cm^{-2}s^{-1}$, respectively. The capability of maintaining a temperature of 1.37 K at a thermal load of 60 W was shown experimentally, while the theoretical load is expected to be 37 W. Calculations show that it is possible to decrease the helium temperature down to 1.2 K at similar heat load. The project includes the development of experimental stations at UCN beams, such as for a neutron EDM search, measurements of the neutron lifetime, and for a search for neutron-to-mirror-neutron transitions. In addition, three beams of cold and very cold neutrons are foreseen. At present, the interchanel part of the UCN source has been manufactured and is waiting for installation to WWR-M reactor.

Modeling of the neutron radiation spectrum of plasma focus chambers

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Plasma focus (PF) devices are widespread pulsed neutron sources which realizes fusion reactions in pinch discharge. Underlying effect of plasma collapse by self magnetic field of discharge current (pinch-effect) leads to generation of high intensity pulses of electromagnetic radiation: light, from infrared to ultraviolet, soft X-ray (1÷5 keV) and hard X-ray to hundreds keV. When the plasma focus chambers are filled with deuterium (D) or deuterium-tritium (DT) mixture, then nuclear reactions D (d, n) He3 and D (t, n) He4 are carried out in them, respectively, and neutrons with an energy of 2.5 MeV or 14 MeV are generated . Neutron yield of plasma focus devices with DT filling reaches 10e13 neutrons per pulse and processes of neutron generation are extremely intensive (to 10e11 neutron/ns) and fast (neutron pulse with 10÷100 ns duration). Therefore plasma focus devices used as multifunctional sources of radiation in different laboratory experiments.

However for some tasks a narrow energy range of plasma focus devices (in fact 2.5 Mev or 14 MeV mono line) is a significant limitation. This paper describes the development of pulse neutron source with wide energy spectrum based on plasma focus devices. The effect of different scattering materials that surrounds plasma focus chamber is considered. It allows to convert 14 MeV neutrons to wide and rather gently slope spectrum with energies up to few MeV's. Also the possibility of neutron spectrum variation by changing of deuterium-tritium ratio in plasma focus filling is considered. Firstly paper shows the possibility of working with pure thritium PF chamber filling that provides neutron energy spectrum in range 1÷10 MeV. Neutron pulse duration on such PF chamber equals to 45 ns that is much higher than mean neutron pulse duration of PF chambers with DT filling (12÷15 ns). Secondly different types of PF chamber neutron spectrum when there are few mixture of T in mostly D filling are considered.

Cold Neutron Sources Historical Review

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The main purpose of the cold neutron sources (CNS) is to increase the flux of low-energy neutrons (below 5 meV) for both existing research reactors and newly created ones with a gain-factor of 10-50 times. This is achieved by installing a low-temperature moderator below 30K in a vacuum containment at the maximum of the thermal neutron flux mostly in the neutron reflector.

Over the past 60 years, cold neutron moderators have been developed and used for both research reactors and accelerator based neutron sources and they are still the most essential scientific multi-user devices for broad spectrum of neutron research. On the basis of literature review the analysis of different approaches was done for the design of cold neutron sources on reactors and accelerators all over the world presented in chronological order of their creation. More than 60 cold neutron sources are compiled in tables, historically starting in 1956 at Harwell until the proposed sources under construction at the research reactors and neutron spallation sources.

There are discussed the main aspects and criteria of design of high-intensity cold neutron sources on stationary reactors such as: the choice of the moderator substance and its optimisation; the gain-factor, flux and brightness; the shape and geometry of the moderator vessel and its optimal location in the reactor; the structural materials and the heat load; various methods of heat removal with their advantages and disadvantages.

Combined pelletized neutron moderator for IBR-2 reactor

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Cold neutrons with wavelengths over 4 Å emitted by high-current neutron sources have been employed in physical research since the 1980s. The cold-neutron flux is enhanced by using neutron moderators cooled to low temperatures. In these, neutrons are retarded when passing through different substances such as water, heavy water, ice, paraffin, beryllium, liquid hydrogen, liquid and solid methane, and various hydrocarbons. A neutron gradually loses its kinetic energy through multiple collisions with the nuclei of the moderator material.

In a modernization of IBR-2 reactor in 2006 was project of creation a cold neutron source. The source included three combine moderators around a reactor core. Moderators have a similar principle of work but different configuration of head part. The combine moderator is a different technical construction witch consist of a cold chamber (20K – 100K) for getting neutrons with long wavelengths and warm chamber (in some of it a water pre-moderator) for thermal neutrons. The substance for slowing neutrons on IBR-2 cold source was choose a mezetilene on solid phase and beads form.

In the presentation will be shown steps of creation the combine moderator of the “central” direction (CM201) of IBR-2 reactor on mezetilene pellets. Calculations and choosing a different various of configuration CM 201 moderator. Technical equipment for the moderator system. Experiment on full scale model of moderator CM201. Will be shown a dependent a neutron spectrum from temperature of moderator. The results of the test exploitation combine moderator (CM202).

Single shot neutron diffraction and spectroscopy at 100 T magnetic field ?

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A neutron source dedicated to pulsed magnetic fields with milli-Hz repetition rate around 5 minutes escapes the cooling and shielding challenges of e.g. the 5MW ESS target. Recent work on so-called high-brilliance sources (HBS) suggest 2 orders of magnitude gains in neutron extraction efficiency by designing target-moderator-guide assembly for maximal neutron delivery to a single guide and a single instrument. Using instead of the economic accelerator in HBS proposals a full intensity ESS or J-PARC proton pulse, would enable a neutron instrument with 2 orders of magnitude more flux than any ESS instrument under construction. Performance estimates from BiFrost at ESS indicate that analyzable statistics can be expected from less than 100 pulses. A milli-Hz neutron source at ESS or J-PARC could thus enable single (or few) shot experiments, opening the possibility of neutron diffraction and spectroscopy at magnetic fields up to 100T. With this poster I wish to plant the idea and initiate discussions about feasibility, science case, funding etc.

The proton linac for DARIA compact neutron source

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The 13 MeV 162.5 MHz 5mA CW proton linac is under development at ITEP. The linac is designed for DARIA [1] compact neutron source and based on linac for BELA project [2] which is also under development at ITEP.

The different linac layouts were considered. The most perspective linac layout is one when the linac includes RFQ and DTL sections with 6D-beam matching between them. The DTL section has modular structure and consists of separated individually phased IH-cavities with beam focusing by magnet quadrupoles between the cavities. This DTL structure provides linac compactness, tuning and commissioning cavity by cavity.

Results of beam dynamic simulation and RF parameters of linac cavities are presented.

1. DARIA - compact neutron sources, Saint-Petersburg, 2018;
2. T. Kulevoy et al., ''Compact Multipurpose Facility - BELA'', in ProcLINAC2018, Beijing, China, pp.349-351;

Update in the design of ASTOR: A cold neutron imaging instrument for the future argentine multipurpose reactor RA-10

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The new instrument ASTOR will be used to apply modern neutron imaging techniques in conventional and nuclear material R&D, fuel cells, lithium and hydrogen associate technologies, paleontology among others. It is being designed by a team of physicists and engineers of the Argentinean Laboratory of Neutron Beam (LAHN), in at Atomic Energy Commission of Argentina.

The instrument will use a cold neutron beam and will be assembled in the reactor hall, directly upon the reactor biological shielding. ASTOR has been designed to have a flexible definition of the beam collimation in order to tailor flux/spatial resolution to the problem being investigated. It will offer a maximum field of view of ~30 cm x 30 cm, and a maximum neutron flux of ~3.10^8 n/cm^{2}s, with conventional pinhole L/D values between 120 and 1500. On top of this, there will be two slit-type apertures optimized (high resolution or high flux) for studies requiring only 1D resolution. Four standard modes will be available for rapid instrument configuration (high resolution, time-resolved, tomography, and Bragg edge imaging). Besides this, a very large experimental room (9 m long, 4 m width and up to 3.5 m high),will allow complex sample environments to be installed, and a large beam conformation room (4 m long, 4 m width and up to 2.5 m high) will offer space to install different systems to collimate the beam (collimator drum), to conform the neutron spectrum incident on the sample (filters, velocity selector, double crystal monochromator), or to discriminate the spectrum of the neutrons in the detector (chopper TOF system). The two rooms will have independent access through shielding sliding doors.

ASTOR collimator system includes a primary beam adjusted collimator made of steel, integrated with the rotating primary shutter of the reactor, inside the biological shielding (with an aperture that defines the lower collimation bound). Outside the biological shielding, a remote controlled device for additional apertures and also beam adjusted secondary collimators will allow simple change between the different collimation modes.

We present here a brief description of the instrument requirements and design principles, together with an update of ASTOR design, describing the main optical parameters, its layout and design of mechanical components, together with its expected performance.

First measurements of neutron spectrum at horizontal experimental channel of reactor PIK

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The aim of the time-of-fight (TOF) measurements is to determine the integrated flux within the defined wavelength range and the peak in the spectrum for thermal neutron beam. For well thermalized thermal neutrons these spectra are broadly Maxwellian in shape and have peaks determined by the effective temperature of the moderator.

The TOF spectrometer is assembled on a standard scheme and consists of the following components: collimator inside the reactor channel, beam chopper, detector. Also TOF spectrometer included adjusted devices (tables) with control electronic, electronic for recording and pre-processing of measurement results. The neutron supermirror Ni/Ti (m=2) was optionally used to filter fast neutrons and gamma radiation from incident beam.

Preliminary were performed calculations of the expected neutron spectrum using the Monte Carlo method. The power of the rector was several tens of kW and taking into account the losses on all elements of the TOF spectrometer. Calculations have shown that the neutron spectrum, using the proposed TOF spectrometer, can be measured in a few tens of minutes with good enough accuracy. Fig. 1 a) and b) show the measured spectra of the neutron beam coming out from the 9th horizontal channel of the PIK reactor. For Fig. 1 a) spectrum without filter mirror Ni/ Ti, and Fig. 1 b) spectrum with using Ni/Ti filter mirror. You can see that the mirror removes the background of fast neutron

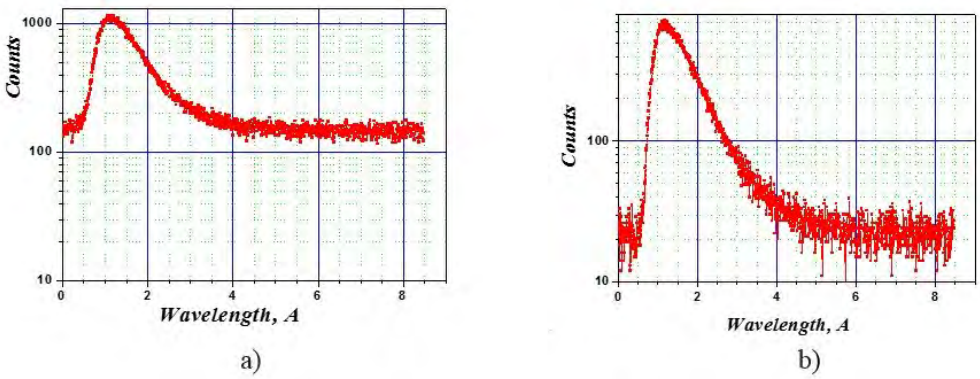

Fig.1. Dependence of the neutron intensity as a function wavelength of neutrons (Å).
a) Spectrum of neutron beam without supermirror Ni/Ti,
b) Spectrum of neutron beam with supermirror Ni/Ti.
The measurement time of each spectrum was 10 minutes.

New developments in the McStas neutron ray-trace simulation package

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The McStas[1,2] neutron ray-tracing simulation package is a versatile tool for producing accurate simulations of neutron scattering instruments at reactors, short- and long-pulsed spallation sources such as the European Spallation Source.

McStas is extensively used for design and optimization of instruments, virtual experiments, data analysis and user training. McStas was founded as an scientific, open-source collaborative code in 1997.

This contribution presents the project at its current state and gives an overview of package features, and developments in McStas 2.5 (December 2018) are discussed. Further, plans for the forthcoming relases in the McStas 2.x and McStas 3.x series are presented.

SINE2020

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000

[1] **McStas : Past, present and future. /** Willendrup, Peter Kjær; Farhi, Emmanuel; Bergbäck Knudsen, Erik; Filges, U.; Lefmann, Kim. In: Journal of Neutron Research, Vol. 17, No. 1, 2014, p. 35-43.
[2] McStas website at http://www.mcstas.org

Tuning of target / moderator / reflector unit for optimized instrumentation at compact accelerator driven neutron sources

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Neutron scattering instruments require specific bandwidths and timing structures according to the experimental resolution conditions. Recent developments of compact accelerator based pulsed neutron sources (CANS) enable an individual optimization of the neutron spectrum and pulse timing to feed every instrument with a suitable phase space volume. This is an advantage compared to today's reactor or spallation sources where many instruments are fed by a single thermal or cold moderator.

In CANS neutrons are produced by the interaction of protons in the 10 to 100 MeV range with a suitable target. This target is embedded in a thermal moderator which is surrounded by a reflector. This increases the thermal neutron flux in the moderator also affecting the moderation time and therefore the pulse structure. Extraction channels inside the moderator and reflector direct the neutrons to the instruments. One dimensional cryogenic moderators can be inserted into the extraction channels and serve just one instrument each. The target / moderator / reflector unit (TMR) is optimized to fulfill the specific requirements of the individual neutron instruments.

We will present the possibility to optimize the neutron spectra and the timing structure for some selected neutron scattering instruments and show the flexibility a CANS offers.

Magnetic field dependence of spin stripe in highly under doped LSCO superconductors

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In the quest to understand the interplay between magnetism and superconductivity (SC), our group investigates the behaviour of spin density waves, so called spin stripes, through elastic and inelastic neutron scattering experiments on $La_{2-x}Sr_xCuO_4$ (LSCO) compounds. It is a well-known fact that one signature of the emergence of superconductivity, is the opening of a spin gap in the excitations spectrum below the superconducting critical temperature[1]. However, in the underdoped region of the phase diagram, where magnetic order co-exists with SC, only a suppression of the low energy excitations, at the onset of SC is observed, also referred to as an incomplete spin gap[2]. In all the studies from the literature[1-4], the effect of applied magnetic field is to induce excited states within the gap while suppressing the superconducting phase.

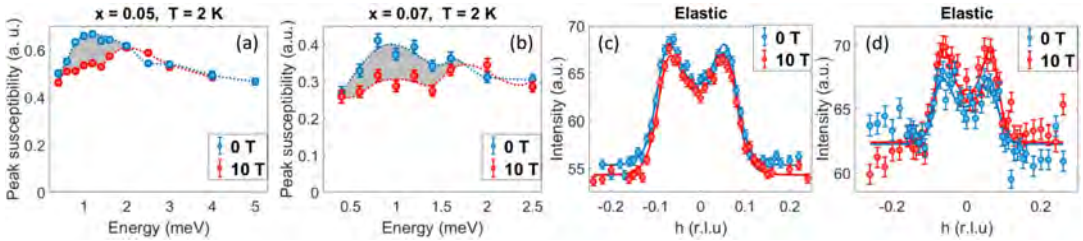

Figure 1 (a) - (b) Integrated intensity as a function of applied magnetic field and energy transfer. The title indicates the sample's doping. (c) - (d) Elastic scans measured at 2K with and without applied magnetic field on the x= 0.05 and x= 0.07 samples respectively. All data was normalized to the 2 meV acoustic phonon.

Our most recent neutron scattering experiments show a change in behaviour of the magnetic signal, namely the stripes along the copper oxide bonds, correlated with the transition, as a function of doping, to SC. We performed measurements on a highly underdoped superconducting LSCO with Sr doping x = 0.07 and non-SC LSCO single crystals with x = 0.05. The SC sample showed a magnetic field induced suppression of the spin fluctuation below 1.5 meV concomitant with an enhancement of the elastic signal (Fig 1). Corroborated with results from the literature, we believe that our findings imply a coherent picture of spectral weight shift towards lower energy transfers for SC samples under applied magnetic field. A similar magnetic field suppression of the inelastic signal, below 2 meV, was observed in our non-superconducting sample, but the lost spectral weight was not recovered in the elastic channel (Fig 1). We speculate that the effect of an applied field on samples outside the SC dome is to move spectral weight towards higher energy fluctuations in contrast to the downward movement on the superconducting ones.

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Magnetic phase diagram of the uniaxial helimagnet $Cr_{1/3}NbS_2$: evidence from small angle neutron scattering

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The magnetic structure of the $Cr_{1/3}NbS_2$ compound was studied by small angle neutron scattering (SANS) under applied magnetic field in the wide temperature range below T_N = 130 K. The magnetic spiral of Cr^{3+} ions is built along the c-axis of the structure belonging to the $P6_322$ space group at zero field [1-3]. As the sample under study is in the powder form, the diffraction ring is detected that is interpreted as scattering on the magnetic spiral with the period of 485 Å at low temperatures

The intensity of the diffraction peak decreases with T and vanishes completely at T = 115 K. Being applied perpendicular to the neutron beam, the magnetic field affects differently the samples grains with helix wave vector **k** along the field and those with **k** perpendicular to the field. The magnetic field, when applied, leads to emergency of the chiral soliton lattice (CSL) for the grains with **k** perpendicular to the field. The period of the CSL increases rapidly as H approaches H_{C1} = 0.25 T. The transition from CSL to the field-induced ferromagnet, however, is not homogeneously smooth but is accompanied by the strong ferromagnetic fluctuations in the wide field range around H_{C1}. These fluctuations are well visible in SANS experiment as scattering at Q = 0. For the grains with **k** parallel to the field systems undergoes a series of the transitions from helimagnet to the conical state, and then to the field-induced ferromagnet at H_{C2} = 1.25 T. The period of the cone increases slightly (for 5 %) with increase of the field, while the transition to the field – induced ferromagnetic state is again accompanied by strong ferromagnetic fluctuations. Magnetic field - Temperature (*H-T)* phase diagram was drown on the basis of the obtained SANS data.

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Low temperature magnetism of the quantum spin ice candidate $Nd_2Ru_2O_7$

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Pyrochlore compounds with general formula A2B2O7, where A is a trivalent rare-earth ion and B is a tetravalent transition-metal ion, have been extensively studied in the past few decades, and various novel magnetic behaviors have been discovered, including spin glass, spin ice, and spin liquid [1]. In the Nd pyrochlores, Nd2Ti2O7 cannot be formed, and Nd2Sn2O7, Nd2Ru2O7, Nd2Ir2O7, Nd2Zr2O7, and Nd2Hf2O7 all show all-in-all-out (AIAO) antiferromagnetic ground state on Nd3 sites. $Nd_2Ru_2O_7$ has a pyrochlore structure and shows magnetic anomalies at 146 K, 22 K and 1.8 K which correspond to the antiferromagnetic order state of Ru^{4+}, ferromagnetic correlation, and antiferromagnetic order state of Nd^{3+} respectively [2]. However, in Nd2Ru2O7 and Nd2Ir2O7, the magnetic structure of Ru^{4+} is an *XY* type [3] and Ir^{4+} an AIAO type [4], which lead Nd^{3+} ordered at 1.8 K and 8 K respectively. Furthermore, Nd2Zr2O7 shows magnetic fragmentation in spin ice pattern (two-in-two-out ferromagnetic correlations) together with the AIAO long-ranged order below the transition temperature ~0.3 K [5].

In the neutron diffraction in applied fields at 50 mK, $Nd_2Ru_2O_7$ has crossed over to a Palmer-Chalker type long-ranged order state above 1.5 Tesla, which is similar to the results of neutron diffraction in fields on Nd2Sn2O7. In this presentation, we will show the results of neutron diffraction in fields of $Nd_2Ru_2O_7$, and the comparisons with other Nd-pyrochlores.

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Phase separation in half-doped manganites with isovalent substitution of rare-earth cations exemplified by $Sm_{0.32}Pr_{0.18}Sr_{0.5}MnO_3$

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Phase separation (PS) in the complex manganite $Sm_{0.32}Pr_{0.18}Sr_{0.5}MnO_3$ was studied by high-resolution neutron powder diffraction, neutron beam depolarization, second-harmonic magnetic response, and magnetization and resistivity measurements from 4 K up to the room temperature and higher. A structural phase transition from the rhombic *Pbnm* phase to a mixture of the rhombic *Pbnm* and monoclinic $P2_1/m$ phases was observed upon cooling, reaching the respective fraction ratio 1:3 at the lowest temperature. The magnetic ground state was found to be phase-separated into three magnetic phases emerging at different temperatures, viz., ferromagnetic (FM), antiferromagnetic *A*- and charge-ordered *CE* types. FM clusters arise far above the room temperature in the paramagnetic rhombic phase and coalesce upon cooling to produce the long-range FM order below 250 K and to arrive at the percolative FM phase below 150 K. The *A*- and *CE*-type orders form in the monoclinic phase at the temperatures ~200 K and ~170 K, respectively. Transfer of electrons from the monoclinic to rhombic phase enhances the growth of clusters and stabilizes the respective magnetic orders in both crystal phases. The isovalent substitution of Sm for Pr enhances the PS tendency and extends it to higher temperatures compared to the parent compounds $Sm_{0.5}Sr_{0.5}MnO_3$ and $Pr_{0.5}Sr_{0.5}MnO_3$.

The resistivity exhibits an insulator temperature behavior of the nonadiabatic small-polaron-hopping type down to ~180 K. Under the magnetic field 7 T, the resistivity becomes of the metallic type below ~120 K, thus, demonstrating colossal magnetoresistance.

Emergence of the perpendicular to the magnetic field magnetization in nickel inverse opals studied by SQIUD, MFM and micromagnetic modelling

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Rapid progress in methods of synthesis and characterization of magnetic nanostructures has encouraged investigations of 3D nanosystems [1]. Such nanosystems can be considered as the base element of the fundamentally new data storage devices. Also, many of them exhibit unusual magnetic behavior. In particular it was found that magnetization distribution in ferromagnetic inverse opals (IO) is governed by the spin-ice rule [2] that was initially stated for magnets with pyrochlore structure - $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ [3]. The validity of the spin-ice rule in IO should lead to the emergence of the magnetization component which is perpendicular to the external field when the field is applied along the special direction of the IO mesostructure. We have studied this property by means of SQUID and magnetic force microscopy (MFM) techniques. Results of the experiments have been explained by micromagnetic simulations.

Nickel IO have been fabricated from colloidal crystal by electrodeposition of nickel into the voids between microspheres. IO have FCC structure with lattice period 700 nm. During SQUID measurements out of plane in plane (along field) magnetization components have been measured. MFM phase shift maps have been registered in the external field applied along [1-21] direction of FCC structure.

Field dependence of the perpendicular magnetization component have been interpreted by micromagnetic calculations. Results have confirmed the validity of the spin-ice model. Based on comparison between calculated and measured phase shift maps we have established the scenario of the magnetization reversal in IO.

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Study of the magnetic properties of arrays of iron-based nanowires by FORC and SANS

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Magnetic nanowires arrays (MNA), until recently, was considered as good candidates for information storage material with high density. The magnetization of a single nanowire in this case plays role of a bit of information.

However, significant demagnetization fields created by long but narrow magnetized nanowires and the intermittent magnetization reversal of a separate nanowire [1, 2] due to pinning of the domain wall on structure inhomogeneities are significant obstacles for correct recording and reading information. Magnetostatic interactions between nanowires often lead to further complication of the magnetization reversal process [3].

To solve the problem of magnetization reversal, it is necessary to use a material with a low anisotropy of the crystal lattice (for example, cubic one), but with a sufficiently high magnetic moment. Iron is an excellent material for this purpose.

In the current work, iron-based MNA synthesized by template electro-deposition method are investigated. Porous anodic alumina (AOA) films of 35 μm thick were used as templates, obtained using two-step anodizing of aluminum. The electro-deposition of iron was carried out at room temperature in a three-electrode cell. The diameter of the nanowires is 30 ± 3 nm, while the distance between them is 100 ± 4 nm. The length of the filaments varies from 400 nm to 35 μm.

The study of magnetic properties of MNA was carried out by the method of first-order reverse curves (FORC) and small-angle neutron scattering. The magnetic field up to 1.2 T was applied both along and across the long axis of the nanowires.

Significant changing of interaction and switching fields distributions depending on the nanowire length have been observed. Additionally, remagnetization curve of magnetic subsystem has been observed.

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Size and lattice distortions as driving agents of long-range magnetic correlation and crystal field excitations of $TbCu_2$ nanoparticles

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Research on magnetic nanoparticles (MNPs) of Rare Earth intermetallics is a discipline where several questions are still to be answered. The latter are related to the facts that those intermetallics constituted a backbone of on the one hand a rich variety of magnetic structures and, on the other, an ample playground to deal with crystal-field effects (CEF) [1]. Among possible families, binary TbX_2 is one which has gathered attention in the last decade in the form of MNPs. Effectively Tb^{3+} with $J = 6$ and ordered moment $\mu = 8.8\ \mu_B$ assures a large magnetic response to be easily recorded by various techniques. When X = Al, the behaviour is pure ferromagnetic in bulk, but disorder appears in MNPs [2]. In the last years we have paid more attention to MNPs of $TbCu_2$ (X = Cu). This is due to existence of an antiferromagnetic (AFM) order in the nanoparticle core ($T_N \approx 46$ K). Hence the response in the nanoparticle shell is enhanced and the role of magnetic disorder is of paramount influence. $TbCu_2$ MNPs are produced by milling; this enables: i) a control of nanoparticle sizes reaching below 10 nm, ii) the appearance of lattice strain, and iii) the production of large quantities of sample, which is handy when using neutron scattering techniques. In this sense, neutron diffraction experiments on those MNPs performed at LLB (France) confirmed the existence of AFM in the particle core and the reduction of the magnetic moment due to the surface moments of the uncompensated AFM chains [3].

With this neutron diffraction characterisation complemented by X-ray diffraction, TEM, DC-magnetisation and AC-susceptibility, we are now aiming to disclose other subtle magnetic effect at the nanoscale. Firstly, magnetic correlations among MNPs will be discussed thanks to data recorded in a series of small-angle neutron scattering (SANS) experiments [4] carried out in SANS2D (RAL-ISIS) in bulk and MNPs milled for 2h (average particle diameter, D = 8(1) nm) and 5h (D = 7(1) nm). There, a peak at $q = 1.14\ nm^{-1}$ has been revealed [4], related to the existence of long-range magnetic correlations. Secondly, inelastic neutron scattering (INS) measurements performed at IN4 and IN6 in the $1.5 \leq T \leq 100$ K range at the ILL (France). These have evidenced a broadening of the inelastic peaks corresponding to CEF excitations. The INS peak-broadening is connected to the presence of the lattice distortions and the surface random anisotropy suffered by the Tb^{3+} moments of the MNPs [5].

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Magnetism and magnetoelectricity in mixed-anisotropy magnets

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Some materials display the magnetoelectric effect where an electric polarization is induced by applying a magnetic field or vice versa, a magnetization is induced by an electric field. This intimate coupling between electric and magnetic properties render magnetoelectric materials interesting for applications in for example data storage and sensors. Our work is focussed on the lithium orthophosphates, LiMPO$_4$ (M = Co, Ni, Fe, Mn). They are a family of compounds with antiferromagnetic and magnetoelectric ground states [1-3] as well as complex magnetic phase diagrams [4-7]. Lately we have started investigating compounds with a mixture of different ions on the magnetic site and we study how the magnetic and magnetoelectric properties of these mixed-anisotropy magnets are affected. In particular we are looking at LiNi$_{1-x}$Fe$_x$PO$_4$ where the Ni^{2+} and Fe^{2+} ions display opposite single-ion anistropies: LiNiPO$_4$ has easy axis c and hard axis b whereas LiFePO$_4$ has easy axis b and hard axis c. Naïvely one would expect spins in the mixed compound to orient in the (b,c)-plane as was also previously proposed for LiNi$_{0.8}$Fe$_{0.2}$PO$_4$ based on second harmonic generation measurements [8]. However, we use polarized neutron diffraction to show that the spins in LiNi$_{0.8}$Fe$_{0.2}$PO$_4$ actually orient with major component along a. This spin orientation is also consistent with the observed magnetoelectric tensor form. To further investigate this somewhat surprising result, we perform Monte Carlo simulations in order to elucidate the interplay and competition between exchange interactions and single-ion anisotropies in LiNi$_{1-x}$Fe$_x$PO$_4$.

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MIEZE neutron spin-echo spectroscopy of strongly correlated electron systems

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We report recent progress in the development of longitudinal Modulation of IntEnsity with Zero Effort (MIEZE) neutron spin-echo spectroscopy at the beam-line RESEDA[1] at MLZ. The key technical characteristics are summarized which highlight that the parameter range accessible in momentum and energy, as well as its limitations, are extremely well understood and controlled[2]. Typical experimental data comprising quasi-elastic and inelastic scattering are presented, featuring magneto-elastic coupling and crystal field excitations in $Ho_2Ti_2O_7$, the skyrmion lattice to paramagnetic transition under applied magnetic field in MnSi, ferromagnetic criticality and spin waves in Fe, and molecular dynamics in H_2O. Taken together, the advantages of MIEZE spectroscopy in studies at small and intermediate momentum transfers comprise an exceptionally wide dynamic range of over nominally seven orders of magnitude, the capability to perform straight forward studies on depolarizing samples or under depolarizing sample environments, as well as incoherently scattering materials.

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Measuring the phonon spectra of single-molecule magnets with inelastic neutron scattering

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Recent work on single-molecule magnets (SMMs) has revealed unprecedented properties such as large energy barriers to magnetic relaxation, U_{eff}, over 2217 K [1] and observable magnetic hysteresis at ever higher temperatures: this has increased from 14 K to 80 K in only a few years [1–4]. However, this marked improvement in magnetic hysteresis has not been consistent, nor is it predictable, on the basis of traditional metrics such as U_{eff}. While the origin of the U_{eff} barrier is well understood, relaxation by this mechanism is not sufficient for explaining SMM performance. Ongoing investigations have postulated that restricted vibrational modes of the newest class of SMMs may play a key role in this step-change [3,5,6]. Therefore, it is necessary to investigate the phonon spectra for a range of SMMs, both with high and low hysteresis temperatures, in order to build a picture of spin-phonon coupling in these materials. Inelastic neutron scattering is used to probe the phonon spectra of these systems.

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Structural and magnetic properties of the Fe-doped layered perovskite $TbBaCo_{1.91}Fe_{0.09}O_{5.5}$ at high pressure

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The structural and magnetic properties of the Fe-doped layered perovskite $TbBaCo_{1.91}Fe_{0.09}O_{5.5}$ (space group *Pmmm* and the unit cell $a_p \times 2a_p \times 2a_p$, where a_p is parameter of perovskite cell) have been studied by means of neutron (at temperature range 5-320 K and pressure up to 6.2 GPa) and x-ray (at ambient temperature and pressure up to 30.05 GPa) diffraction.

Pressure dependences of the structural parameters were obtained. The compressibility of $TbBaCo_{1.91}Fe_{0.09}O_{5.5}$ was found to be anisotropic. The average compressibility ($k_{ai} = -(1/a_{i0})*(da_i/dP)|_T$, $a_i = a, b, c$) of the a – parameter is about twice larger in comparison with those of the b- and c- parameters. The bulk modulus $B_0 = -V(dP/dV)_T$ of $TbBaCo_{1.91}Fe_{0.09}O_{5.5}$ was 138.0(1.7) GPa.

Upon cooling below ambient temperature in all neutron diffraction spectra at investigated pressure region 0 – 6.2 GPa the reflection (112) appeared at Neel temperature, indicating antiferromagnetic (AFM) ordering of G-type (magnetic cell $2a_p \times 2a_p \times 4a_p$). At ambient pressure between 290 - 150 K additional ferromagnetic component is formed.

Upon compression up to 6.2 GPa the Néel temperature decreased with a pressure coefficient $(1/T_N)dT_N/dP \approx -0.001(1)$ GPa^{-1}. The ferromagnetic component is suppressed and G-type AFM order only is observed. The ordered magnetic moments remain about the same under pressure indicating the absence of the spin-state transition.

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Measurements of the spin wave stiffness in helimagnets by small-angle polarized neutron scattering

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We have developed a method for measuring the spin wave stiffness in helimagnets with Dzyaloshinsky-Moriya interaction in a completely polarized state using small-angle scattering of polarized neutrons [1]. It has been experimentally proved that the dispersion of magnons in this state has an anisotropic appearance, since the neutron scattering intensity pattern is registeres as two circles for neutrons with the gain and loss of magnon energy, respectively. The centers of the circles are shifted by the momentum transfer value equal to the helix wave vector ± ks, which is oriented along the applied magnetic field H. The radius of the circles is directly related to the spin wave stiffness of the magnetic system, but depends on the magnitude of the magnetic field. This scattering depends on the polarization of neutrons, showing the chiral nature of the spin waves in the Dzyaloshinsky-Moriya helimagnet in the polarized state. We have measured the temperature dependence of the spin wave stiffness of the following compounds: MnSi [1], $Mn_{1-x}Fe_xSi$ with x = 0.03, 0.06, 0.09, 0,10 [2],$Fe_{1-x}Co_xSi$ with x = 0.25, 0.30, 0.50 [3], FeGe [4], $Mn_{1-x}Fe_xGe$ with x = 0.80 [5] and other concentration x = 0.10, 0.20, 0.30, as well as Cu_2OSeO_3 .

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Magnetic structure of the ternary $GdMn_2Si_2$ compound

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RMn_2X_2 (R is a rare-earth ion, X = Ge, Si) compounds crystallize in a natural layered crystal structure (SG *I4/mmm*) and exhibit a rich variety of magnetic structures and magnetic phase transitions. In case of $GdMn_2X_2$ compounds, theoretical modeling predicted five possible types of magnetic order [1] but their experimental study by means of neutron diffraction is hampered by highly absorbing Gd atoms. In this work, a detailed study of magnetic structure of the $GdMn_2Si_2$ compound has been performed by means of magnetic measurements on the single crystal sample and neutron powder diffraction with a short neutron wavelength l=0.4959 Å.

Fig. 1(left panel) shows temperature dependences of magnetization measured for an external magnetic field applied along the *c* crystallographic axis and along the basis plane. Neutron diffraction patterns for $GdMn_2Si_2$ plotted as a function of temperature are represented using a colored 2D map in Fig. 1(right panel). Below the Neel temperature T_N = 480 K, Mn magnetic moments adopt a canted antiferromagnetic structure which can be described by the Shubnikov group *Pnnm*'. Further cooling below T_{Gd} = 52 K results in the emergence of an in-plane ferromagnetic ordering of the Gd magnetic sublattice that triggers a complex transformation of magnetic structure due to the interplay of two competing interactions. Firstly, the strong Mn-Mn interlayer exchange interaction tends to form a canted antiferromagnetic structure observed at high temperature above T_{Gd}. Secondly, the RKKY exchange interaction forces the Mn and Gd magnetic sublattices to be antiparallel to each other. The resulting canted ferrimagnetic structure can be described by the Shubnikov group Pm'm'n. It exhibits both ferrimagnetic in-plane ordering of the Mn and Gd magnetic sublattices as well as an out-of-plane antiferromagnetic component inherited by Mn magnetic sublattice from the high temperature magnetic phase.

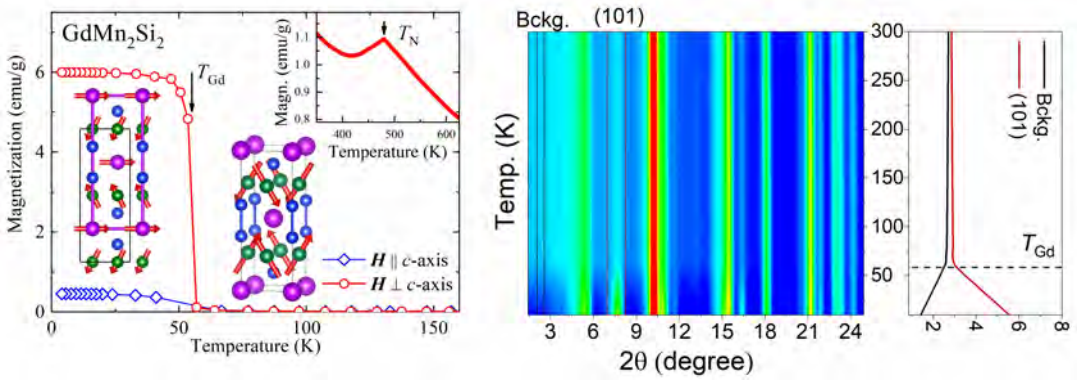

Fig. 1 (left panel) Temperature dependences of magnetization of $GdMn_2Si_2$ in a magnetic field of 50 Oe applied along the *c*-axis and in the basis plane of the single crystal. (right panel) Neutron diffraction patterns for $GdMn_2Si_2$ plotted as a function of temperature represented using a colored 2D map.

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Magnetic triplon excitations in the alternating chain system $(VO)_2P_2O_7$

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Vanadyl pyrophosphate ($(VO)_2P_2O_7$, also abbreviated VOPO) is a low dimensional quantum system, where no magnetic long range order is observed at low temperatures, even though it has significant antiferromagnetic exchange interactions between the spins 1/2 of the V^{4+}.

Early susceptibility and inelastic-neutron-scattering (INS) data on VOPO powder were consistent with both a spin ladder and an alternating spin chain system. The assumption that the strongest exchange interactions would be between the V^{4+} spins with the smallest separation lead to a preference for a ladder along the crystallographic *a*-axis [1]. Single crystal INS showed that the dominant exchange couplings are in fact along the *b*-axis ruling out the ladder model in favour of alternating chains along the *b*-axis [2]. Intriguingly, their measurements showed two excitations, where the energy gap of the second mode is approximately twice as large as the first. The origin of this second branch became a matter of debate. One possibility, is that the two sets of magnetic chains in the unit cell are decoupled and inequivalent and in this case it is purely fortuitous that the second gap has twice the value of the first [3]. Alternatively, the second branch could be a two-triplon bound state, predicted by some theories in the presence of frustrated interchain couplings [4]. High field magnetisation and NMR data [5,6] were interpreted using the two chain model, however this simple model of inequivalent and decoupled chains has not been reconciled with the significant *a*-axis dispersion.

Taking the *a*-axis dispersion into account, VOPO can be considered as a 2D strongly coupled dimer system where the ground state should be a macroscopic singlet with a gapped excitation spectrum. The two triplon modes could arise from two inequivalent dimers in the unit cell. The 2D exchange interaction scheme could allow cubic interactions and favour more exotic excitations [7]. Here we would like to present a detailed INS study of the magnetic excitations in VOPO and compare the experimental S(Q,ω) to a theoretical model based on a harmonic triplon approximation.

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From Nuclear SRO and Incommensurate Magnetic LRO in $SbVO_4$ Catalyst to non-magnetic ground state in SbV_9O_{20}

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$Sb_xV_{1-x}O_2$ ($0 \leq x \leq 0.5$) rutile related system shows a full panoply of subtle structural changes and multifunctional properties. On the rich Sb side, $SbVO_4$ series of compounds could be a promising catalyst for the production of 20% cheaper acrylonitrile by the ammoxidation of propane compared to current method from propylene producing 8×10^6 ton/year, *i.e.* more than 1Kg per human inhabitant of the planet. Composition, oxidation state and restrained structural features influence the activity and selectivity of the highest performance catalyst.

In the non-stoichiometric series described as $Sb_{0.9}V_{0.9+\delta}[]_{0.2-\delta}O_4$ ($0 \leq \delta \leq 0.2$), cation vacancies ([]) in the basic rutile type-structure balance V^{3+} V^{4+} charges while antimony remains as Sb^{5+}. A reduced phase (richest in V^{3+}) has been reported to be $Sb_{0.9}V_{1.1}O_4$, which shows by electron diffraction (ED) superlattice reflections characteristic of a 2-fold rutile superstructure along *c*. The careful reciprocal lattice study by ED has revealed the following unit cell for the rutile superstructure: $a=\sqrt{2}a_r$, $b=\sqrt{2}b_r$, $c=2c_r$. (subindex *r* refers to the basic rutile unit cell). Its space group, $I4_1md$, was determined by CBED. A structural model based on alternating Sb and V cations ordering along *c* in the chains of edge-sharing octahedra was proposed. No cation vacancies have been observed for this reduced phase, while for the compounds synthesized in oxidizing conditions the presence of vacancies has been confirmed. Magnetic susceptibility data indicate possible magnetic ordering in reduced phases rich on V^{3+} which are close to the nuclear superstructure by Sb-V ordering. For the simultaneous crystal and magnetic structure determination we have performed a neutron diffraction study on different samples of the series with composition ~$SbVO_4$.

Below $T_N \leq 50K$, new Bragg reflections of pure magnetic nature appear due to the 3D-AF interaction of the vanadium spins changing gradually from the paramagnetic disorder to the magnetically ordered state as the temperature decreases. The periodicity of the magnetic structure develops being close to doubling again the two-fold commensurate supercell of rutile type described by the alternate ordering of Sb and V along the rutile ***c***-axis in $SbVO_4$, giving rise to a final 4-fold rutile superstructure. However, the exact periodicity of the spin arrangement is clearly not commensurate with the nuclear cell but close to that. The refinement of the incommensurate magnetic propagation vector to $\boldsymbol{k}=[0, 0, \pm k_z]$ with $k_z=0.266(1)$ *r.l.u.* is close to the commensurate value ¼. It accounts both for the magnetic satellites and it is compatible with the absence of a commensurate nuclear 2-fold supercell but the observed modulated chemical structure with modulation vector $\boldsymbol{q} = 0.532\ c^*$.

Using joint refinement of X-ray and high resolution neutron diffraction data the nuclear cell could be fitted under basic rutile structure, space group $P4_2/mnm$, chemical modulations observed by ED correspond to short range order SRO phenomena in the cation sublattice coexisting with the magnetic long range order LRO evidenced by neutron diffraction.

On the other hand, V rich side like SbV_9O_{20} , shows a non-magnetic ground state and possible MIT related to both spin Peierls and structural phase transitions.

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Magnetic characterization of oblique angle deposited Co/CoO on gold Nanoparticles

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The magnetic anisotropy in exchange biased thin films deposited under an oblique angle on homogeneous and Au nanoparticle decorated substrates, was studied.
The Au nanoparticles (NPs) form an ordered array and promote Co-nanoparticle growth in addition to lateral structuring of the Co film. This leads to a complex magnetic system with potentially competing anisotropies originating from oblique angle deposition, nanostructuring and exchange bias. Using the complementary techniques of SQUID magnetometry and polarized neutron reflectometry (PNR) we attempt to disentangle the different contributions to the magnetic hysteresis of this system.

For the sample with NPs, that was grown simultaneously with a control sample, we found an in-plane magnetic anisotropy along the deposition direction, for the sample without NPs no preferential magnetization direction could be established.

Magnetic structures of $RCuAl_3$ (R = Ce - Nd) compounds

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RTX_3 compounds, where R = rare-earth, T = transition d-metal and X = p-metal, belong to the most intensively studied systems in the field of condensed matter physics for several decades. Amidst them, a considerable attention has been dedicated to – mostly, however not exclusively Ce-based – compounds crystallizing in the tetragonal non-centrosymmetric $BaNiSn_3$-type structure (space group *I4mm*). A spectrum of physical properties such as valence-fluctuations, heavy-fermion antiferromagnetic orderings and complex magnetic structures, superconductivity and pressure induced superconductivity or strong magneto-elastic coupling leading to the formation of a new quantum quasi-bound state represents the reason behind the still not ceased interest in this family of intermetallics. The latter feature, occurrence of the so called 'vibron' quasi-bound state which displays itself as an additional magnetic excitation in energy spectrum, stimulated detailed investigations of the physical properties of $CeCuAl_3$[1], $CeAuAl_3$[2] and $Ce(Cu,Al)_4$ [3]. To search for further compounds exhibiting 'vibron' states, other RCuAl$_3$, where R = Pr and Nd, crystallizing in the tetragonal $BaNiSn_3$ structure-type were investigated[4]. However, no additional magnetic excitation, i.e. no clear sign of a 'vibron' state, was observed in powder time-of-flight neutron scattering spectra[4].

The physical properties of $PrCuAl_3$ and $NdCuAl_3$ have been studied on polycrystalline samples so far and there exists only a handful of previous results, frequently very brief and not convincing. We prepared single crystalline samples of both analogues for the first time and investigated their physical properties in detail[5]. Our neutron diffraction experiment allowed us to confirm both the antiferromagnetic ordering in $NdCuAl_3$ below T_N = 2.45 K and $PrCuAl_3$ remaining paramagnetic down to low temperature (< 1.5 K). The magnetic structure of $NdCuAl_3$ was described by two propagation vectors $\boldsymbol{k_1}$ = (1/3 - δ_1, 0, 0) and $\boldsymbol{k_2}$ = (1/7 - δ_2, 1/7 - δ_2, 0), where δ_1 = 0.035(1) and δ_2 = 0.007(1). The magnetic moments (of both magnetic modulations) are arranged within the basal plane with eventually a small tilt of the moments into the c-axis, which is allowed by the symmetry. Sum of magnetic moments' amplitudes (1.62(2) μ_B/Nd^{3+} + 0.96(4) μ_B/Nd^{3+} = 2.58(6) μ_B/Nd^{3+}) is significantly lower than the moment of a Nd^{3+} free ion (in agreement with magnetization data)[5]. Such a reduction can be ascribed to the crystal electric field. The presented data are discussed with respect to our previous results on physical properties and the magnetic structure of $CeCuAl_3$[6]. The magnetic structures of Ce and Nd based RCuAl$_3$ have a few common characteristics: (i) magnetic structures are incommensurate, (ii) magnetic moments are arranged within the basal plane and (iii) amplitudes of magnetic moments are significantly reduced compared to the free ion values. The investigation of magnetic structures of other RCuAl$_3$ with R = Sm and Gd would be desirable, but extremely difficult employing neutron diffraction techniques due to neutron absorption issues.

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Magnetic Ordering in the 2-dim Quantum Antiferromagnet alpha-CuV_2O_6

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So far, he magnetic properties of the spin S=1/2 quantum antiferromagnet αlpha-CuV_2O_6 have been analyzed bin terms of an one-dimensional Heisenberg model with uniform nearest-neighbor antiferromagnetic spin exchange interaction.[1,2,3] We have carried out extensive DFT GGA+U *ab initio* calculations to derive the spin exchange parameters and find that an anisotropic two-dimensional square planar model with $J_y/J_x \approx 0.8$ is rather adequate to describe the spin lattice of αlpha-CuV_2O_6. We present recent neutron powder diffraction measurements, single-crystal magnetization, and ESR data, carried out in order to conclusively establish the magnetic structure. These results are in best agreement with the *ab initio* theoretical predictions.[4] Magnetoelastic effects occurring at the onset of long-range order below 22.5K will be discussed.

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Half Replacement of Bismuth by Neodymium in Half-Hole Doped Bismuth-Based Manganites $Bi_{0.25}Nd_{0.25}X_{0.5}MnO_3$ (X=Sr, Ca): A Neutron Diffraction Study

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The impact of half substitution of diamagnetic Bi^{3+} with rare earth magnetic Nd^{3+} ions on the structural and magnetic properties of polycrystalline $Bi_{0.25}Nd_{0.25}Sr_{0.5}MnO_3$ (BNSMO) and $Bi_{0.25}Nd_{0.25}Ca_{0.50}MnO_3$ (BNCMO) has been investigated by X Rays and neutron diffraction and magnetic measurements. Both substances belong to the family of mixed-valence manganites for which the rich electric and magnetic properties have been explained by means of the double exchange (DE) interaction theory, Jahn–Teller effect, polaron theory and phase separation. The striking feature that distinguishes the Bi-based manganites from the RE-manganites (RE is a rare earth cation) with similar perovskite-like structure is the much higher temperature of onset of long-range charge ordering (CO). For $Bi_{0.5}Sr_{0.5}MnO_3$ the record-breaking T_{CO}=525 K for manganites was reported [1]. Reflecting on the structural consequences of setting in charge ordering, the role of the highly polarized $6s^2$ character of Bi^{3+} was advanced as most important. A dominant character of the lone pair was inferred for $Bi_{0.5}Sr_{0.5}MnO_3$ (hereafter BSMO) with a consequence that the effective radius of Bi^{3+} is $r_i \approx$ 1.24 Å in contrast to ri≈ 1.16 Å for screened lone pair. The latter value is just the effective radius of Nd^{3+} ions ($r_i \approx$1.163 Å). In $Nd_{0.5}Sr_{0.5}MnO_3$ (NSMO) the CO also sets in but at T_{CO} = 150 K and is stable only for 0.45<x<0.51. Moreover, there are coexisting nanosized AFM and FM clusters. The half doped manganites is expected to adopt a CE-type charge/orbital/spin superstructure [2] and, indeed, at $T_N < T_{CO}$ a CE antiferromagnetic (AFM) ordering occurs in BSMO[1,2] and NSMO [3]. An interesting point to address is that both compositions are good examples for the structural phase-separation conception [4]. For $Nd_{1-x}Sr_xMnO_3$ the CE AFM-phase is stable in a very narrow range 0.49<x<0.5 [4] and similarly to BSMO it coexists with the layer AFM arrangement (A-type) due to spontaneous segregation of two phases below T_{CO} with different magnetic behaviour. In both compositions each one of the separated phases is orthorhombic but of different symmetry - Pnma space group is valid for BSMO [1] whereas Imma is more adequate for NSMO [2]. We correlate the structural response of $Bi_{0.25}Nd_{0.25}X_{0.5}MnO_3$ (X=Sr, Ca) to charge and spin ordering with reduced amount of Bi^{3+} which beside its peculiar contribution to itinerant e_g electrons leads to modified average size of the A-site cations <rA> and mismatch between A-site cations (size variance, σ^2).

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Complementary Neutron Diffraction and μSR Studies of the Static and Dynamic Magnetic Properties of New Spin-frustrated Chiral Magnet $MnSnTeO_6$

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The new $MnSnTeO_6$ tellurium was experimentally investigated by neutron powder diffraction and muon spin spectroscopy. This compound belongs to quasi-two-dimensional frustrated layered magnets with a triangular superstructure of magnetic ions in the layer. Recently, $MnSb_2O_6$, a magnet with a chiral crystal structure and a cycloidal magnetic structure, was predicted as a multiferroic with a unique ferroelectric switching mechanism [1]. $MnSnTeO_6$, studied by us, in its electronic structure is closest to the $MnSb_2O_6$ prototype, since Sn and Te are neighbors of Sb on the left and right in the periodic system. It was found that $MnSnTeO_6$ crystallizes in *P321* sp.gr. similar to the chiral phase of the related $MnSb_2O_6$ oxide. The distribution of Sn and Te ions over equivalent positions in the crystallographic unit cell is determined. The complexity of the refinement of the crystal structure consists that the atomic scattering factors for tin and tellurium are very similar not only for X-rays (Z_{Sn} =50, Z_{Te} =52), but also for neutrons (b_{Sn} = $0.62 \cdot 10^{-12}$ cm and b_{Te}=$0.58 \cdot 10^{-12}$ cm). Therefore, it is difficult to define the location of tin and tellurium ions directly in nonequivalent sites from the full-profile analysis, and the main attention was paid to finding out the oxygen positions and the corresponding bond lengths. It is important to note that the layer with magnetic ions is highly ordered due to the large difference in the formal charges of Mn^{2+} and Te^{6+} cations. The appearance of new reflections on the low-temperature neutron diffraction patterns at temperatures below 10 K unambiguously indicates the long-range antiferromagnetic nature of the spins ordering of manganese ions. As a result of the full-profile analysis of the neutron diffraction pattern measured at 3 K, it was shown that the magnetic structure in an ordered state is incommensurate with crystallographic one and describes the propagation vector k = (0, 0, 0.183) characterizing a spiral spin order, which completely coincides with the propagation vector of the magnetic structure of the related $MnSb_2O_6$ oxide. Such structure is organized due to competition and frustrations in several possible ways of exchange interaction.

Additional information on the spin dynamics and ground state properties was obtained from μSR measurements. For the analysis of the longitudinal data, a dynamic version of the Kubo-Toyabe function was used. In particular, the situation was recorded when the spectra in the longitudinal field are not easily separated and remain Gaussian in shape. This “inseparable Gaussian” indicates the presence of a transition field in the muon site, which exists only for a very small fraction of the muon residence time. Above T_N, μSR implies a short-range order of spins, as evidenced by a slight increase in the muon asymmetry intensity on a time scale of several μs. With a decrease in temperature, the increase in the relaxation rate indicates a slowing down of the spin dynamics, which is probably associated with the creation of short range correlations. The saturation of the relaxation rate at the lowest temperatures is a common feature of highly frustrated magnets, which signal the preservation of slow spin dynamics on approaching T = 0 K.

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Theory of Multiple Small-Angle Neutron Scattering in Ferromagnets

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The small-angle neutron scattering method is often used to study nanoscale inhomogeneities of materials. The multiple small-angle neutron scattering theory based on the eikonal approximation was built and experimentally tested [1]. The theory takes into account interference and correlation effects in multiple scattering. Based on the constructed theory, the limit of small values of the Born parameter — the limit of diffraction — was studied in detail [1,2]. At the same time, the refraction limit remains less studied, although it is theoretically interesting (the scattering is determined not only by the pair correlation function, but also by higher-order functions) and is realized experimentally in scattering on the ferromagnetic domains.

In the classical theory [3], developed in the works of Shilstein et al., it is assumed that scattering occurs on domains whose spatial arrangement and orientation are random and not correlated. In this case, either the refraction is calculated at a randomly oriented domain boundary, or the theory of small-angle diffraction on spheres is applied. The same approach is applied in later works [4].

In this work, a more realistic theory is developed, which allowed us to take into account that, within the limits of the correlation radius, the location and orientation of the domains are ordered. The natural forms of the corresponding correlation functions are considered.

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Doping evolution of the gap structure and spin-fluctuation pairing in $Ba(Fe_{1-x}Co_x)_2As_2$ superconductors

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Doping dependence of the superconducting state structure and spin-fluctuation pairing mechanism in the iron-based superconductors $Ba(Fe_{1-x}Co_x)_2As_2$ is studied. We show that the overdoped compounds $Ba(Fe_{1-x}Co_x)_2As_2$ have a three-gap structure with substantially different order parameters and a weak interband spin-fluctuation coupling. In the three-gap state of $Ba(Fe_{1-x}Co_x)_2As_2$, the s+d anisotropic electronic gap has an intermediate value between two isotropic hole gaps. During transition to the optimal regime, the electron gap strongly increases (by a factor of two) and gets close to the largest hole gap value, while the electron gap anisotropy sharply decreases pointing to a strong increase in the interband interaction, with spin fluctuations accompanying the antiferromagnetic transition. The same two-gap state with close values of the electron and largest hole gaps is preserved even with further decrease in doping. The performed study shows that in the regime when antiferromagnetism and superconductivity coexist, the spin-fluctuation pairing mechanism has a significant effect on superconductivity in the electron band, but its role in elevating the critical temperature of the $Ba(Fe_{1-x}Co_x)_2As_2$ compounds is relatively small.

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Neutron diffraction study in magnetic fields of the antiferromagnetic spin-1/2 trimerized chain compound $Cu_3(P_2O_6OD)_2$

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We can investigate magnetism on each site even in magnets without magnetic long-range order using neutron diffraction. Magnetic moments are induced by magnetic fields and generate magnetic reflections. We can evaluate a field-induced magnetic moment (magnetization) on each site from analyses of the magnetic reflections.

We have paid our attention to $Cu_3(P_2O_6OD)_2$. No magnetic order appears down to 2 K. Two types of Cu^{2+}-ion sites (Cu1 and Cu2) exist. The J_1 interaction between two spins on Cu2 sites and J_2 interaction between two spins on Cu1 and Cu2 sites are dominant. The antiferromagnetic (AF) spin-1/2 trimerized (J_1-J_2-J_2) chain with J_1 = 111 K and J_2 = 30 K can explain magnetization and inelastic neutron scattering results [1,2]. The J_1 interaction is larger and forms Cu2-Cu2 AF dimers. Therefore, the field-induced magnetic moment on Cu2 sites is expected to be much smaller than that on Cu1 sites.

We measured diffraction patterns at 1.8 and 20 K in 6 T using the DMC diffractometer at PSI and observed several magnetic reflections generated by field-induced magnetic moments. We evaluated the moments on Cu1 and Cu2 sites to be 0.4 and 0 mu_B.

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A Possible Magnetic Structure of the Hexamer-Based Haldane Compound $K_2Cu_3O(SO_4)_3$

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We performed neutron powder diffraction experiments on the hexamer-based Haldane compound fedotovite K2Cu3O(SO4)3 using the SIKA spectrometer at ANSTO. The space group of the crystal structure is monoclinic C2/c (No. 15). Although the ground state was reported to be spin singlet [1], we observed a few magnetic reflections caused by magnetic long-range order below TN = 3.1 K. We looked for magnetic structures that were consistent with the reported magnetic properties [1,2]. Probably, the Shubnikov group C2'/c with the propagation vector k = 0 is applicable to the magnetic structure of K2Cu3O(SO4)3. Among the three types of Cu sites, Cu1 and Cu2 sites have ordered magnetic moments. The a components of the magnetic moments are dominant.

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Some aspects of the magnetism in $Dy_{1-x}Ho_xMnO_3$

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Magnetic multiferroic materials (or type-II multiferroics) are the subjects of intense research activity due to their property of possessing coexisting and interacting ferroic orders. These features being attractive from the point of view fundamental studies, at the same time offer wide ranging potential for technical applications. The manganites $RMnO_3$ (R = Dy, Ho) belong to this multiferroic family but the emergence of ferroelectric polarization in the compounds $DyMnO_3$, $HoMnO_3$ is described by different microscopic mechanisms, respectively, by the inverse Dzyaloshinskii-Moriya interaction and the exchange striction [1,2].

The studies of $DyMnO_3$ and $Dy_{0.8}Ho_{0.2}MnO_3$ single crystals were carried out by neutron scattering, including the diffraction of polarized neutrons.

The temperature evolution of the magnetic structures parameters of both investigated compounds demonstrate a significant dependence on the measurement mode — heating or cooling. The probable origin of this is the strong interaction of two magnetic subsystems, namely, manganese and rare-earth ones. However, the type of such hysteresis differs for $DyMnO_3$ and $Dy_{0.8}Ho_{0.2}MnO_3$, which indicates a stronger effect of the rare-earth magnetic subsystem on the manganese one in the “parent” compound than in the substituted one.

The determination of the magnetic structures of $DyMnO_3$, which are realized under different heating/cooling modes, has been carried out. The magnetic structure of $DyMnO_3$ at 4 K is a spin cycloid with components of the manganese subsystem A_yA_z type and G_xA_y one of the dysprosium subsystem. Along with the incommensurate structure, below T_{NR} Dy^{3+} is also ordered into the collinear magnetic structure G_xA_y type with the wave vector (0 0.5 0).

The magnetic structure of the compound $Dy_{0.8}Ho_{0.2}MnO_3$ at 4 K was determined. The manganese subsystem is ordered into the structure of a spin helix of the $A_xA_yA_z$ type with a total magnetic moment of 3.5 (4) μB. The magnetic structure of the rare-earth subsystem also represent an inclined spin helix of $G_xA_yA_z$ type. The magnetic structure of the substituted compound inherits the type of magnetic configuration from both parent compounds — $DyMnO_3$ and $HoMnO_3$. Replacement dysprosium with holmium leads to suppression of the ordering of the rare-earth subsystem with its own wave vector. The results of the calculations are in good agreement with the measurements of the magnetization.

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Cr and Ce magnetic ordering in $CeCrO_3$: revisited

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We have investigated the magnetic structure of bulk rare earth orthochromite $CeCrO_3$ using neutron diffraction technique. The $CeCrO_3$ crystallize with the $GdFeO_3$ structure-type (space group *Pbnm*) which originates from a slight orthorhombic distortion of the cubic perovskite structure. Earlier neutron diffraction measurements on nanocrystalline powder sample of $CeCrO_3$ have proposed *G*-type antiferromagnetic structure for Cr sublattice and *C*-type for Ce sublattice [1]. The analysis of the magnetic structure for Ce - sublattice is based on one magnetic peak (102) at $d \sim 3.152$ Å. However, the proposed *C*-type coupling for Ce will generate primarily two magnetic peaks at (100) at $d \sim 5.47$Å and (102) at $d \sim 3.152$ Å. We have recorded neutron powder diffraction patterns on a high-purity sample of $CeCrO_3$ [2] using ILL's medium resolution high-intensity D20 diffractometer and did observe the previously reported magnetic Bragg $d \sim 3.152$ Å, however significantly less intense than reported before. Simulations indicate that only the presence of magnetic coupling of *C*-type on the Cr- and the Ce- sublattices can lead to a situation where the magnetic peak (102) at $d \sim 3.152$ Å is a lot stronger than the (100) Bragg peak at $d \sim 5.47$Å. Following this proposal we have analyzed our neutron diffraction data very carefully at low temperature (1.5K), and conclude a C_yG_z type magnetic ordering for the Cr sublattice with a very small C_y - component and C_y type coupling for Ce - sublattice.

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Spin waves in a rare-earth orthoferrite $HoFeO_3$

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The multiferroic properties of rare-earth orthoferrites RFeO3 (R is a rare-earth ion) have been discovered in recent years and the ferroelectric polarization was observed at rather high temperatures [1]. This can bring RFeO3 closer to use them as new functional materials of advanced technologies. The coexistence of two magnetic subsystems - iron and rare-earth ones leads to a complex structure of magnetic interactions. The role of the Fe-R or R-R interactions increases with temperature change, leading to spin-orientational transitions [2]. An antisymmetric Dzyaloshinsky-Moria interaction (DMI) also makes a significant contribution to magnetic interaction scheme, providing the appearance of weak antiferromagnetism. It is assumed that magnetic interactions in RFeO3, and, apparently, DM, are the origin of the ferroelectric polarization.

This work presents the results of experiments on inelastic neutron scattering on the holmium orthoferrite HoFeO3, which were performed at ILL on the spectrometers IN12 and IN22. The exchange interaction parameters were obtained which show that the main contribution to the formation of the magnetic structure is determined by the exchanges inside the Fe3+ subsystem where the exchange of Fe-Fe between the nearest neighbors is J1 = -5.071 meV, and the next-nearest neighbors exchange is J2 = -0.042 meV. The distortion of the collinear structure is caused by the interaction of the DMI with the components Dx = -0.01 and Dz = -0.11 meV. The estimate of the exchange interaction Fe-Ho gives J3 = 0.026 meV and the exchange interaction within rare-earth system estimated to be J4 = 0.048 meV. These parameter values are in a good agreement with the data obtained by optical spectroscopy [3] and Raman spectroscopy [4].

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Magnetic structures of the $La_{1-x}Tb_xMn_2Si_2$ compounds

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Intermetallic compounds RM_2X_2 (R is the rare earth metal or Y; M is the 3*d*-, 4*d*- or 5*d*-transition metal; *X* is Si or Ge) crystallize in the naturally layered body-centered tetragonal $ThCr_2Si_2$-type structure (space group *I*4/*mmm*). In this structure, the single-atomic layers of different elements are stacked along the crystallographic *c*-axis in the strict sequence -*M*-*X*-*R*-*X*-*M*-. The layered structure is considered to be responsible for very exciting variety of physical properties observed in these compounds [1-3]. Systematic study of different ternary and pseudoternary RMn_2X_2 compounds shows that exchange interactions strongly depend on the in-plane Mn-Mn distance $d_{Mn\text{-}Mn}$ The spontaneous and field-induced change of the interlayer Mn-Mn magnetic ordering in the compositions with $d_{Mn\text{-}Mn} \approx d_c$ are accompanied by considerable volume and anisotropic lattice deformations.

In this paper, to clarify the origin of different type of magnetic orderings in RMn_2X_2, we studied magnetic structures of the $La_{1-x}Tb_xMn_2Si_2$ compounds using powder neutron diffraction and magnetization measurements for single-crystalline samples. We demonstrate that at 4.2 K with increasing the Tb concentration a canted ferromagnetic structure of $LaMn_2Si_2$ changes to a canted antiferromagnetic structure at $x > 0.2$. The antiferromagnetic in-plane component of the Mn magnetic moment decreases with increasing x and vanishes at $x > 0.5$. $TbMn_2Si_2$ is characterized by a collinear in-plane Mn ordering and the ferrimagnetic structure, for which the Mn sublattice possesses the interlayer ferromagnetic alignment, the net magnetic moment being oriented along the easy *c*-axis. Neutron diffraction study does not reveal a long-range magnetic order of the Tb moments for the compounds with $x \leq 0.4$. Our results show that for the Tb content $0.2 < x \leq 0.4$ a competition of the interlayer Tb-Mn and Mn-Mn exchange interactions and strong uniaxial magnetic anisotropy lead to formation of a frustrated magnetic state of the Tb ions, which prevents magnetic ordering in the Tb sublattice.

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Neutron diffraction of nano-laminated rare earth containing i-MAX phases

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The i-MAX phases[1] are a class of materials with the chemical formula $(M^1_{2/3}M^2_{1/3})_2AlC$ where M^1 and M^2 are metals. The magnetic properties of these phases are of great interest as precursors to their potential 2D counterparts,[2,3] which are obtained by selective etching of the Al layer, and may lead to functional 2D magnetic materials. We report on a magnetic neutron diffraction study of the $(Mo_{2/3}Er_{1/3})_2AlC$ i-MAX phase using the high flux E6 diffractometer (HZB, Germany), and the high resolution HRPT diffractometer (PSI, Switzerland). The magnetic structure is found to be an incommensurate transversal (static) spin wave, which is described by the propagation vector k = (0, ~0.68, 0) with the spins oriented perpendicular to k. The ordered magnetic moment, ~5.8 μ_B/Er^{3+} atom, is reduced compared with the free ion. The temperature evolution of this structure is studied, and a phase transition is observed at 4 K, where the onset of short range magnetic ordering is observed. Below this temperature, additional reflections appear in the diffraction pattern, signaling the appearance of a long range order. Evidence for an additional phase transition is observed below ~ 1.5 K, where an additional magnetic reflection appears. This new reflection is found to be consistent with a q = (1/2, 0, 1/2) propagation vector and an ordered magnetic moment of ~ 1 μ_B.

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Monoclinic super-space group description of the magnetic modulations in bulk $BiFeO_3$ at ambient conditions

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Among numerous multiferroics, $BiFeO_3$ is currently the only ABO_3-type simple perovskite that exhibits room-temperature multiferroism. $BiFeO_3$ has a highly disordered perovskite-type structure. The Fe ions are octahedrally coordinated by six O ions. The neighboring octahedra rotate in opposite direction around the [111] axis of the pseudo-cubic cell (see e.g.[1]). The relative displacement of Bi, Fe and O makes a crystal non centro-symmetric. The R3c group was ascribed to the $BiFeO_3$ structure. The crystal structure with the space group R3c is a double perovskite-like unit cell [2]. The electric polarization emerges along cubic [111] axis or hexagonal [001] axis. The magnetic structure is close to that in G-type antiferromagnet (T_N= 643 K) in which all the adjacent spin are antiparallel (e.g.[1]). A detailed investigation of the spin structure revealed that the spins form a cycloid structure with a periodicity of 62 nm [3]. Using the polarized neutron SANS technique the additional modulation (spin density wave) was found that the magnetic cycloid is tilted away from the hexagonal *c*-axis at an angle of 1°, corresponding to a SDW with $0.09(1)\mu_B$ amplitude [4]. A high resolution diffraction experiment at synchrotron source shows that the crystal structure of bulk BiFeO3 at ambient conditions should be interpreted in lower symmetry group than R3c, namely in the monoclinic Cc [5] or triclinic P1 [6]. Our synchrotron diffraction data did not reveal any modulation of crystal structure [5]. The long range magnetic modulated ordering of bulk $BiFeO_3$ at ambient conditions can be quantitatively described within the magnetic superspace group formalism [7,8] by using the monoclinic super-space group Cc'(0β0)0. This quantitative model based on Cc'(0β0)0 is in agreement with both: G-type antiferromagnetic superimposed on a cycloid structure with a periodicity of 62 nm [3] and with a ferromagnetic type superimposed on a spin density wave with the same periodicity observed in SANS studies [4].

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Spin-wave stiffness of Dzyaloshinskii-Moriya helimagnets $Fe_{1-x}Co_xSi$ studied by small-angle neutron scattering

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The spin wave stiffness was measured by small-angle neutron scattering method in the Dzyaloshinskii-Moriya helimagnets $Fe_{1-x}Co_xSi$ with x = 0.25; 0.30; 0.50. It has been shown that the spin wave dispersion in the fully polarized state is anisotropic due to Dzyaloshinskii-Moriya interaction. It is reflected in the neutron scattering pattern as two circles for neutrons obtaining and losing the magnon energy, respectively. The centers of the circles are shifted by the momentum transfer oriented along the applied magnetic field **H** and equal to the wave vector of the spiral

$\pm k_S$. The radius of the circles is directly related to the stiffness of spin waves and depends on the magnetic field. We have found that the spin-wave stiffness A changes weakly with temperature for each individual compound. On the other hand, the spin-wave stiffness A increases linearly with x in contrast to the x dependences of the critical temperature T_C and the low-temperature ordered spin S.

It has been demonstrated that in the B20 compounds, the magnetism correlates closely with the structure, and the DM interaction in $Fe_{1-x}Co_xSi$ and $Fe_{1-x}Co_xGe$ can be effectively controlled by the Co composition. It is instructive to compare the magnetic properties of the $Fe_{1-x}Co_xSi$ [1,2] compounds with those of $Fe_{1-x}Co_xGe$ compounds [3]. In the Co-rich compounds the magnetic properties duplicate each other: the CoGe and CoSi are both nonmagnetic isolators, the ordered magnetism emerges with 80% of the Co content, the sign of the DM interaction changes at x = 0.6 in $Fe_{1-x}Co_xGe$ [3] and at x = 0.65 in $Fe_{1-x}Co_xSi$ [2], the critical temperature decreases monotonously with increase of x from 0.4 to 0.8.

On contrary, the Fe-rich compounds are different: FeGe is helimagnetic metal with very high Tc =278 K, while FeSi is nonmagnetic semiconductor. The Co doping results in the decrease of the critical temperature and the average spin S for the $Fe_{1-x}Co_xGe$ compounds, while 5-10% of Co doping results in appearance of the helimagnetic structure in the $Fe_{1-x}Co_xSi$ compounds. Nevertheless the magnetic structure of the Fe-rich part of the $Fe_{1-x}Co_xSi$ phase diagram are rather well understood being described by the Bak-Jensen model, but the Co-rich part remains a puzzle.

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1D Magnetism in the Russian Mineral Pauflerite

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Pauflerite, or β-$VOSO_4$ was discovered among volcanic products of the Tolbachik volcano in Kamchatka, Russia [S. V. Krivovichev, et al., Canad. Mineral 2007, 45, 921]. It crystallizes in the Pnma orthorrobic group and its structure represent three dimensional frameworks built up from distorted $V^{4+}O_6$ octahedra and SO_4 tetrahedra. The $V^{4+}O_6$ octahedra share the O(2) corners to form [$V^{4+}O_5$] chains extending along the *a*-axis [Paufler, et al., Z. Kristallogr. 2014; 229(11): 725–729]. The vanadium arrangements form low dimensional ladders with a nearest neighbor distance of 3.7Å and next near neighbor distance of 4.89Å (see Fig. 1). We have grown mm-sized single crystals of in β-$VOSO_4$ by following the method described by Peter Paufler, et al., [Z. Kristallogr. 2014; 229(11): 725–729]. V^{4+} ions have spin ½, and present a well-defined orbital ground state, a spin only magnetism and weak spin-orbit coupling. Magnetic susceptibility and high field magnetization are in perfect agreement with theoretical expressions for 1D s-1/2 Heisenberg chain with an exchange parameter of 3.85meV and saturation fields over 60T. Powder inelastic neutron scattering shows clear gapless spinons with a continuum spanning up to 12meV (see Fig. 2). In this poster we will discuss whether Pauflerite is a realization of an ideal 1D s-1/2 Heinsenberg chain.

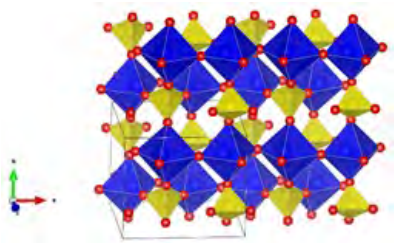

Fig. 1 Crystal structure of β-$VOSO_4$. The red balls represent O ions, the blue represent the magnetic V^{4+} ions and the yellow S. Spin chains extend along the *a*-axis

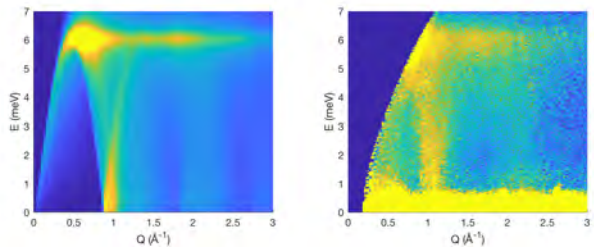

Fig. 2 Spinon excitations in β-$VOSO_4$. Right: Inelastic neutron scattering data measured on NEAT-HZB at 3K. Left: Algebraic Bethe ansatz model.

Mapping complex superstructures in the co-doped high-temperature superconductor family La(2-x)Sr(x)CuO(4+y)

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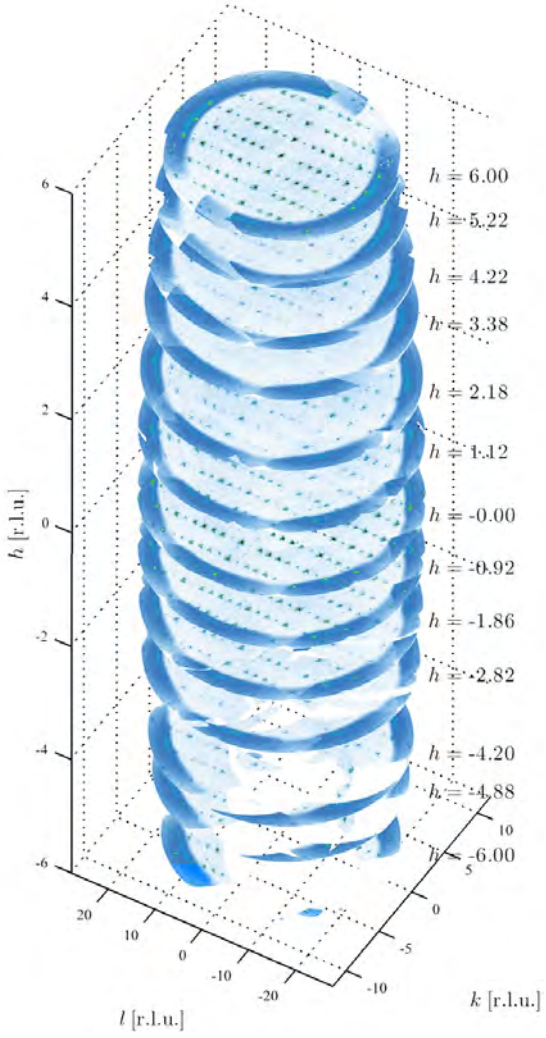
The family of high-temperature superconductors $La_{2-x}Sr_xCuO_{4+y}$ offer a great opportunity to investigate the relationship between crystal structure and superconductivity [1-3]. One of the earliest found high-T_c superconductors, hole-doped La_2CuO_4, could be key to understanding the relationship between crystal structures and the complex interplay of magnetism and superconductivity. This material can be doped by substituting some of the La with Sr or by intercalating O, making $La_{2-x}Sr_xCuO_4$ or La_2CuO_{4+y}. The intercalated O in the latter are mobile to low temperatures (<200 K), and tends to favor modulated structures.

Previous work on these modulations primarily focus on a single or a few specific observed superstructures, e.g. a concommittant 1D structure along the *c* axis – called staging – or a 3D structure assumed to originate directly from the interstitial O [4-6].

Instead, we have focused on a larger overview of the large number of superstructures, including both the previously mentioned as well as novel modulations that have never before been observed. We have mapped reciprocal space of several good quality single crystals of super-oxygenated co-doped $La_{2-x}Sr_xCuO_{4+y}$ with varied Sr doping *x*, all with remarkably coinciding $T_c \sim T_N \sim 40$ K [7-8]. We have used several different both neutron and X-ray instruments, and measurements have been done at varying temperatures in order to cover several structural phases.

We will here present our fascinating new overviews of the complex superstructures, discussing their importance to further our knowledge of the cuprate superconductors.



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Magnetic spiral in $ZnCr_2Se_4$ under pressure up to 56kbar

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The compound with the spinel structure ZnCr2Se4 is of interest as one from objects with a magnetoelectric effect [1], in which at TN = 21K a weak tetragonal distortion occurs [2] and below this temperature a simple magnetic spiral structure of the SS type [3] is formed, the period of which decreases synchronously with an increase in spontaneous deformation with decreasing temperature [4]. To determine the effect of high pressure on the magnetic spiral, we made neutron diffraction studies at T = 1.5-50K and pressures P = 0-56 kbar using cells of the piston-cylinder type and sapphire anvils with a hole. The sample was a mixture of powders ZnCr2Se4 and NaCl immersed in a liquid (Fluorinert). It was obtained that the Neel temperature increases, and the period of the spiral decreases with in pressure. The lattice parameter is close to 10A, and, it may be that period magnetic spiral at a pressure of 75 kbar will almost coincide with it and the magnetic structure will become commensurate.

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Analysis of the intermediate valence of Eu and Sm in SmB_6 and $EuCu_2Si_2$ compounds

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The work presents a cumulative analysis of experimental data on inelastic magnetic neutron scattering for intermediate-valence systems based on Sm (SmB6, Sm (Y) S) and Eu (of the EuCu2Si2 type) from the point of view of the applicability of the generalized approach based on a theoretical model of an exciton of a finite radius.

A model of a finite-radius exciton for a quantum-mechanical mixed ground state was proposed by K.A. Kikoin to describe the properties of SmB6. The model was developed and expanded to correctly understand the essential details of the spectrum of inelastic magnetic neutron scattering in the presented systems. The basis of the new approach is the idea of hybridization, as the driving force for the formation of an intermediate-valence (IV)state for Eu.

As a result, an explanation was found for the experimentally observed features of the dynamic magnetic susceptibility of EuCu2Si2, in particular: the formation of a resonant mode in the spectrum; quadratic renormalization of the energy of the resonant mode in europium compounds by changing the valence of Eu; specific Q-dependence of magnetic form factors for f-electronic excitations.

Thus, for the first time, a hole analogue of a model of a finite radius exciton was proposed and analyzed, which makes it possible to adequately describe the IV properties of the Eu state using a single (for Eu and Sm) approach to representing the structure of the ground-state wave function.

This work is supported by the Russian Science Foundation (Project No. 18-12-00133).

Magnetic structures of Li-Ni/Co-P-O

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An incommensurate (IC) – commensurate (C) antiferromagnetic (AFM) transition has been found in the $LiNiPO_4$ single crystal. The IC phase occurs over a narrow range of intermediate temperatures (20.8–21.8) K between the C magnetic structure and the paramagnetic phase [1-3]. The transition to the paramagnetic state for $LiCoPO_4$ occurs without the incommensurable phase [4]. The aim of our work is to study the effect of 10% replacement of nickel ions by cobalt on the magnetic structure of Li-Ni/Co-P-O. We present results of neutron scattering of $LiNi_{0.9}Co_{0.1}PO_4$ single crystal.

The single crystal $LiNi_{0.9}Co_{0.1}PO_4$ has been synthesized by a conventional solution growth in a LiCl flux [5]. Neutron experiments performed at the IBR-2 reactor of the Frank Laboratory of Neutron Physics using a DN-2 diffractometer [6] with cryostat on the basis of closed-cycle helium refrigerator. We have carried out neutron scans along (0k0) direction for $LiNi_{0.9}Co_{0.1}PO_4$ single crystals from 10 K up to 25 K with temperature steps 1 K and 0.2 K.

$LiNi_{0.9}Co_{0.1}PO_4$ crystallize in the orthorhombic olivine crystal structure, with the space group *Pnma*, in which the 4a position are occupied by Li ions; the Ni/Co ions are located at the 4c site; and the O ions are found at the 4c and 8d positions. Magnetic structures of $LiNi_{0.9}Co_{0.1}PO_4$ are third states: C AFM, IC AFM and paramagnetic. The C magnetic structure is such that Ni^{2+} and Co^{2+} ions located at [¼ + ε, ¼, − δ], [¼ − ε, − ¼, ½ − δ] are antiparallel to one another and the ions at [− ¼ − ε, − ¼, δ], [− ¼ + ε, ¼, ½ + δ] are anti-parallel to the first pair. Here ε = 0.02577(3) and δ = 0.01714(7), for example, at 300 K. Magnetic moment of a C structure AFM oriented along c-axis and disappear with temperature from 2.4 μ_B at 10 K down to zero at 21.0 K. The IC state is characterized by magnetic satellites (01±τ0) which are indexed by the propagation vector $\boldsymbol{\tau} \neq 0$. The long-range ordering IC structure described perpendicular spin wave along the b-axis. Magnetic satellites of the IC structure of $LiNi_{0.9}Co_{0.1}PO_4$ exist over temperature range (20.2–21.0) K. The module of the propagation vector increases with a heating of the sample from 0.097 up to 0.112 r.l.u. The 10% doping of cobalt ions decreases the transition temperature, while the temperature range of the incommensurate phase narrows.

This work was supported by MES of RF (contract No. 3.6121.2017/8.9) and by Act 211 Government of RF (contract No. 02.A03.21.0006), and supported in part by FASO of Russia (theme “Flux” No. AAA-A18-118020190112-8).

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Optical conductivity of quantum spin liquids

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We analyze optical conductivity of the herbertsmithite. Our analysis is in agreement with the corresponding measurements [1], which provide important experimental evidence of the nature of quantum spin liquid (QSL) composed of spinons. Our theoretical consideration of the optical conductivity allows us to reveal the physical mechanisms responsible for its temperature and magnetic field dependences. We show that at elevated temperatures the low-frequency optical conductivity is a decreasing function of T. This observation is consistent with the experimental data [1]. We also demonstrate that the optical conductivity diminishes under the application of magnetic fields. This observation seems to contradict the experimental results since no systematic magnetic field dependence is observed [1]. To elucidate the magnetic field dependence, we note that the measurements of the optical conductivity have been taken at 6 K and the magnetic fields B=7 T [1]. In such a case the system is still in the transition regime and the magnetic field dependence cannot be observed [2,3,4]. We predict that the B-dependence of optical conductivity can be observed at B=7 T provided that T is less or equal to 1 K. Thus, we predict that the optical conductivity diminishes at growing magnetic fields. Since the contribution coming from phonons does not depend on magnetic fields, we suggest that measurements under the application of different magnetic fields. In our report we expose a state of the art in the investigations of physical properties of 2D geometrically quantum frustrated magnets. As QSL excitations are fermions, the most appropriate description of observed phenomena is based on some spinon formalism. Our analysis permits to describe the multitude of experimental results obtained in measurements on frustrated magnets including inelastic neutron scattering

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Stability of the Q-phase of $CeCoIn_5$ in the presents of localized magnetic impurities

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In heavy fermion superconductors, the strong interlocking of charge and spin degrees of freedom creates unconventional superconductivity in the vicinity of complex magnetic ground states - an ideal test bed to study quantum phase transitions. A special case for the coexistence of superconducting and magnetic order is the well-known Q-phase in $CeCoIn_5$ [1] where the antiferromagnetism coexists at low-temperature and high field with the superconducting phase [2] and is a rare example of cooperative coexistence [3]. The magnetic order was evidenced to be an incommensurate spin density wave (SDW). For a 5% substitution of Ce with Nd, an antiferromagnetic phase is stabilized within the superconducting phase already at zero magnetic field. Previous experimental evidence suggests that both antiferromagnetic phases are separated by a quantum critical point (QCP) that separates two antiferromagnetic states with identical symmetry [3]. We present our recent studies on 2% and 3.5% Nd-doped $CeCoIn_5$ which both feature the Q-phase magnetic order at high-field region along (0.554, 0.554, 0.5) as well as a low-field SDW phase with the same order. Interestingly, the low-field SDW phase vanishes with increasing magnetic fields before the Q-phase is stabilized. This suggests that these two phases are separated by a disordered magnetic phase for low Nd-doped $CeCoIn_5$. The separation of SDW phases represents for two magnetic instabilities in the $Nd_xCe_{1-x}CoIn_5$ series, suggesting different origins of the two phases. Our study presents a unique case where two magnetic phases of identical symmetry are separated by a disordered phase.

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High pressure neutron diffration study of magnetic and structural transitions in anion deficient cobaltites

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Anion deficient cobaltites with an oxidation state close to 3+ have been studied by neutron diffraction in the wide range of temperatures and applied external pressure.
A gradual magnetic phase transition from antiferromagnetic to ferromagnetic through the mixed magnetic phase has been observed. A structure transition from rhombohedral to orthorhombic phases has been also observed. Possible mechanisms of phase separation and magnetic transition between high and low spin state of cobalt are discussed

Investigation of the magnetic structure of $Rh_{1-x}Fe_xGe$ by small-angle neutron diffraction

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The temperature evolution of the magnetic structure of the $Rh_{1-x}Fe_xGe$ compounds was studied by the small-angle neutron scattering (SANS) method. These compounds, synthesized at high pressure, crystallize into a non-centrosymmetric B20 cubic structure [1], which resultsin the appearance of the antisymmetric Dzyaloshinsky-Moriya interaction (DMI) and the formation of a magnetic spiral [2, 3]. Howeverthe RhGe compound exhibits a superconducting state below Tc = 4.5 K and weak ferromagnetism below Tm = 140 K [4] and does not possess any traces of the helical structure. It turned out that the replacement of Rh atoms by Fe in $Rh_{1-x}Fe_xGe$ compounds leads to helical magnetic ordering. The temperature of the transition from paramagnetic to helical state Tc increases with x from zero for RhGe to 278 K for FeGe [5]. At the same time, in the $Rh_{1-x}Fe_xGe$ compounds with iron concentrations $0 < x \leq 0.3$, the helicoidal magnetic structure is observed only at temperatures below 30 K.For compounds with x = 0.4 and 0.5 the scattering from the helical magnetic state was not registered with SANS. That indicates that the value of k_S is less 0.01 nm^{-1} for compounds with x = 0.4 and 0.5 and the transition of the magnetic system into the ferromagnetic state appears.The value of the wave vector at concentrations of $0.6 \leq x \leq 1.0$, increases with x up to $k_S = 0.09 \pm 0.005$ nm^{-1} at x = 1.0 [5]. Since the helical wave vector k_S is small and is almost constant with temperature for concentrations of $0.6 \leq x \leq 1.0$, it can be consideredthat the helical structure of these compounds is satisfactorily described by the model developed for FeGe [3]. Similar conversion of the wave vector to zero for intermediate concentrations was found in the study the magnetic structure of the compounds $Fe_{1-x}Mn_xGe$ and $Fe_{1-x}Co_xGe$ [5,6]. This phenomenon was interpreted as a reversal of magnetic chirality with a change in concentration x and later confirmed by the theoretical calculations [7]. The question of the nature of the helicoidal magnetic structure in compounds with a large content of Rh ($0.0 < x \leq 0.3$) requires additional theoretical and experimental studies.

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Magnon-polaron excitations in the noncollinear antiferromagnet Mn_3Ge

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We discuss the full spin-wave spectrum of the noncollinear antiferromagnet Mn_3Ge obtained using neutron time-of-flight and triple-axis spectroscopy. The sublattice of magnetic ions in hexagonal Mn_3Ge can be viewed as two adjacent kagome layers stacked along the crystallographic [001] axis (Fig. 1). Below T_N of 370 K the Mn atoms form the coplanar triangular 120-deg. antiferromagnetic order. Our measurements revealed a magnon mode with a spin-wave gap of 5 meV and a very steep anisotropic dispersion. The obtained spectrum allows one to build an effective model of magnetic interactions in the system. We found two coupled magnon-phonon excitations seen in the vicinity of the zone center on the energies of 14 meV and 17.5 meV. We argue that this mixed excitations represent a strong magneto-elastic coupling in Mn_3Ge.

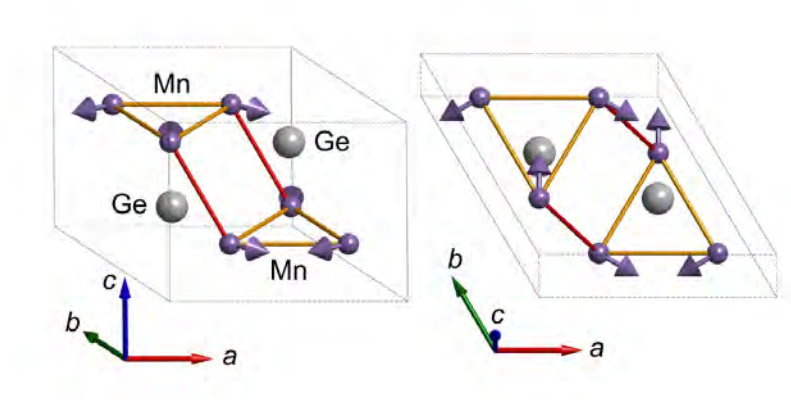

Fig 1. The chemical and the magnetic unit cells of the noncollinear AFM Mn_3Ge shown from two sides. Arrows depict the orientation of the magnetic moments, first two shortest Mn-Mn distances are shown by red and orange lines, respectively.

Crystal and magnetic structure of layered orthorhombic Li_2MnGeO_4

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The studied Li_2MnGeO_4 compound belongs to the A_2MXO_4 (where A – alkali metal, M - transition metal and X = Si, Ge) family which is diverse in types of structures and physical properties. In particular, some of them have been intensely studied as materials for positive electrodes of alkali-ion batteries. The magnetic ions form a frustrated subsystem which makes these compounds interesting in terms of magnetism. However, the mechanism of magnetic ordering and magnetic properties of Li_2MnGeO_4 are insufficiently studied.

Crystal structure precise details were established by refining the synchrotron powder diffraction data that were measured on BM25, ESRF (λ = 0.621 Å). Li_2MnGeO_4 belongs to the orthorhombic space group $Pmn2_1$. The structure is based on structural motives of the corner-sharing oxygen tetrahedra with magnetic Mn, nonmagnetic Ge and Li atoms. Magnetic susceptibility and specific heat measurements demonstrated clear anomalies associated with the antiferromagnetic phase transition at a temperature T_N = 8 K [1]. Since manganese ions are in isolated tetrahedra, the magnetic exchange interaction implies to be weak super-super-exchange with the participation of lithium and germanium cations. In the presence of the antiferromagnetic interaction between manganese ions Mn - O - X - O - Mn (X = Li, Ge), one should expect frustration of the magnetic subsystem.

The low-temperature neutron powder diffraction (NPD) experiment was carried out on diffractometer DMC (PSI, Switzerland; λ = 2.46 Å). The presence of additional neutron magnetic Bragg reflection was found below T_N. The corresponding propagation vector was found equal to k = (½, ½, ½), that is, the magnetic cell is twice along all crystallographic directions. The following group theory analysis allowed us to establish magnetic symmetry and the type of magnetic ordering. Thus Li_2MnGeO_4 has a long range antiferromagnetic ordering with a tetrahedral structure. The magnetic moment value determined from NPD refinement at 1.6 K is equal to 4.47(1) μ_B/Mn which corresponds to Mn^{2+} in high-spin (S=5/2) state. Besides, some diffuse neutron scattering was found above T_N that is located near the first magnetic reflection. This is expected to be due to the presence of short-range spin correlations above the phase transition temperature.

The study was funded by Russian Science Foundation according to the research project № 18-12-00375.

[1] Nalbandyan V. B. et al. //Inorganic chemistry. – 2017. – Т. 56. – №. 22. – С. 14023-14039.ear the first magnetic reflection.

$Ba(TiO)Cu_4(PO_4)_4$ - a neutron scattering journey towards the understanding of a chiral magnet family

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The chiral quantum magnet family $A(b\mathrm{O})Cu_4(PO_4)_4$ is an exciting series of compounds to study quantum effects in a magnetoelectric chiral system. Indeed, substitution of A^{2+} cation allows quantitative control of the degree of chirality in this family, leading to concomitant changes in the magnetic interactions. The nuclear structure is rather complicated, consisting of square cupolas stacked along the (001) direction. It crystallises in a tetragonal structure that orders at 9.5K. It is important to note that its crystallographic structure makes it a good experimental realisation of the 2D square lattice. Knowledge of the Hamiltonian of these compounds is a significant step towards the understanding of low dimensional quantum magnets.

Both diffraction and inelastic neutron experiments have been performed on several members of this family. These emphasised the presence of complex behaviour such as non colinear magnetic moments, and the existence of many spin waves in the magnetic excitations spectrum.

In this talk, I will present how we took advantage of Spherical Neutron Polarimetry (SNP) in order to solve the magnetic structure of A = Ba, Sr, Pb, b = Ti. I will also show our advance in the analysis of the complex magnetic spectrum of BaTi.

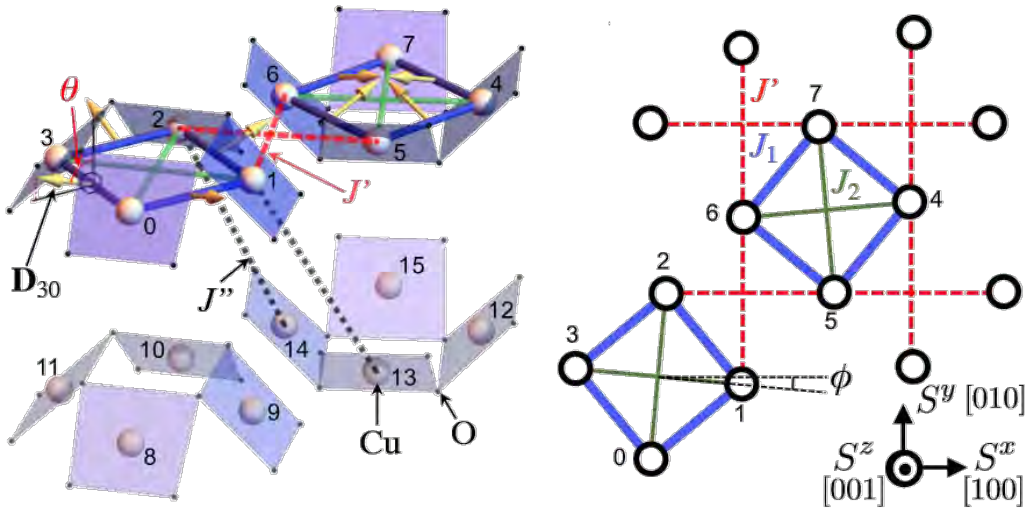

Figure 1: (left) Sketch of the crystal structure of $A(b\mathrm{O})Cu_4(PO_4)_4$. (right) Hypothetical magnetic interactions.

Effect of grain-boundary diffusion process on the geometry of the grain microstructure of Nd−Fe−B nanocrystalline magnets

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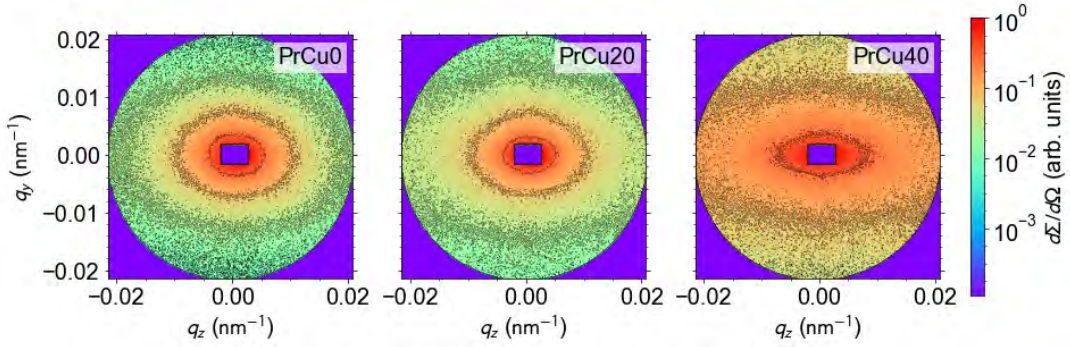
Hot-deformed anisotropic Nd-Fe-B nanocrystalline magnets have been subjected to the grain-boundary diffusion process (GBDP) using a $Pr_{70}Cu_{30}$ eutectic alloy. The resulting grain microstructure, consisting of shape-anisotropic Nd-Fe-B nanocrystals surrounded by a Pr-Cu-rich intergranular grain-boundary phase, has been investigated using unpolarized small-angle neutron scattering (SANS) and very small-angle neutron scattering (VSANS). The neutron data have been analyzed using the generalized Guinier-Porod model and by computing model-independently the distance distribution function. We find that the GBDP results in a change of the geometry of the scattering particles: In the small-q regime the scattering from the as-prepared sample exhibits a slope of about 2, which is characteristic for the scattering from two-dimensional platelet shaped objects, while the GBDP sample manifests a slope of about 1, which is the scattering signature of one-dimensional elongated objects.



Two-dimensional total nuclear and magnetic SANS cross section dΣ/dΩ of Pr-Cu doped hot-deformed Nd-Fe-B nanocrystalline magnets (logarithmic color scale). Data in the remanent state are shown. Applied-field direction was along the horizontal direction, parallel to the c-axis (pressing direction).

Non-destructive determination of critical temperature distribution in LSCO superconductor by means of polarized neutron imaging

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One of the most important aspects in condensed matter research is the use of high quality and purity single crystals. Such samples are essential for fundamental studies where the analysed physical properties can be drastically affected by defects, impurities or inhomogeneities. When it comes to type II superconductivity, the fact that the fundamental pairing mechanism is not understood has driven a great amount of research into the characterization of intrinsic properties of these materials. The synthesis method of choice in the field of cuprate superconductors is the Traveling Solvent Floating Zone technique (TSFZ)[1], the advantages being the fact that no crucibles are used in the crystallization process, keeping contamination to a minimum and the possibility to grow centimetric size single crystals essential for neutron scattering investigations.

In $La_{2-x}Sr_xCuO_4$ (LSCO) compounds, which are of interest in this project, the distribution of Sr atoms is fixed after crystallization. However, the dopant concentration is difficult to monitor or control during the growth. Because of this, it is important to test the doping homogeneity throughout the crystals.

Here we demonstrate the use of polarization neutron imaging[2] as a non-destructive method for determining the superconducting critical temperature distribution along the sample length. In the presented experiment, we have trapped the applied magnetic field inside the single crystal by cooling the system below the critical temperature. We then measured the change in beam polarization caused by the local field within the sample. This way we were able to distinguish between the superconducting areas, where the magnetic field was present, and non-superconducting areas of the sample as a function of increasing temperature. The data show an inhomogeneous distribution of critical temperatures along the crystal length, which is also the growth direction. We attribute this to a heterogeneous Sr doping throughout the sample.

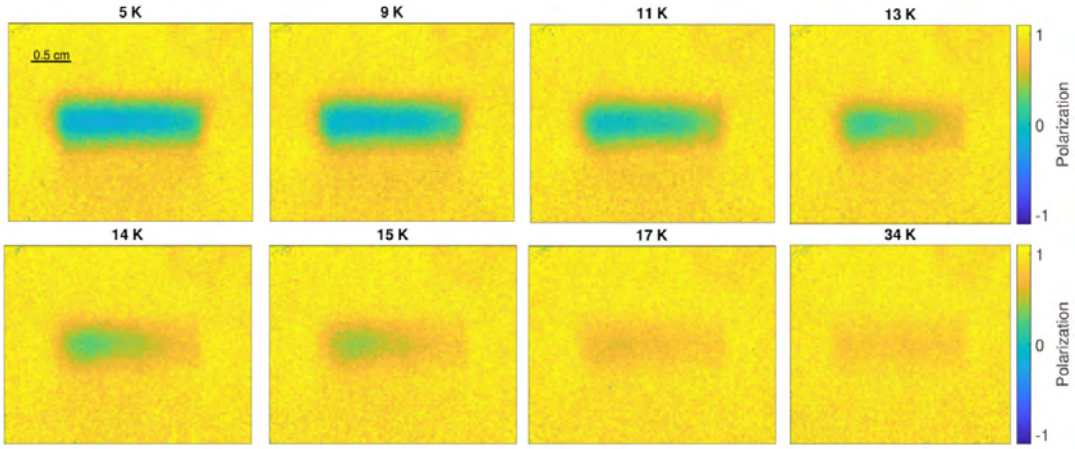

Figure 1: Temperature evolution of the recorded polarization. At the sample position, the trapped magnetic field induces a spin precession of the incoming neutron beam creating the visible contrast after passing through the spin analyser.

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Features of magnetic phase transitions in lithium-nickel orthophosphate

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$LiNiPO_4$ is the multiferroic, having co-existing antiferromagnetic and ferroelectric phases at low temperatures. In addition, in this material was found an incommensurate – commensurate antiferromagnetic transition [1]. The incommensurate phase (the propagation vector $\mathbf{k} = (0, \tau, 0)$) occurs over a narrow range of intermediate temperatures (20.8–21.8) K between the commensurate magnetic structure and the paramagnetic phase [2, 3]. As opposed to that, in the $LiMnPO_4$ compound, there is only a transition from a commensurate antiferromagnetic phase to a paramagnetic state (T_N = 33.85 K) [4]. In given work, we present results of neutron diffraction study of a magnetic phase transition in $LiNi_{0.9}Mn_{0.1}PO_4$ single crystal.

High-quality $LiNi_{0.9}Mn_{0.1}PO_4$ single crystals were grown by standard flux growth technique. The phase purity was confirmed by x-ray powder diffraction [5]. To investigate the magnetic phase boundaries, neutron diffraction experiments have been performed using the IBR-2 reactor (JINR, Dubna) on the DN-2 diffractometer [6] with a closed-cycle helium refrigerator.

The crystal structure of the $LiNi_{0.9}Mn_{0.1}PO_4$ orthophosphate is described within the orthorhombic cell (space group *Pnma*), as that of the $LiNiPO_4$ compound is. The Li^+ ions occupy the 4*a* position with the coordinate (0, 0, 0), the Ni^{2+}/Mn^{2+}, P^{5+}, $O1^{2-}$ and $O2^{2-}$ ions are located at 4*c* (*x*, 0.25, *z*) site, and $O3^{2-}$ are situated at the 8*d* (*x*, *y*, *z*) position.

According to neutron scattering data for $LiNi_{0.9}Mn_{0.1}PO_4$, magnetic satellites were not detected in magnetic ordered state. The main magnetic reflex (010) corresponding to the commensurate phase disappears at $T_N \approx 24.6$ K. This value is higher than that obtained from magnetic measurement data. It can be assumed that in $LiNiPO_4$ the 10% replacement of Ni ions by Mn ions suppresses the incommensurate phase and increases the transition temperature from the commensurate antiferromagnetic to the paramagnetic state.

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Magnetic phases in the $Cs_2CuCl_{4-x}Br_x$ mixed system

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Low dimensional spin systems have been a central concern in the last decades. The $Cs_2CuCl_{4-x}Br_x$ mixed system is very rich in magnetic phases, which can be separated by their tetrahedral or octahedral Cu^{2+} environment. For the tetrahedral Cu^{2+} environment, the neutron diffraction investigation of the magnetic phase diagram of $Cs_2CuCl_{4-x}Br_x$ provides detailed information about the influence of a specific Br concentration on the magnetic structure. This helps to clarify, how small modifications of the local Cu^{2+} environment influence the exchange couplings and frustration in such compounds. Two different long-range ordered magnetic phases are found in this mixed system. An overview of the low-temperature magnetic phases of $Cs_2CuCl_{4-x}Br_x$ will be presented [1]. For the octahedral Cu^{2+} environment of the $Cs_2CuCl_{4-x}Br_x$ mixed system, the compounds are typical quasi 2-D antiferromagnets. The realisation of the new tetragonal phase of Cs_2CuCl_4 is possible using specific crystal growth conditions at a temperature below 281K. The susceptibility measurements of Cs_2CuCl_4 show similar magnetic behaviour as the magnetic susceptibility and the magnetisation curves of the tetragonal compounds $Cs_2CuCl_{2.9}Br_{1.1}$, $Cs_2CuCl_{2.5}Br_{1.5}$ and $Cs_2CuCl_{2.2}Br_{1.8}$ and present consistent results for typical quasi 2-D antiferromagnets [2]. For the structure investigation of these compounds, synchrotron powder diffraction was used. The structure analysis down to 4K for $Cs_2CuCl_{2.2}Br_{1.8}$ shows no phase transition and the tetragonal symmetry $I4/mmm$, which is also the same for this composition at room temperature. However, the new neutron single crystal diffraction investigation presents very small orthorhombic splitting. Several magnetic reflections corresponding to the propagation vector $k = (0, 0, 0)$ are observed for this compound with neutron diffraction experiments below the magnetic phase transition at $T_N = 11.3$K confirming its antiferromagnetic nature.

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Incommensurate magnetic structure of Ho_7Rh_3

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The binary intermetallic compound Ho_7Rh_3 crystallizes in the hexagonal Th_7Fe_3-type structure with the space group $P6_3mc$ where Ho ions occupy three non-equivalent sites. This compound exhibits a complex magnetic phase diagram with three successive magnetic phase transitions at T_N = 32 K, T_{t2} = 23.5 K and T_{t1} = 9 K [1, 2]. In this work, the Rietveld refinement of the high-temperature incommensurate magnetic structure of Ho_7Rh_3 has been done using the magnetic superspace group formalism.

Figure 1 (left) shows the neutron powder diffraction pattern for Ho_7Rh_3 in the paramagnetic state at the temperature T = 70 K as well as in the antiferromagnetic state at T = 28 K. The Rietveld refinement of the magnetic structure at T = 28 K was carried out using the program JANA2006. The incommensurate magnetic structure can be well described by the magnetic superspace group P63.1'(00g)hs and the propagation vector $\boldsymbol{k}_1$ = (0, 0, 0.388). Figure 1 (right) shows the visualization of the refined magnetic structure. It has been found that magnetic moments of Ho atoms occupying 2b Wyckoff site are arranged into a circular helix-type structure propagating along the *c* crystallographic axis, while the Ho moments at the 6c Wyckoff sites form transverse spin waves propagating along the *c*-axis. Additional magnetic peaks indexed by third harmonic $3\boldsymbol{k}$ emerges on the neutron diffraction pattern measured at the low temperature T = 4.5 K indicating emergence of the squared-up magnetic structure.

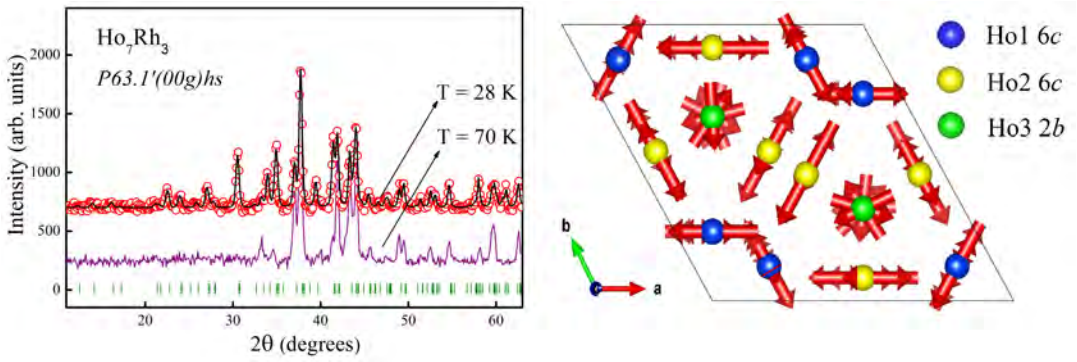

Figure 1. (left) Neutron powder diffraction patterns for Ho_7Rh_3 measured at T = 70 and 28 K. (right) Visualization of the magnetic structure of the Ho_7Rh_3 compound at T = 28 K

This work was supported by the RSF project No 18-72-10022.

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Magnetization distribution in noncollinear systems

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A large number of compounds exhibit complex magnetic behavior, including non-collinear as well as incommensurate magnetizm. Recently the great effort has been made to investigate the magnetic properties of such a systems. Unfortunately, due to vectorial character of magnetization, the experimental reconstruction of magnetization can be easily performed for the systems with the ferro- or at least antiferromagnetic ordering. The studies of the noncollinear magnetic systems which cannot be reduced to the linear problem are avoided or not published [1]. Here we present a simple method that allows us to reconstruct the magnetization distribution in any crystallographic system with any ordering of magnetic moments.

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Persistence of the roton minimum into the disordered state of a square-lattice antiferromagnet

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$Cu(DCOO)_2 \cdot 4D_2O$ (CFTD) is known to be an excellent representation of the square-lattice S = 1/2 Heisenberg antiferromagnet. The low energy spin excitations in the magnetic ordered state can be well understood within the framework of linear spin wave theory [1], but there is presently no consensus on the high energy spin-dynamics: In the vicinity of the zone boundary wavevector (π, 0) there is a minimum in the single-magnon dispersion resembling the roton minimum of ^{4}He, and a broad spin-isotropic continuum [1, 2]. Dalla Piazza and coauthors interpreted this anomaly as due to unbound spinons, which bind to form a conventional magnon spectrum upon moving away from the special zone-boundary point (π, 0) [2].

Although this idea is supported by a recent QMC study [3], theoretical methods such as CUT [4] and DMRG [5] attribute the roton minimum to the hybridization of one-magnon states with a three-magnon continuum. This process is enhanced by a strong attraction between magnon pairs.

Here we report on measurements of the magnetic excitation spectrum of CFTD at 20K, slightly above the Néel temperature T_N=16.5K. We extracted the dispersion relation and compared it to the excitation spectrum in the ordered state (T=6K). Figure 1 shows that the roton minimum at (π, 0) persist in the paramagnetic state indicating that broken spin rotation symmetry is not essential for the existence of the zone boundary dispersion anomaly, and posing a challenge to theory.

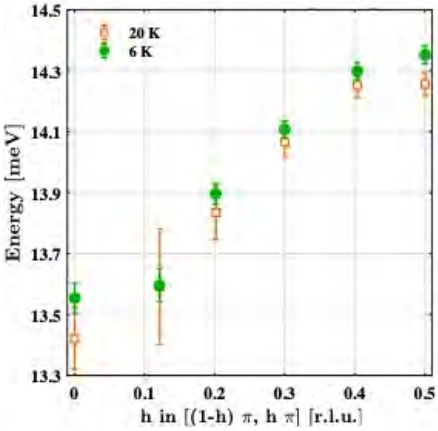

Figure 1: Magnetic dispersion along the zone boundary direction from (π, 0) to (π/2, π/2).

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Disordered skyrmion phase stabilized by magnetic frustration in a chiral magnet $Co_7Zn_7Mn_6$

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Magnetic skyrmions are vortex-like topological spin textures often observed to form a triangular-lattice skyrmion crystal in structurally chiral magnets with the Dzyaloshinskii-Moriya interaction. Recently, beta-Mn structure–type Co-Zn-Mn alloys were identified as a new class of chiral magnet to host such skyrmion crystal phases, while beta-Mn itself is known as hosting an elemental geometrically frustrated spin liquid. Here we report detailed small-angle neutron scattering, ac susceptibility and Lorentz microscopy measurements that show the intermediate composition system $Co_7Zn_7Mn_6$ to be a unique host of two disconnected, thermal-equilibrium topological skyrmion phases; one is a conventional skyrmion crystal phase stabilized by thermal fluctuations and restricted to exist just below the magnetic transition temperature T_C, and the other is a novel three-dimensionally disordered skyrmion phase that is stable well below T_C. The stability of this new disordered skyrmion phase is argued to be due to a cooperative interplay between the chiral magnetism with Dzyaloshinskii-Moriya interaction, and the frustrated magnetism inherent to beta-Mn [1].

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Magnetic structure of 2D Dirac fermion antiferromagnet $EuMnBi_2$

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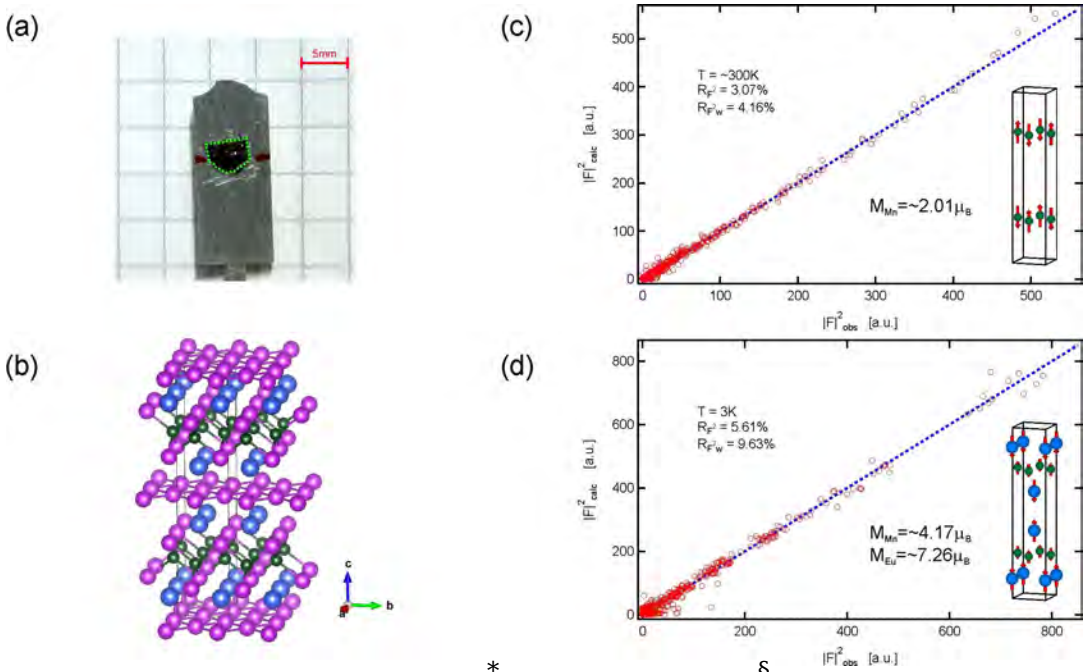
The layered bulk antiferromagnet $EuMnBi_2$ was recently reported possessing 2D Dirac fermions in its Bismuth layer [1], and the reported magnetic field dependent transport experiments show that the antiferromagnetic order has a marked impact on the topological transport properties [2,3]. Following an earlier study of the magnetic order in $EuMnBi_2$ via resonant X-ray scattering [1], we report here a comprehensive determination of the magnetic structures of both the Eu and Mn magnetic sub-lattices by using both polarised and non-polarised single-crystal neutron diffraction methods [4]. Since Eu has a quite large thermal neutron absorption cross-section, the intensities of diffraction peaks are quite sensitive to the shape of sample due to the different absorption path. To solve the absorption problem, a 3D model of the same shape and size as the real sample was established, and the absorption paths were also calculated for each reflection by dividing the sample model into 20 x 20 x 20 subsections. After absorption correction, the magnetic structures are refined as shown in Fig. (c)-(d). The ordered magnetic moments are 7.26(8) μB and 4.17(8) μB for the Eu and Mn ions respectively at 3K. At room temperature, only the Mn moments order and the size of the ordered magnetic moment is ~2.00(4) μB. Furthermore, the magnetic phase transition temperatures are found at T_N(Eu) = 22 K and T_N(Mn) = 337 K. The interplay between the Eu and Mn magnetism as well as possible coupling between the magnetic order and Dirac fermions will also be discussed.



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4. Fengfeng Zhu, et al. (in preparation)

Polarized neutron reflectometry in China spallation neutron source

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The multi-purpose reflectometer (MR) at China spallation neutron source (CSNS) is an instrument optimized for examining thin films with nanometer scale structure, especially in regard to their magnetic properties with the removable polarized neutron devices. The commission of MR is finished in 2018. Although the current beam power of CSNS is about 50 kW,the MR can measure lowest reflectivity down to 10^{-5}.

Several kinds of user proposals have been done. The minimum sample up to 10×10 mm^2 had been used. The followings are some examples.

First, I report a polarized neutron reflectometry (PNR) study on W/CoFeB/MgO/CoFeB/W thin film, which exhibited a perpendicular magnetic anisotropy (PMA). The results show that PNR is a technique sensitive to the compositional and magnetic depth profiles of thin film samples which enables us to discuss the role of boron in the formation of PMA.

Second, I report a PNR study on YIG/Pt thin film. The dead layer between the GGG substrate and YIG film has been discussed.

The MR at CSNS will accentuate the polarized/un-polarized neutron reflectivity with low background, which is a powerful technique to study the structure of thin flims.

Branched polyethyleneimine/TEMPO-oxidized cellulose nanofibers xerogels for water remediation: a Small Angle Neutron Scattering (SANS) study

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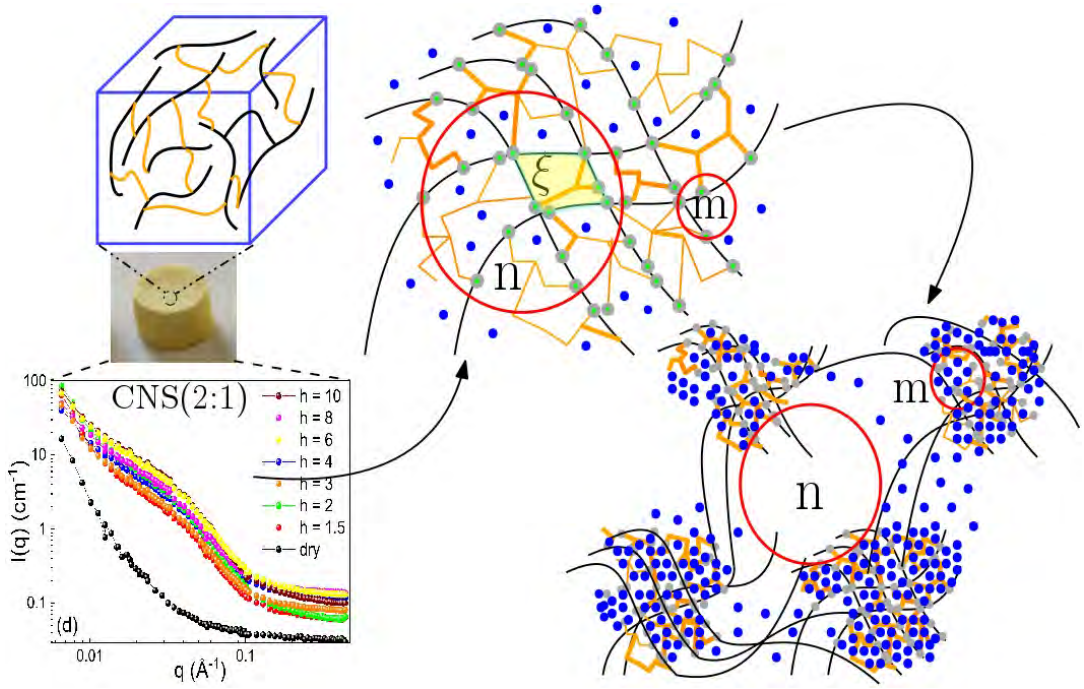
Adsorbent sponges for water remediation, prepared using 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) oxidized and ultra-sonicated cellulose nanofibers (TOUS-CNFs) as three-dimensional scaffolds, and branched polyethyleneimine (bPEI) as the cross-linking agent, underwent to a systematic Small Angle Neutron Scattering (SANS) investigation, by varying the amount of cross-linker and the water content. The aim was to provide an experimental evidence of nano-porosity in these cellulose nano-sponges (CNS) by investigating the water nano-confinement geometries in the adsorbent material. Moreover, we also verified how the breaking/reformation of specific intermolecular hydrogen bond interactions between water and the chemical groups present in the architecture of the CNS can contribute to regulate the water adsorption process observed at macroscopic level.

The short-range correlation length interpreted as a very first indirect estimation of the effective nano-dimension of the cavities produced by the cross-linking of the reticulated cellulose nanofibers. From the model, the Porod (*n*) and Lorentz (*m*) exponents have been also obtained, respectively associated to the density of TOUS-CNFs at high (~100 nm) and low (1 - 10 nm) spatial scale. These parameters are sensitive to the structural variations induced by the progressive uptake of water on the bPEI/TOUS-CNFs xerogels with different CNS ratios.

Finally, the effect of the addition of citric acid in the CNS formulation was investigated, confirming its role in increasing cross-linking density and xerogel rigidity. The obtained results appear crucial in order to rationalize the design of these sponges and to track the changes in the ability of the final products as efficient nano-confinement systems for water.



Interaction of Fe-Ni alloy with amorphous fullerene C60 in sintering

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The interaction of the amorphous phase of fullerene C_{60} (1.7 at.%) with austenitic Fe – Ni alloy was studied during sintering at high pressures of 2–8 GPa and high temperatures of 800–950 °C using the methods of neutron diffraction, neutron tomography and microstructural analysis. After sintering (2 GPa and 950 °C, 4.5 GPa and 900 °C, 8 GPa and 800 °C), the metal matrix in all samples retained the original fcc structure, fullerene dissolved in the alloy and formed carbide Fe_3C. At 2 GPa, compact regions of the carbon phase were formed.

Structural changes during sintering of composites with a low concentration of amorphous fullerene (1.7 at.%) in a number of parameters are similar to changes in the case of a composite with a high concentration of amorphous fullerene (25 at.%) [1]: the fcc lattice of an iron-nickel alloy is preserved; carbon dissolves in the alloy; carbides are formed. But there is a significant difference: at low pressure (2 GPa), the carbon component in the metal matrix localized, which lowered the composite hardness. An increase in pressure (4.5 and 8 GPa) led to the dispersion of the carbon component, its transformation into a harder component than the metal component, and an increase in the hardness of the composite. This indicates that the amorphous fullerene phase can be a promising reinforcing additive. High hardness can be associated with the formation of carbides and the transformation of amorphous fullerene at high pressures and temperatures into hard disordered (amorphous) graphite.

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Ab initio study of lattice dynamics of rear-earth borides

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Cluster-network systems are complex compounds with a wide range of ground state types, which predetermines the functional properties and possibilities for considering them as promising materials. One of the typical examples of such systems are hexa- and dodecaborides of rare-earth metals, where, along with the unusual physical properties of the f-electron subsystem, a number of anomalies and features of atomic dynamics [1] are observed in the experimental spectra of phonon excitations. The present-day *ab initio* calculations of the phonon spectrum in RB_{12} dodecaborides (for example, [2]) do not very well describe the density of phonon states measured in neutron experiments. In particular, this refers to a peak in the phonon density of states of LuB_{12} near 5 THz, corresponding to lower optics. However, it is precisely this energy region that is of interest due to the unusual physical properties of these systems, such as intermediate valence, the formation of Kondo-insulator properties, etc.

Here, we present an *ab initio* study of lattice dynamics of cluster-network compounds. Our calculations are performed using the Quantum Espresso package, with PAW-type pseudopotentials. We determine the phonon dispersions and atom-projected density of phonon states for several high borides of rear earths (see, e.g., Fig. 1). The obtained results are compared with available experimental and theoretical data.

This work was supported by Russian Science Foundation (Grant RSF 18-12-00438).

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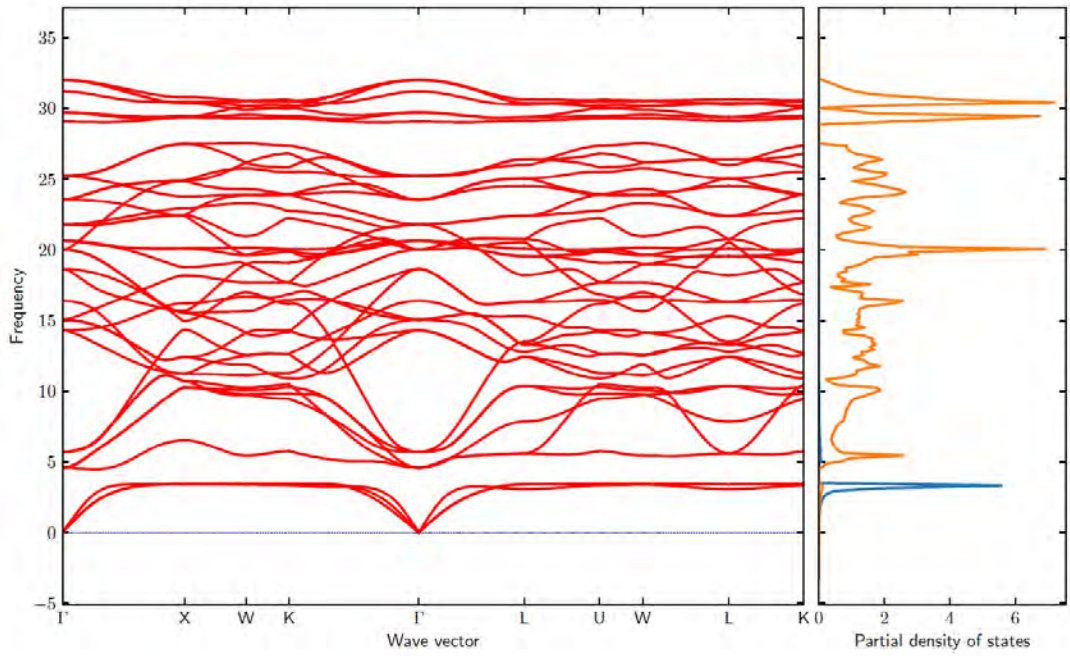

Fig. 1. Phonon dispersions and atom-projected density of phonon states in LuB_{12}.

Defective hierarchical porous copper-based metal-organic frameworks synthesised via facile acid etching strategy

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Introducing hierarchical pore structure to microporous materials such as metal-organic frameworks (MOFs) can be beneficial for reactions where the rate of reaction is limited by low rates of diffusion or high pressure drop. This advantageous pore structure can be obtained by defect formation, mostly via post-synthetic acid etching, which has been studied extensively on water-stable MOFs. Here we show that a water-unstable HKUST-1 MOF can also be modified in a corresponding manner by using phosphoric acid as an etching agent and a mixture of dimethyl sulfoxide and methanol as a dilute solvent. More interestingly, we demonstrate that the etching process which was time- and acidity- dependent resulted in defective HKUST-1 with extra interconnected hexagonal macropores forming in this MOF without compromising on the bulk crystallinity. These findings can suggest an intelligent synthetic method of hierarchical porous MOFs with improved molecular accessibility and diffusion for catalysis.

New possibilities of time resolved X-Ray studies of defect structure of crystals

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At present report time resolved methods and measurements of shape and full width half maximum (FWHM) of rocking curves (RC) under external ifluences are described.

Fast control of X-ray parameters, including scanning diffraction conditions and controlling by times much shorter than possibilities of traditional approaches, is a very relevant scientific task. We overcame limitation of traditional approach, such as complex goniometric systems, by using of non-mechanical adaptive X-ray optic elements, such as X-ray acoustic resonators of longitudinal oscillations or bimorph piezo-actuators [1]. It allows fast and precise variation of X-ray diffraction parameters, varying the angular position of the X-ray beam and controlling its wavelength. An important feature of the method is the possibility of conducting experiments not only in laboratory conditions, but also at synchrotron stations.

The method has been successfully applied to the study of processes occurring in crystals under the action of both static and dynamic loads. Using this method, studies of a silicon crystal subjected to quasistatic mechanical load were carried out [2]. The studies of the evolution of the defective structure of lithium fluoride single crystals under the conditions of dynamic ultrasonic loading in a wide range of amplitudes have also been studied [3]. It is shown that the diffraction pattern (shape and FWHM of rocking curves) under the action of ultrasound can differ significantly from the original, and the proposed method allows monitoring its changes with a temporal resolution of up to 10 μs, inaccessible when using mechanical goniometric systems. Studies of the evolution of the defective structure using the new method showed its significant (at least 3 orders of magnitude on a laboratory source) superiority in speed over existing methods.

The reported study was funded by RFBR and DFG 19-52-12029 and by RFBR according to the research project №18-32-20108.

QENS studies of Reorientational Hydrogen Dynamics in Complex Hydrides

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All-solid-state batteries employing solid-state electrolytes (SSE) promise higher energy densities through the use of high voltage cathodes and metallic anodes and improved operational safety compared to batteries based on liquid organic electrolytes [1]. Moving beyond lithium electrochemistry also offers more sustainable and cost-effective solutions. Development of practical SSEs with high conductivity is, however, a major challenge, which requires a synergistic experimental and computational approach.

QENS has proved to be an informative method for describing reorientational dynamics in a recently emerged SSE class of borohydrides and polyborates, contributing to the increased understanding of fundamental mechanisms underlying superionic conductivity in these materials. A profound characterization of complex systems can, nevertheless, be achieved only with the input from complementary methods. Thus, in this work we demonstrate detailed dynamical portraits of novel SSEs for Li [2,3], Mg [4] and Na [5] batteries obtained by means of the QENS analysis supported by DFT simulations, IR, Raman and NMR spectroscopy. Using deuterium labeling we disentangle contributions of different components of the studied electrolyte systems and build comprehensive models of molecular motions.

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Structure of oxy-halide glasses for solid state batteries

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Discovering new chemistry and materials to enable rechargeable batteries with higher capacity and energy density is our priorities. The novel inorganic and thermally stable glasses are potential substitutes for the toxic and flammable organic liquid electrolytes that are used in the Li-ion batteries. The oxy-halide glasses/amorphous solids are derived from the precursors of crystalline anti-perovskites of metal hydroxides and have the highest reported Li^+ and Na^+ conductivity, $\sigma > 10^{-2}$ S cm^{-1} at room temperature (25ºC) [1].

Here we study a new glass family with nominal composition: $A_xM_{1-x}O_{1+y}Cl_{1-2y}$ (where A=Li, Na and M=Ba, Ca), which were prepared from commercial precursors: NaCl, LiCl, NaOH and $Ba(OH)_2$ etc, applied multi-step heat treatments.

The structure characterization is challenging, first of all we intend to understand the atomic structure of the new materials. Neutron and X-ray diffraction experiments have been performed. Neutron diffraction experiments were carried out at the 10 MW Budapest research reactor using the PSD diffractometer, λ_0 = 1,069 Å [2]. Microstructure were analyzed on powder samples, by laboratory X-ray diffraction technique using a Brucker axs type diffractometer operating with Co Kα radiation (λ = 1,97 Å, Co Kα), stepsize was 2θ = 20-100°.

Since electrode materials are inherently nano-scale materials, local observations of these materials at high resolutions can be helpful to understand the microscopic processes that occur inside nano-particles and their interfaces with the electrolyte. Scanning electron microscopy coupled with energy dispersive X-ray spectroscopy was used to visualize and study the structural morphologies and atomic distribution.

Neutron- and X-ray diffractions already showed that both Li and Na based compositions has a well-defined structure. All Li/Na based samples possess good hydrolytic stability, no any hydrogen bonds were detected. Details of the structural characteristics will be presented.

Acknowledgement - This work was supported by the NKFIH, Nr. 2017-2.3.7-TÉT-IN-2017-00023.

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Self-assembly of iron oxide nanoparticles in magnetic field studied by Small-Angle Neutron Scattering

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Magnetic nanoparticles (NPs) as responsive materials are widely used for various applications, for example as contrast agents for magnetic resonance imaging and as core constituents for magneto-responsive nanocomposites [1,2]. To better understand and be able to tailor the properties of these materials, a better knowledge about their behaviour in a magnetic field is needed. Therefore, we studied the self-assembly of iron oxide nanoparticles in a magnetic field of up to 3 T by small-angle neutron scattering.

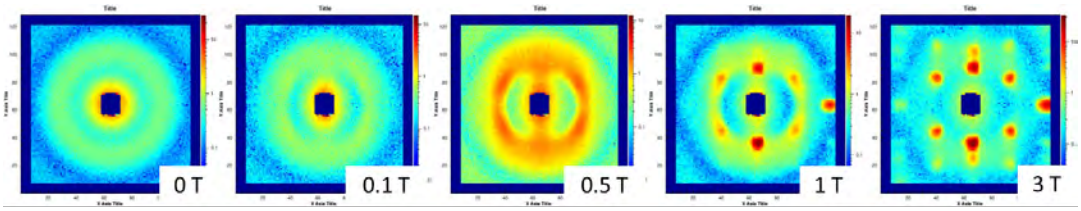

Figure 1 Scattering images from iron oxide nanoparticles in magnetic field

The NPs show completely isotropic behaviour at zero field (Figure 1). Applying a field of 0.1 T already leads to an ordering of the NPs which can be seen in the anisotropic pattern of the scattering image. Increasing the field strength leads to more pronounced ordering effects.

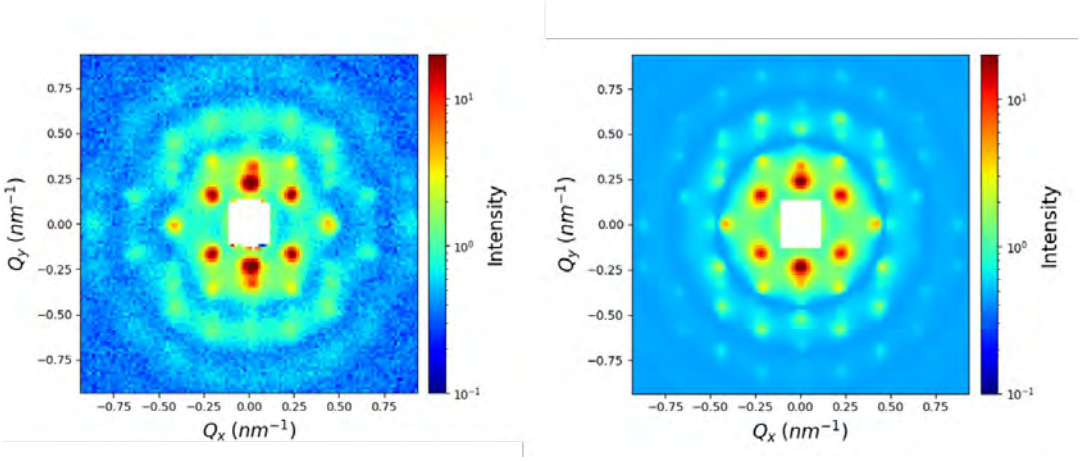

Figure 2 Fit results using a bct crystal lattice of NPs in BornAgain

Using the BornAgain software, we were able to evaluate our data by directly fitting the obtained 2D scattering images, taking into account a body-centered tetragonal crystal lattice (Figure 2). Without field, the data can be described by a simple core-shell form factor. The NPs tend to form chain-like structures when a low field is applied. These can be considered as building blocks for their supercrystalline structure at the highest field strengths.

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In situ synchrotron study of layered double hydroxides loaded with chloride and sulfate anions

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The studies of layered double hydroxides (LDHs) are a very promising field in the search for new non-toxic corrosion protective materials. These materials can be used as nanocontainers for corrosion inhibitors with their subsequent controlled release. LDHs have high anion exchange ability and in general case can be represented by formula $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}[A^y]_{x/y}\cdot zH_2O$, where $M^{II,III}$ and A^y are metal cation and interlayer anion, respectively. LDHs can be used as highly effective corrosion protective materials if they loaded with corrosion inhibitors [1].

This work is related with study of kinetics of Cl^- and SO_4^{2-} anions intercalation to Zn-Al LDH grown on Zn substrate. As a result of *in situ* synchrotron experiment with anion exchange processes two data sets were obtained: nitrate anion (NO_3^-) in host LDH was replaced by chloride (Cl^-) and sulfate (SO_4^{2-}) anions. The crystal structure analysis shows that LDH-NO_3 and LDH-Cl are described by R-3m space group with unit cell parameters a=3.0771(2) Å, c=26.862(9) Å and a=3.081(2) Å, c=23.359(5) Å, respectively. The structure of LDH-SO_4 is described by P-3 space group with unit cell parameters a=5.3338(4) Å, b=11.109(2) Å.

In the intercalation process for both cases the parent LDH-NO_3 phase disappeared completely, and formation of new crystal phase is accompanied by the appearance of intermediate one. At the end of the $NO_3 \rightarrow Cl$ exchange process the intermediate phase disappeared completely, while at $NO_3 \rightarrow SO_4$ exchange reaction the intermediate phase exists until the end of the process.

Using Avrami-Erofe'ev model [2] the analysis of anion exchange process was performed and it shows that in the case of $NO_3 \rightarrow Cl$ exchange the disappearing of NO_3^- and emerging of the intermediate phase with Cl^- is 2D process, which is phase boundary controlled. Further processes of disappearing of the intermediate phase and emerging of the final one are 1D diffusion controlled reactions. The $NO_3 \rightarrow SO_4$ anion exchange reaction is described by the similar way.

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Effect of crystallographic textures on the functional properties of TiNi shap memory alloy

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TiNi alloys became one of the most technologically important shape memory alloy due to the excellent combination of attractive properties like the shape memory effect (SME), superelasticity effect (SE), high damping capacity, biocompatibility and excellent mechanical properties, as well as a very high resistance to corrosion. The thermoelastic martensitic transformation enables the SME and SE. Homogeneous semi-finished products of TiNi alloy were obtained by sintering of hydride-calcium powder. The sintered blanks were subjected to rotary swaging at temperatures of 600, 900 and 1000 °C with a total deformation of 53 … 56% (e = 1.5). Measurements of the crystallographic preferred orientations (CPO's) of alloys were performed at the neutron time-of-flight texture diffractometer SKAT (FLNP JINR, Dubna, Russia). The degree of preferred orientations and space characteristics of textures are directly depend on the type of plastic deformation of sample. The martensitic transformations temperatures were determined by mechanical spectroscopy, and temperature spectra of elastic and inelastic properties were obtained. The shape memory characteristics at torsion deformation (g_{pr}=2…14 %) are determined. We observed the correlation between patterns of CPO's and functional properties of alloy, namely, the degree of shape recovery and the temperature displacement of martensitic transformation points.

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A New Class of Low Surface Energy Anionic Surfactant for Enhanced Oil Recovery (EOR)

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A highly branched green low surface energy surfactant (LSES), stable in harsh conditions, was synthesized for enhanced oil recovery (EOR). Oil recovery factors were determined using a glass micromodel and indicated 72% increase in oil recovery in both low and high brine solutions, a remarkable result for only a single chain surfactant flooding. The surface-interface analysis of brine and brine-surfactant solutions were carried out, while small-angle neutron scattering measurements were used to determine the changes in surfactant structure in different brine solutions, and zeta potential experiments revealed the effect of monovalent and divalent cations in each solution. Adsorption analysis on crushed glasses was evaluated to see the maximum amount of surfactant adsorption in the system, and finally, oil recovery factors were discussed according to the interfacial tension and contact angle measurements. Based on our inclusive study we conclude that the cost-effective and environmentally friendly LSES present a class of potentially important material for use in various EOR scenarios, such as the low salinity, smart water, alkaline-surfactant-polymer, and nanoparticle-surfactant flooding.

Supercritical vs subcritical drying of silica aerogels: Structural considerations

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Aerogels are unique materials possessing low density, high specific surface area, and high porosity, allowing their wide practical applications as sorbents, heterogeneous catalysts, heat and sound insulators, etc. A key stage in the synthesis of aerogels, is the removal of solvent from the wet gel matrix. To avoid high mechanical stresses due to the action of the capillary forces, which may lead to complete destruction of the gel structure, aerogels are produced using supercritical drying. Our previous results have shown that the removal of the solvent at the temperature slightly lower than the critical one can produce monolythic silica aerogels with even higher specific porosity and specific surface area in comparison with the similar aerogels obtained using supercritical drying. Until now, the effect of the drying temperature on the structure of aerogels has not been analyzed in detail. In this work, we focused our efforts on the comprehensive structural studies of silica aerogels prepared from isopropanol media and dried in a wide temperature range - from 85°C to 265°C.

The silica gels were prepared by slow hydrolysis of tetraethoxysilane in water-ethanol mixtures in the presence of HF. The gels were thoroughly washed by isopropanol and heated to 85°C, 115°C, 145°C, 175°C, 205°C, 235°C or 265 °C (critical temperature of isopropanol is 235°C). Then autoclaves were slowly depressurized, evacuated (15-20 torr) and cooled to obtain silica aerogels. Using low-temperature nitrogen adsorption measurements, X-ray diffraction, thermal analysis, scanning electron microscopy, small-angle neutron scattering, we have carried out the comparative analysis of the structural characteristics of SiO2 aerogels prepared from isopropanol media and dried in a wide temperature range - from 85°C to 265°C. Analysis of the obtained data showed that the these aerogels are porous systems with the mass-fractal organization of the structure. It has been established that both the fractal dimension D_m and the upper limit of self-similarity R_c of mass-fractal clusters increase with increasing temperature of aerogels synthesis.

This work was supported by the Russian Science Foundation (grant no. 19-73-20125).

A quasi-elastic and inelastic neutron scattering study of alkaline and alkaline-earth borohydrides $LiBH_4$ and $Mg(BH_4)_2$

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Quasielastic neutron scattering was used to investigate the low energy transfer dynamics of the complex borohydrides $Mg(BH_4)_2$ in the alpha and beta-modifaction, $LiBH_4$ in the low and high temperature crystal structure, and the 1:1 molar mixture of $LiBH_4$ + alpha- $Mg(BH_4)_2$. All investigated compounds show a rich dynamic behavior below energy transfers of E = 10meV with the superposition of rotational dynamics of the constituent BH_4 anions and low lying lattice modes. For $Mg(BH_4)_2$, the rotational diffusion of the BH_4 units was found to be much more activated in the metastable beta-polymorph compared to the alpha-phase, and the low lying lattice modes are even softer in the former crystal structure. In $Mg(BH_4)_2$, the structural phase transition is mainly governed by the lattice dynamics, while alkaline $LiBH_4$ exhibits a transition of the BH_4 rotations around the phase transition temperature. Ball milled $LiBH_4$+-$Mg(BH_4)_2$ remains a physical mixture of the parent compounds and each component retains its characteristic dynamic signature up to the melting temperature.

Time-Resolved X-Ray Diffraction for Investigation of Effects Induced in Non-Centrosymmetric Crystals by External Electric Field

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INTRODUCTION: This work is devoted to investigation of the near-surface thin structures formation processes, which occurs in non-centrosymmetric crystals under external electric field. The relevance of the work lies in the perspectives of this effect applying for control of defect structure and functional properties of the crystalline materials. The understanding of the nature of the structure behavior caused by the perturbation of external electric field is the key for development of the such technological direction as defects engineering, that has direct relationship to the design of multilayer functional systems, applied in microelectronics and srtaintronics. For example, the reversible process of migration-induced field-stabilized polar phase (MFP) formation was discovered and investigated in strontium titanate single crystals under external electric field [1]. This process has been caused by the oxygen vacancies migration to the near-cathode area of the sample followed by phase transition to the piezoelectric state and corresponding X-Ray rocking curve broadening. The similar behavior of diffraction pattern was observed by us in other crystals that allows to expect the same mechanisms of real structure transformations.

EXPERIMENTAL: The samples under investigation were perspective piezoelectric crystals of oxides: the crystals of lanthanum-gallium silicate family, paratellurite and lithium tetraborate. The basic instruments of structural diagnostics were X-Ray diffraction techniques, which are non-destructive and have a high sensitivity to interatomic distances changings and real structure. Among the lots of existing methods the most modern have been used: reciprocal space mapping in triple-axis diffraction scheme, which makes it possible to separate angular misorientation of domains from interplanar distance variation, and time-resolved X-Ray diffractometry of high resolution, which allows to observe real crystal structure dynamics with high (up to microseconds) time resolution by diffraction pattern changing and was realized both at the synchrotron radiation facility and at the laboratory sources.

RESULTS AND DISCUSSION: The results of X-Ray diagnostics have been supplemented by the electrophysical measurements. Spatial and time parameters of the near-surface structural phases induced by electric field were investigated in the crystals with different types of conductivity. In lanthanum-gallium silicate only fast process of piezoelectric effect was observed after applying of external electric field which appear as rocking curve angular shift while in paratellurite and lithium tetraborate crystals slower (tens of minutes) process of rocking curve broadening caused by charge carriers migration and real structure transformation in near-surface area was observed additionally to piezoelectric effect.

CONCLUSIONS: Multiscale diagnostics of electric field-induced near-surface phases and time-resolved studies of their nucleation processes have been carried out. We can conclude that the reason of the observed effect is the field-induced real structure transformation due to the migration of the oxygen vacancies or ions, because its dynamics corresponds to dynamics of electric conductivity. Migration of charged defects to near-surface area was followed by a sharp increase in the electric field intensity there. As a result of piezoelectric deformations mechanical strains appears which can significantly change real structure up to phase transition in all samples except lanthanum-gallium silicate which has a higher elecric conductivity.

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Investigating the SEI in silicon-based anodes with contrast-matched SANS

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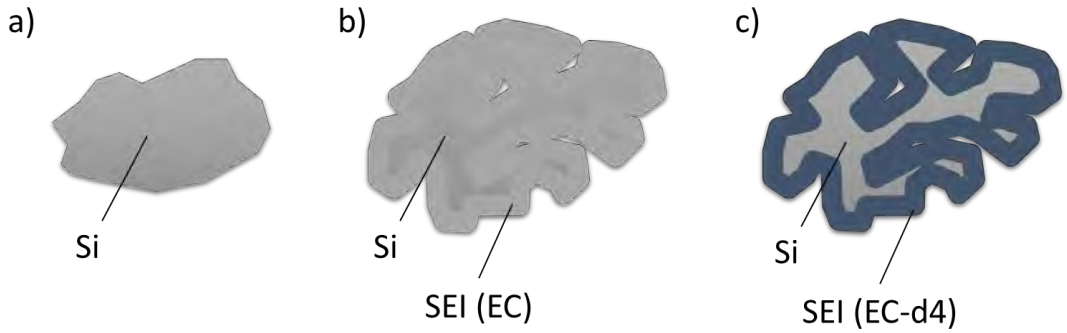
Silicon-based electrodes are attractive candidates as anodes for Li-ion batteries due to their high theoretical specific capacity. However, repeated lithiation/delithiation causes significant morphological changes of the silicon particles which results in the formation of highly porous silicon structures and severe side reactions at the silicon/electrolyte interface. To quantify the morphological changes of silicon electrodes, we applied small-angle neutron scattering (SANS) with selective contrast matching of silicon particles and the solid-electrolyte-interphase (SEI). Using either deuterated or protonated ethylene-carbonate based electrolytes allowed us to obtain SEI products with scattering length densities either perfectly matching or mismatching with that of the silicon particles. The resulting contrast-matching SANS spectra provide quantitative insights into the SEI coverage around the silicon particles and filling of the evolving porosity within the electrode.



Determination of the morphology modification of zwitterion doped PEDOT:PSS with neutron scattering techniques

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Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is arguably the most used conducting polymer across a wide range of applications due to its superior processability compared to most conducting materials. However, the enhancement of its relatively low electrical conductivity remains a dynamic field of research. One of the most common ways to improve the conductivity of PEDOT:PSS is by adding asymmetrically charged dopants to the PEDOT:PSS dispersion. However, the morphological changes of the PEDOT:PSS structure induced by such dopants are still not completely understood due to the use of surface rather than bulk morphology characterisation techniques to study the mechanisms of conductivity improvement. This is because most bulk techniques are not very sensitive to disordered polymer blends composed of two materials close in nature such as PEDOT and PSS. In this study we have synthesized PEDOT:(deuterated)PSS and doped it with different concentrations of the asymmetrically charged zwitterion 3-(N,N Dimethylmyristylammonio)propanesulfonate (DYMAMP). We then conducted small angle neutron scattering to study the morphological changes that PEDOT and PSS experience as the dopant concentration increases. We found that the correlation distance between PSS rods decreases linearly as the concentration of DYMAP increases. This improves the packing of the PSS molecules and the spacing between PEDOT chains allowing for a more ordered network that provides a more favourable electrically conductive pathway. Additionally, we spun-cast the different doped PEDOT:PSS dispersions into thin films and conducted neutron reflectivity to study the thin film structure of PEDOT:PSS as a function of DYMAP doping concentration. We determined that at low doping concentration the film separates into a quasi bi-layer structure that slightly decreases the conductivity of the film. However, at higher doping concentration the film forms into a homogeneous layer experiencing an enhanced conductivity by more than a order of magnitude. These findings provide insight on the morphological mechanisms of conductivity improvement of doped PEDOT:PSS to develop more efficient PEDOT:PSS for its different applications.

Microstructure Study of Ti-6Al-4V Additively Manufactured using Neutron Diffraction

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This study presents a detailed characterization of room temperature bulk microstructure and texture of additively manufactured Ti-6Al-4V alloy samples with the neutron time-of-flight diffractometer HIPPO. A comparison is made between samples that were manufactured by two different methods utilizing selective laser melting and electron beam melting. Analysis of the orientation distribution function shows a dependency upon the particular fabrication technique used as well as on the location within the built body and orientation relative to the build direction. It is shown that the texture components strength in the hexagonal phase depends on the relative tilt angle between the build direction and that the overall texture of samples prepared with the electron beam method is weaker than those prepared with the selective laser melting. Such knowledge on the bulk microstructure allows to optimize additive manufacturing process parameters.

Microporous (guest-host) systems: from (micro-)structure to optical properties

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Inorganic zeolites and organometallic MOFs are widely used as catalysists in petrochemistry and selective sorbants in gaz separation process or depollution, but also exhibit good transparency in visible-IR range for optical applications.

While possessing similar framework topologies, zeolites are characterised by SiO_4 / AlO_4^- based structure whose global negative charge has to be compensated by cations M^{q+} sparse throughout the cavities. The flexible Si/Al ratio and easy exchange of cations M allows to tune the Coulombian force that interacts with guest molecules. In MOFs, the large choice of linkers (terephthalate, biphenyl, benzene-dicarboxylate…) gives rise to larger and richer structures where hydrogen bonding or Van der Waals force stabilises more weakly the guests. Contrary to usual applications as selective sorbants or catalysts where the (guest-host) system has only a transient character and where adsorbed molecules are highly mobile, in (chromophore-zeolite) systems a permanent and controlled arrangement of molecules is advisable. In all cases, detailed understanding of the guest-host interactions (hydrogen bonding, ion pairs) is a primary step to tailor-made functional materials at a molecular level.

Despite frequent defects or disorder induced by the sample preparation, diffraction remains the main source for structural information for these crystalline materials, supplemented by local spectroscopies (XAFS, UV-Visible) or Monte-Carlo simulations.

We will present X-Ray and neutron diffraction studies on (guest@zeolite) systems used as pigments, for Second Harmonic Generation or as enhancers for probing pollutants and discuss the influence of sample preparation and structural defects on the properties.

Highly sensitive estimation correlation scale of magnetic impurities or phase in functional materials by means of SANS of polarized neutrons

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The examples of measuring magnetic correlations and phases by small-angle polarized neutrons scattering (SAPNS) in different functional materials are given. High efficiency of this measuring is based on the possibility to study nuclear-magnetic scattering, i.e. measuring of cross-correlation part in scattering which proportional to product $A \bullet B$, where A is nuclear scattering amplitude and B – magnetic. In turn, the mutual magnetic-nuclear contrast enhancement of scattering due to: 1) by linear law of magnetic or nuclear amplitude; 2) the interference scattering is measured as the difference in the intensity of scattering with polarized neutrons up/down to the magnetic field applied to the sample, thus the effect of the interference is measured at zero background if A or B in searching area is zero. Examples of studies magnetic correlation are shown in the report: 1) 3-d impurities in nonmagnetic matrix [1]; 2) the evolution of magnetic-nuclear contrasting fraction in magnetic alloy under treating [2]; 3) impurity magnetic phase in high-quality LiFePO4; 4) ferromagnetic nanoparticles in the polymer, and others.

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Magnetic phase separation and unusual scenario of its temperature evolution in porous carbon-based nanomaterials doped with Au and Co

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Two porous glassy carbon-based samples doped with Au and Co were investigated. Neutron diffraction indicated amorphous structure of both specimens and long-range ferromagnetic ordering of Co-doped sample at low temperatures [1]. The magnetization study as well as measurements of the nonlinear longitudinal response to a weak ac field (NLR) and electron magnetic resonance give evidences for a presence of magnetic nanoparticles (MNPs) embedded in paramagnetic/ferromagnetic matrix respectively, both samples being in magnetically phase-separated state at temperatures above 300 K [2]. Matrix, forming by paramagnetic centers located in matrix outside the MNPs, reveals exchange interactions providing its ferromagnetic (FM) ordering below $T_C \approx 210$ K in Au-doped sample and well above 350 K in Co-doped one. For the former, NLR data suggest a percolation character of the matrix long-range FM order, which is mainly caused by a porous amorphous sample structure. Temperature dependence of the magnetization in the Au-doped sample evidences presence of antiferromagnetic (AF) interactions of MNPs with surrounding matrix centers. At magnetic ordering below T_C these interactions promote origination of ‘‘domains” involving matrix fragment and surrounding MNPs with near opposite orientation of their moments that decreases the magnetostatic energy. On further cooling, the domains exhibit AF ordering below $T_{cr} \sim 140$ K $< T_C$, resulting in formation of a peculiar ‘‘ferrimagnet”. The porous amorphous structure leads to absence of translational and other symmetry features through the samples that allows canted ordering of magnetic moments in domains and in whole sample providing ‘‘canted ferrimagnetism”. At low temperatures $T_{tr} \sim 3$ K, ‘‘order-oder” transition, evidencing the non-Heisenberg character of this magnetic material [3], occurs from ordering like ‘‘canted ferrimagnet” to FM alignment, which is stimulated by external magnetic field. The data for Co-doped sample imply the similar evolution of magnetic state but at higher temperatures above 350 K. This state exhibits more homogeneous arrangement of the FM nanoparticles and the FM matrix. Order-order transition occurs in it at higher $T_{tr} \sim 10$–15 K as well and followed by formation of long-range FM ordering found earlier by neutron diffraction. Doping of carbon-based nanomaterials by magnetic metals provides advantages for their possible practical applications as Co-doped sample with higher T_C (> 350 K) and larger remanent magnetization evidences.

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Operando neutron diffraction improves understanding of lithiation dynamics in graphite anodes

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Current lithium ion batteries typically use graphite as an anode material. Understanding the dynamical processes during lithiation and delithiation is crucial for understanding performance and degradation of such cells, especially in regard to the detrimental effects of fast charging or charging at low temperatures of the cells [1]. Many aging processes, like lithium plating, depend intrinsically on the lithiation properties [2]. It has been shown that even small effects can trigger such lithium plating and severely enhance cell aging and even impose a security issue in commercial cells [3]. Therefore, a detailed understanding of the material properties and the dynamic lithiation processes in commercial type cells is important to optimize cell design and avoid security issues as well as unexpected performance deterioration due to occurrence of Li plating or phase inhomogeneity [4-6]. We have studied the temperature dependence of the lithiation dynamics in 18650-type graphite/NMC cells with operando neutron diffraction [5, 7-9]. In the scope of the ExZellTUM II project (funded by BMBF, grant no. 03XP0081) we found that intermittent Li plating and phase inhomogeneity in graphite anodes can be observed even under unexpectedly mild conditions, although the effects are often hidden due to the fast relaxation processes at room temperature [7]. While Li plating occurs mainly during charging the majority of lithium is only intermittently plated and dissolves again during very short relaxation times at room temperature [8]. Similarly, phase inhomogeneity, i. e. simultaneous occurrence of different intercalation stages of graphite, is observed during cell discharge and can remain even for many hours at very low temperatures [7, 8]. The relaxation of phase inhomogeneity can be completely inhibited due to geometric effects or slowed down at low temperature [9]. The temperature dependence of the relaxation times in these cases is well known, though the role of other effects like charge rate, or applied current density respectively, are not well studied yet. Our new study therefore focused on the lithiation dynamics and phase inhomogeneity depending on temperature and current density at the same time [10]. The operando neutron diffraction of $LiCoO_2$/graphite pouch bag type cells was done at the Instrument Stress-Spec at the neutron source FRM II at the MLZ facility in Garching. The ability of neutrons to deeply penetrate into large samples allows investigating these effects in large scale battery sizes and not only lab prototypes. The observed phase coexistence of multiple stages is followed by relaxation into a single phase or a two phase mixture close to the mean lithium content. We confirm that these phase changes are not only visible in diffraction but are also discernible from the voltage response during the relaxation period. The effects of temperature (-10 °C to 25 °C) and current density (0.9C to 5.3C) on the occurrence of inhomogeneity and subsequent relaxation were studied. While barely recognizable at room temperature, the graphite lithiation became strongly inhomogeneous after discharge at −10 °C with the relaxation processes lasting for a few hours. The observed effects are best explained due to the slowdown of lithium diffusion in the solid phase depending on temperature. Through analysis of the relaxation times, the effective solid diffusion constants at room temperature and -10 °C could be derived. The observed relaxation times are in good agreement to expected values for solid diffusion constants.

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Cerium(IV) hydrogen phosphate ultralight aerogels

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Aerogels are highly porous materials with low density and high specific surface area. Aerogels can be obtained on the basis of a number of simple substances, inorganic and organic compounds, hybrid organic-inorganic aerogels are also known. Recently, a significant number of papers devoted creation of aerogels containing anisotropic 1D and 2D structural units have appeared. Cerium phosphates could be a promising candidates for 1D aerogels preparing. It is known that cerium(IV) hydrogen phosphates, unlike phosphates of rare-earth metals and transition metals, tend to form amorphous fibers with a significant anisotropy coefficient (up to 1: 100). Due to its fibrous structure, cerium(IV) hydrogen phosphates can form bulk highly porous materials with extremely low values of their geometric density. Aerogels based on cerium(IV) hydrogen phosphates, because of their structure features and chemical properties, are of interest for the creation ion-exchange materials, proton conductors, sorbents and catalysts.

The present work was aimed at elaboration of methods to obtain a novel class of ultralight aerogels based on cerium hydrogen phosphates with quasi-one-dimensional fibrous structure. The tasks were follow: 1) selection of inorganic mineralizers for the monolithic ceric phosphate gels preparation; 2) drying of monolithic gels in supercritical conditions; 3) analysis of the obtained aerorgels by a complex of physico-chemical methods.

During the synthesis, 0.02 g of nanocrystalline CeO_2 was dissolved in 1 ml of H_3PO_4 (85%) under a constant stirring at 80°C. Then, the obtained cerium-containing phosphate solution was mixed with a 3 M HNO_3 aqueous solution or a 3 M H_3PO_4 aqueous solution in a volume ratio of "initial solution: mineralizer solution" = 1: 8, as well as 1:20. As a result, a gel was formed, which was aged for 2 days, then the solvent was replaced by keeping the gel in acetonitrile for one week, with a daily solvent change. The samples were dried under supercritical conditions, to obtain the aerogels. As solvents for the supercritical drying, we used carbon dioxide. As a reference sample, a xerogel was used, the synthesis of which included mixing the cerium-containing phosphoric acid solution and water, purifying the resulting gel by dialysis against deionised water and drying the purified gel at 60 °C under atmospheric pressure.

It was shown that supercritical drying in CO_2 leads to the successful preparation of monolithic aerogels. The geometric density of the aerogels obtained using the volume ratio "initial solution: mineralizer solution" = 1: 8 was ~ 5.5 mg/cm^3, while the geometric density of aerogels synthesized with the volume ratio "initial solution: mineralizer solution" = 1:20 - only about 2.2 mg/cm^3. The skeletal density of aerogel samples, as measured using a Pycnomatic ATC helium pycnometer, was equal to 2.98 ± 0.04 g/cm^3. The calculated porosity of the monolithic aerogels was ~99%.

According to X-ray diffraction analysis, aerogels obtained were mostly X-ray amorphous. In the diffraction pattern of these samples, at 2θ ~8°, one can observe a pronounced broadened maximum, which mayindicate the existence of short-range order in cerium-containing hydrogen orthophosphate aerogels with a characteristic distance of ~1.2 nm. The specific surface area of the samples was about 70 m^2/g. According to the results of scanning electron microscopy (SEM), aerogels are characterized by a large fiber diameter (~ 40 nm) compared to xerogel (~ 20 nm). At the same time, transmission electron microscopy (TEM) data show that aerogels fibers also consist of smaller diameter fibers, up to 5 nm. The structure of xerogel and aerogels was independently analysed by means of small angle neutron scattering in the range $0.02 < q < 0.15$ Å^{-1}. Analysisof the scattering in this q-range enables an estimation of the R_C value, which is equal to 25.9 ± 0.6 nm for xerogel, that correspond to the upper estimate of the fibrillae radii in the gels and are in line with TEM and SEM data.

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A New Measuring Cell for Operando Neutron Diffraction on Li-Ion Battery Cathode Materials

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The use of operando diffraction has taken a major step forward, in no small part due to the increase in flux at large scale facilities such as synchrotrons and neutron spallation sources. While the X-rays are absorbed by the battery casing which necessitates special cells with windows, neutrons have a penetration depth large enough to probe the entirety of cell. This has allowed measurements directly on commercial batteries, giving unique insights into the evolution of cell parameters and composition of the cathode and anode phase, but also showing Li-consumption by decomposition of the electrolyte and plating of lithium metal.

When measuring on commercial cells, contributions from all parts of the cell are observed which complicates the analysis of the diffraction data. A desire also exists to measure on non-commercial electrode materials prepared in the lab. Thus, there exists an incentive to develop a measuring cell which allows easy measurement on a variety of different cathode materials, either commercial or synthesized.

In this work, we present a new operando neutron diffraction battery cell, especially designed for the new beamline ErwiN at the FRM-2 research reactor outside of Munich, Germany. The cell uses a Zr/Ti-alloy with negligible scattering strength to eliminate contributions from the casing. We present data on the commercial cathode materials $LiFePO_4$ and $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ to demonstrate the capabilities of the cell, as well as on the non-commercial cathode material $Li_3V_2(PO_4)_3$. $Li_3V_2(PO_4)_3$ is interesting, as it has the highest gravimetric capacity among the known phosphates (197 mAh g^{-1}). The material displays a complex series of phase transformations during charge and discharge, and interestingly, these transformations are very dependent on the number of Li-ions extracted during charging. The material has been investigated using operando synchrotron X-ray diffraction, but operando neutron diffraction is important to uncover the exact nature of the Li-ion dynamics.

Lattice parameter changes under ordering in Fe-Al(Cr) and Fe-Ga alloys

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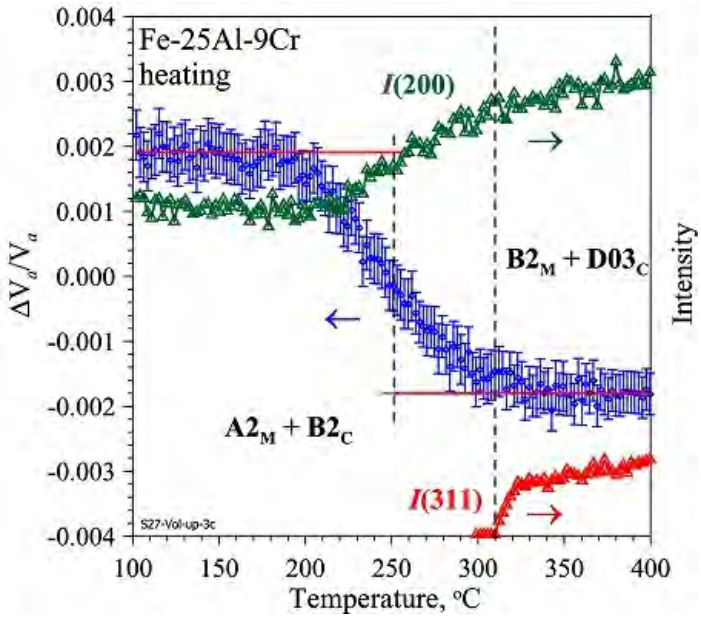
For intermetallic compounds, the fact of decreasing of the unit cell parameters during the transition from a disordered to an ordered state is well known. The reasons for this effect are still under discussion, mainly on the basis of models involving its energy or geometric mechanisms (see review article [1]). Theoretical calculations by means of the Bragg–Williams model based on embedded atom method potentials led the authors of [2] to the conclusion that in the case of a structural transition of the second order, changes in the cell parameter are not linear.

We have studied the processes of atomic ordering in Fe-Al(Cr) and Fe-Ga alloys by neutron TOF-diffraction at the HRFD instrument (IBR-2 pulsed reactor, JINR, Dubna) in wide temperature range (20 – 850) °C. For instance, in the Fe-25Al-9Cr composition it was found that during the second order transition from the partially ordered B2 state to the ordered $D0_3$ state the relative decrease in the atomic volume is about 0.4% (Fig.1). The high sensitivity of the method made it possible to clearly observe a similar change in the lattice parameter down to 0.08% in others Fe-Al(Cr) alloys, as well as in the Fe-*x*Ga compositions. Earlier, it was found that the microstructure of both types of studied alloys is organized in the form of a disordered matrix and clusters of nanoscopic size with an ordered atomic structure dispersedly embedded in the matrix (see [3] for details). In contrast to the conclusions of [2], our results indicate that the relationship between the cell parameter and the ordering factor of the structure is linear.



Pic.1. Changes in the intensities of the main (200) and superstructural (311) diffraction peaks (right scale) and atomic volume (left scale) during the Fe-25Al-9Cr alloy heating. In the initial state, the clusters of the partially ordered $B2_C$ phase are distributed in the $A2_m$ matrix. After the completion of the ordering process (at $T > 300$ ºC), clusters of the ordered $D0_3$ phase in the B2 matrix are formed. The nonlinear change of the atomic volume starts almost 100 °C below the temperature of $D0_3$ phase occurrence.

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Adaptive X-ray optical elements based on combination of longitudinal and transverse acoustic waves in the kHz and MHz frequency ranges

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X-ray acoustic interactions allowing to implement the control of X-ray parameters are widely studied. Among the numerous researches, it is possible to highlight the ability of controlling the spatial and energy spectrum of X-ray radiation [1] and the effect of redistribution of intensity between transmitted and diffracted beam [2]. This paper describes the implementation of a combination of these two possibilities.

The effects of the redistribution of intensities between the diffracted and transmitted X-ray beams under the conditions of excitation of resonant acoustic thickness oscillations in quartz crystals were investigated. It has been established that the effect of increasing the intensity of a diffracted beam almost linearly depends on the amplitude of ultrasound (the FWHM of the rocking curves does not change at the same time) and is observed for all the studied reflexes.

The time characteristics of the observed effects upon excitation and relaxation of ultrasonic oscillations were investigated for the first time: the process of increasing intensity takes about 250 microseconds, then its oscillation is observed for about 1 millisecond, and the process of complete relaxation takes about 1.5 milliseconds.

Preliminary design of elements combining thickness and longitudinal oscillations are considered, several schemes of implementation are proposed. The effect of intensity redistribution in Potassium and Rubidium hydrogen phthalate crystals, which are emerging materials for creating a two-frequency element, was studied for the first time.

Prospects of implementation of such elements at synchrotron radiation as well as laboratory sources will discussed.

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The morphology of the structure of calcium carbonate CaCO3, obtained in the process of biomineralization

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Various environmental factors lead to the formation of cracks in concrete materials. One of the recovery methods is biomineralization, i.e. the formation of minerals by living organisms due to reactions of their metabolism with the environment [1]. In the last decade, the ability of some bacterial strains to precipitate Ca^{2+} ions in the form of CaCO3, which can fill the microcracks formed in the walls of buildings, has been revealed. In the process of the vital activity of some bacteria capable of raising the pH of the environment, CO_3^{2-} is formed from CO_2. If free Ca^{2+} ions are present in the medium near the bacterial cell, $CaCO_3$ precipitates, due to the fact that the cell wall carries a negative charge, and thus attracts positively charged Ca^{2+} ions. Thus, the surface of bacterial cells plays an important role as a nucleation center [2].

In the present work, the bacterial strain *Bacillus licheniformis* 8782 was cultivated using special solid and liquid media containing urea and calcium acetate in order to obtain $CaCO_3$ crystals. After 2 weeks of cultivation, the *Bacillus licheniformis* 8782 strain was found to demonstrate the ability to produce significant amounts of $CaCO_3$ of different morphology and colors. X-ray phase analysis, scanning electron microscopy, low-temperature nitrogen adsorption, small-angle neutron scattering, and small-angle x-ray scattering were used to study the structure of samples of biogenic anhydride CaCO3, depending on the environment and the culture conditions of bacterial cells. It has been established that when cultivated in a liquid medium containing urea and calcium chloride, $CaCO_3$ precipitates in the form of crystals of vaterite (hexagonal syngony, space group $P6_522$), and in the case of liquid and solid media containing calcium acetate, calcite is formed (trigonal syngony, space group R-3c).

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Multiple ultra-small-angle neutron scattering on materials obtained by selective laser melting: theory and experiment

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Materials obtained using additive technologies are promising for a wide range of industries. Therefore, an important issue is the study of the internal structure of such materials, including the method of small-angle neutron scattering (SANS). Due to the inhomogeneities size of the order of microns and the samples thickness from millimeters and more, multiple ultra-small-angle neutron scattering (MUSANS) takes place. The most suitable USANS measurement technique is the double-crystal neutron spectrometer.

Traditionally, when the inverse scattering problem is unsolved, the method for determining the inhomogeneity parameters is based on an approximation of the experimental model curve by the least squares method.

The MUSANS curve was simulated by the method developed in [1] and based on the theory [2]. The theoretical curves are in qualitatively agreement with the experimental results obtained by the double-crystal STOIK diffractometer at the IR-8 reactor at NRC "KI".

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Martensitic transformation in NiTi(Hf,Zr) shape memory alloys studied by TOF neutron diffraction

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Among shape memory alloys, NiTi systems demonstrate good dimensional stability, ductility and workability, superelasticity and high damping capacity. Currently, they are most commercially viable alloys, being widely used in industry and engineering, as well as in various biomedical applications. The basis of all unique properties in NiTi based alloys is reversible thermoelastic martensitic transformations [1]. Unfortunately, practical applications of NiTi are limited to a temperature below 100°C. Alloying NiTi by hafnium or zirconium is the most promising way to increase the transformation temperatures [2]. However, the effect of joint alloying by hafnium and zirconium has not yet been studied in detail.

Bulk samples of NiTi(Hf,Zr) alloys of different composition have been studied in a wide temperature range by time-of-flight neutron diffraction at the HRFD diffractometer (IBR-2 reactor, FLNP JINR, Dubna) [3]. Recent upgrade of this instrument significantly increased flux at the sample position, and also allowed seamless transition from high resolution ($\Delta d/d \approx 0.001$) mode of experiment to high intensity mode, where acquisition of TOF diffraction spectra is possible within the time of ≈1 minute, which is particularly important for *in situ* studies of phase transitions in crystalline materials.

We report details of structure and microstructure changes in several NiTi(Hf,Zr) alloys with different Hf and Zr content as they undergo forward and reverse martensitic transformations.

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A determination of CO_2 molecule sites in $K_{2x/3}Cu[Fe(CN)_6]_{2/3}$ with x = 0 and 1 at various temperatures and CO_2 gas pressures

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Prussian Blue analogues (PBA) have attracted much attention as potential gas adsorbents [1]. In our previous study, we showed that the PBA $K_{2x/3}Cu[Fe(CN)_6]_{2/3}$ has a significant uptake for CO_2, with ~4.5 mmol/g [2]. The location of the CO_2 molecules in its crystal structure was not known though.

In order to determine the CO_2 positions, a series of in-situ neutron powder diffraction (NPD) measurements were performed. NPD data was collected on the Polaris instrument at ISIS for two samples of $K_{2/3x}Cu[Fe(CN)_6]_{2/3}$, with $x = 0$ or 1. The dehydrated samples were measured in-situ with a gas stick under vacuum and at the following CO_2 pressures: 150 mbar, 500 mbar, and 1000 mbar.

According to the chemical formula, $K_{2/3x}Cu[Fe(CN)_6]_{2/3}$ has 33% of vacancies in the framework, formed by the missing $Fe(CN)_6$ groups. The most common structure model assumes a random distribution of those vacancies which results in a face-centered cubic structure and space group *Fm*-3*m*. However, the NPD time-of-flight spectra reveal additional Bragg peaks which can be indexed with a primitive unit cell and space group *Pm*-3*m*. This indicates correlations between the $Fe(CN)_6$ vacancies which result in a domain formation. Moreover, the primitive Bragg peaks are much broader than the average structure peaks which implies a small domain size.

Figure 1a shows that the intensity of the primitive peaks (100) and (110) decreases with the CO_2 uptake whereas the highest peak (200) slightly increases. In case of the samples with the K^+ cations (Figure 1b), the primitive peaks are much weaker, and they do not change that much with the higher CO_2 pressure.

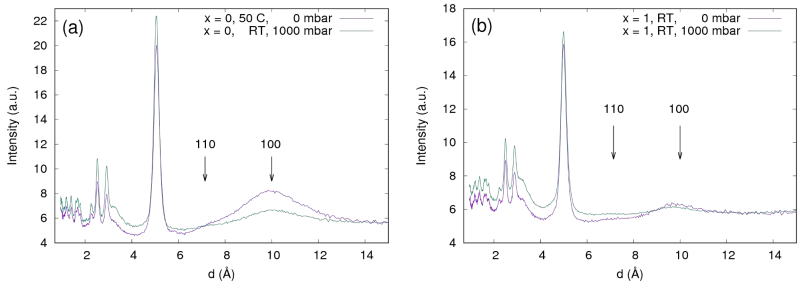

Figure 1: NPD patterns (Polaris, bank 1) obtained for samples x = 0 (a), and x = 1 (b). The data collected before and after CO_2 adsorption. The patterns show additional broad peaks which can be indexed with a primitive unit cell.

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Elucidation of the structural geometries and the ammonia-responsive behaviors of Zr-based metal-organic frameworks

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Understanding the structural responses of Metal-organic frameworks (MOF) upon the inclusion of guest molecules has gained increasingly attention in several applications, such as gas storage, drug delivery, and molecular sensing. MOFs have been recently reported to show a remarkable uptake for ammonia gas.[1] However, the ammonia-induced structural changes and the adsorption geometries of this MOF-guest system are still questionable. In our recent work, robust Zr-based MOFs, including UiO-67, m-UiO-67, and UiO-bpydc, were selected for ammonia sorption. These MOFs are consisted of Zr_6 clusters coordinatively bond with either biphenyl-4, 4′-dicarboxylate or 2, 2′- bipyridine-5, 5′-dicarboxylate linkers. We observed the alteration of stepped ammonia adsorption isotherms when the phenyl groups were replaced by the pyridine ones (Fig. 1). *In situ* neutron diffraction and *in situ* synchrotron powder X-ray diffraction combined with Rietveld refinement reveal that this unusual adsorption transition is induced by reorientation of the bipyridine linkers via hydrogen bonding interactions with the ammonia molecules. The details of the atomic positions and the geometrical interactions between the MOFs and the adsorbed ammonia will be also discussed.

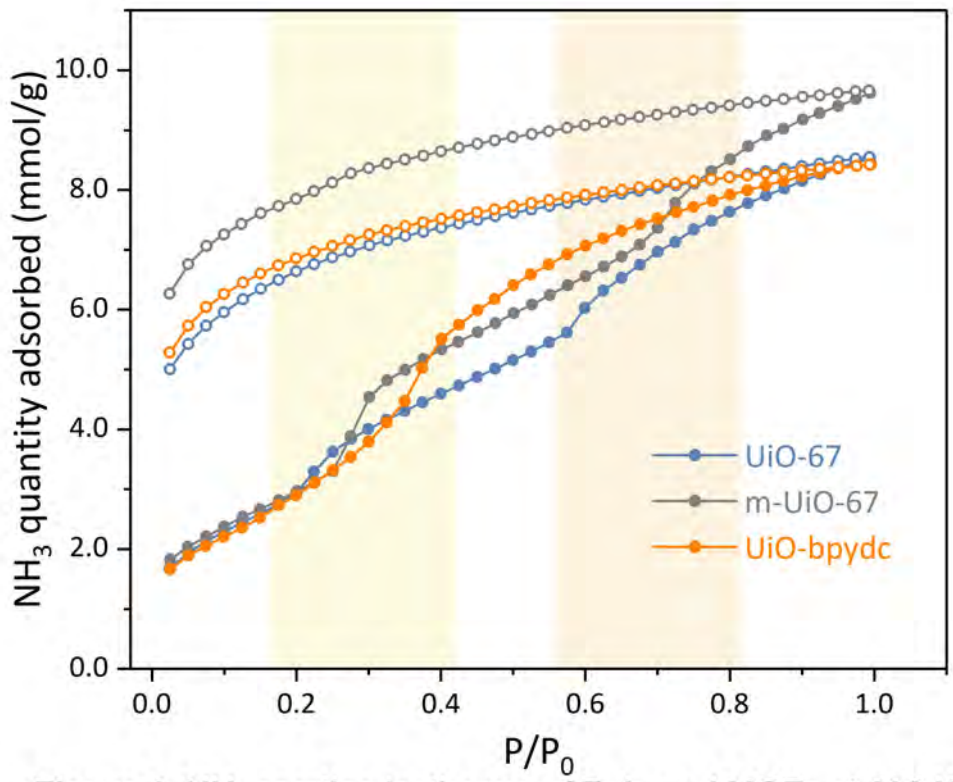

Figure 1. NH_3 sorption isotherms of Zr-based MOFs at 298 K.

Keywords: Ammonia adsorption, Zr-based metal-organic frameworks, neutron diffraction, synchrotron X-ray diffraction, Rietveld refinement

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Structure of quaternary type-I clathrate $Ba_8(Al_xGa_{1-x})_{16}Ge_{30}$

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Inorganic clathrates are among the best thermoelectric materials. They can be regarded as realizations of the phonon-glass electron-crystal concept, combining relatively large electrical conductivities (“electron crystal”) with very low thermal conductivities (“phonon glass”). Clathrates exhibit complex host-guest crystal structures containing cages, which are formed by host elements from the group 13, 14 and 15 of the period table, that can host large guest ions for example from the alkaline earth groups. The extremely low thermal conductivity makes clathrates especially attractive for thermoelectric application. The origin of that has been debated, but most studies attribute it to the ‘off-centering’ of the guest ions, which refers to that guest ions can be located away from the cage center and hybridize with the acoustic phonon of the host framework. However, the position of guest ions is highly correlated with the chemical environment, for example, the bond length between host and guest atoms, as well as the elemental distribution of the host atoms in the cages which results in different bond energy. Furthermore, the existence of vacancy makes it more difficult to solve the crystal structure.

In order to study the impact of host atom distribution on the guest atom behaviour, a quaternary type-I clathrate $Ba_8(Al_xGa_{1-x})_{16}Ge_{30}$ was synthesized and characterized by energy-dispersive x-ray spectroscopy (EDX), single crystal and powder synchrotron x-ray, as well as single crystal neutron diffraction. EDX indicates no vacancy existing in either host or guest sites. Two models, ‘on-centering’ and ‘off-centering’, are used to describe the position of guest ion Ba at the large cage. Both models show that trivalent elements (Al and Ga) preferentially occupy 6c Wyckoff site, but the ‘on-centering’ model gives higher Al content than the ‘off-centering’ model. For ‘on-centering’ model, Ba at the large cage is assigned to have anisotropsic atomic displacement (ADP), and a linear temperature dependence is observed. Taking the ADP into account, a linear temperature dependence of bond length between host and guest atoms is observed, for both models.

Stress distributions in P91 martensitic steel and in AISI 316LN steel welds for Gen IV nuclear applications

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This contribution will present experimental results obtained in the frame of the European Energy Research Alliance - Joint Programme Nuclear Materials (EERA-JPNM) to non-destructively characterize the stress field, by means of neutron diffraction, in two different welds developed for nuclear applications. Namely, a martensitic TIG P91 weld (Cr 9 Mn 6 Mo 1 C 0.1 Fe bal wt%) and an hybrid laser-arc AISI316LN steel (17.8 Cr, 12.3 Ni, 1.7 Mn, 2.4 Mo, 0.3 Si Fe bal wt%) have been investigated. Their sizes were 100 x 50 x 12 mm^3 for the P91 weld and 220 x 160 x 15 mm^3 for the 316LN weld; unstrained references were prepared for both welds. The neutron diffraction measurements have been carried out utilizing the E3 diffractometer, at the BER II reactor in Berlin. These measurements were carried out along a line perpendicular to the weld direction, at different depths inside the material and at different distances from the weld center; measurements were extended inside the HAZ and the welded zone, with a gauge volume of approximately 10 mm^3. Strain and stress values were determined in the three principal directions. In the P91 weld the stresses are almost completely relieved after PWHT of 1 h at 750°C; a more complex stress distribution is found within a range of approximately 3 mm around the center of the AISI316LN weld, with nearly balancing longitudinal and transverse components as high as 300 – 400 MPa. These experimental results will be discussed with reference to the expected service conditions of such welds.

Residual Stresses and Temperature Fields in AA6082 Friction Surfacing

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Friction Surfacing (FS) is a solid-state process, which allows deposition welding at temperatures below the melting range. It can be used, e.g., for property enhancement or repair purposes [1]. FS uses a consumable stud that is rotated and pressed on a substrate surface while moved forward. The combination of materials used for stud and substrate defines the windows of process parameters: stud rotational and translational speeds and axial force. The rotational and translational stud speeds together with substrate geometry determine the temperature regime during deposition and the geometry of the coating. The residual stress (RS) field and its relation to the deposition parameters has already been investigated for Ti-6Al-4V FS coatings [2]. The study has shown that low deposition velocities lead to more substrate plastification and lower RS. However, this is not the case for AA6082 on AA2024 coatings, where RS appear to be independent of the deposition velocity. Hence the focus of this investigation is the mechanism of RS formation in AA6082 on AA2024 coatings. Neutron and synchrotron diffraction combined with the finite element T field modelling were used to probe the RS field and correlate it with its formation conditions. Results show insights into the timing scale of the heat processes during the deposition, RS formed in different substrate geometries, and possible approaches to manipulate the process efficiency and design the RS state in the substrate.

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Efficiency upgrade of separator-superheaters in NPP with pressurized water and boiling water reactors by physical-modeling based modernization

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In the development of the first separator for the No. 1 unit at the Novovoronezh NPP, a complex of experimental studies was conducted which made it possible to provide output moisture content of steam ≤0.1%. This apparatus operated reliably until the unit was decommissioned. In separator-superheaters, in order to dry (separate) and superheat the steam that has passed through the high-pressure step of the NPP turbines, moisture separation from the steam in a baffle or mesh type separator and superheating of dried steam to moisture content 0.2–1% in the superheating part are implemented successively.

The latter consists of tubular heat exchangers with the warming steam moving inside or outside vertical or horizontal tube bundles, condensing at high pressure 2–6 MPa, and transferring heat to the superheated steam at low pressure 0.3–0.8 MPa. Supplying moisture at this level is of great importance because an increase of such moisture results in inadmissible efficiency loss of the NPP unit. At the entry into the steam superheater, the flow is a steam-droplet flow and drops of moisture evaporate, after which the flow becomes single phase. Since heat emission to single-phase flow of steam is 10–100 times lower than heat emission from the condensing steam side, the heat transfer coefficient is increased by, for example, finning (longitudinal or transverse) the tubes and steam-superheating heat exchangers – modules.

The separation part of SPP-500-1 was modernized at the Smolensk, Leningradskaya, and Kursk NPPs and ensured that they operate reliably. The testing of the modernized SPP-500-1 at the Leningradskaya and Smolensk NPPs made it possible to determine the moisture content of the separated steam along its perimeter. Analysis showed that the moisture distribution along the perimeter is uniform, the moisture content decreased by factor of 3 and approached the design value ~0.5%; the particulars of the design of the separation blocks do not affect the moisture content.

Modernization whereby the separation blocks are replaced by an old design based on blocks with baffle elements Powervane (Germany) and changes in the arrangements for delivering heated steam made it possible to decrease the non-uniformity of the load on the blocks, ensure the design moisture content after the separator, and increase the superheating temperature of the steam.

Physical modeling ensuring efficient organization of the low-pressure steam flow into the entry chamber of SPP-500-1 made it possible to propose design improvements for the separation part: changing the configuration of the barrier surfaces of the steam flow in the chamber and organizing drainage of the separated material from the floor of the chamber through a system of indentations with holes in the bottom. These improvements decrease the moisture content of the steam at the Leningradskaya, Smolensk, and Kursk NPPs – the measured moisture content of the steam in the No. 4 unit of the Leningradskaya and No. 1 unit of the Smolensk NPP decreased from 1.5–2 to 0.2–0.85%.

The modernized separation part of SPP-500-1 can be regarded as one of the promising designs for separator-superheaters of the turbines at NPPs.

In-situ neutron diffraction study of engineering materials under thermo-mechanical treatment at STRESS-SPEC

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The understanding of structure-property relationships is essential for the development and improvement of engineering materials. *In-situ* characterization of materials under external thermo-mechanical treatment is usually required. The materials science diffractometer STRESS-SPEC at FRM II (Garching, Germany) is designed to be applied equally to structure, texture and residual stress analyses by virtue of its very flexible configuration. In order to meet the needs of *in-situ* characterisation STRESS-SPEC has been dedicated with mechanical loading and dilatometry equipment.

First a unique load rig was designed for *in-situ* structure and lattice strain analysis both at ambient and high temperatures (~ 1000 °C). This rig is also fully rotatable to emulate Eulerian cradle like sample positioning, which allows intensity and peak position pole figure measurements. Second is a quenching and deformation dilatometer has been recently adapted. It offers simultaneous high-precision measurements of length changes while heating/cooling or deforming the sample, and thus adding an additional measurement quantity that is sensitive to phase transformations. The combination of neutron and dilatometry measurements yields a unique view on the microstructural evolution during thermomechanical treatment. As examples the *in-situ* measurements of a high ductility Mg alloy, a shape memory Ni-Mn-Ga alloy, and newly selective laser beam manufactured Ti will be presented in this contribution.

Diffraction based determination of single-crystal elastic constants on polycrystalline titanium alloys

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The components of the 4th rank elasticity tensor (= single crystal elastic constants) are of fundamental importance for any engineering material as they define the bulk elastic properties like Young's modulus, shear modulus etc. Furthermore, precise knowledge of elastic constants is needed for various methods such as diffraction-based residual stress analysis or crystal-plasticity numerical simulations.

Using the classical diffraction based stress analysis in reverse way, diffraction elastic constants (DEC's) can be obtained by diffraction under mechanical load while the lattice strains are measured during various sample orientations and load steps. The single-crystal elastic constants can then be determined from the DEC's based on model assumptions for polycrystal – single crystal relationships - such as approaches by Voigt, Reuss, Hill etc. - using a χ^2 minimization technique. Various authors have already applied such an approach to obtain single-crystalline elastic constants on polycrystalline materials by neutron or synchrotron diffraction under mechanical load [1-3].

In this contribution we present the determination of single-crystalline elastic constants on titanium alloys Ti-6V-4Al (near alpha alloy), Ti-6Al-2Sn-4Zr-6Mo (alpha + beta alloy) and Ti-3Al-8V-6Cr-4Zr-4Mo (beta alloy). The investigations were carried out on diffractometers D20 (ILL), SPODI (MLZ/FRM II) and STRESS-SPEC (MLZ/FRM II) using a load frame which allows an orientation of the load axis in an Eulerian cradle like manner [4]. By this setup, lattice strains of various reflections could be analyzed under various orientations between the scattering vectors and the load axis. In addition, the orientation distribution function of grains was determined and included in the analysis.

To our best knowledge the study on Ti-6Al-2Sn-4Zr-6Mo is the first example to reveal all eight elastic constants in a two phase h.c.p. + b.c.c. alloy. The results for Ti-6V-4Al agree quite well with previous studies by neutron diffraction [3] as well as ultrasonic studies on Ti single crystals. Various approaches for the grain-interactions were implemented in the analysis, namely the models of Voigt, Reuss, Hill, Kröner, De Wit and Matthies.

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In-situ neutron diffraction study on compressive behavior of solution heat-treated Mg-Ca alloys at room and elevated temperature

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The addition of Ca to Mg can improve the creep resistance at elevated temperatures and the mechanical properties of Mg alloys at both room and high temperatures. In current study, the *in-situ* compressive deformation behaviors of solution treated Mg-0.5Zr and Mg-0.3Ca-0.5Zr alloy were investigated both at room and elevated temperature (~200°C) at STRESS-SPEC neutron diffractometer (MLZ, Garching). Calendric samples with 6 mm in diameter and 11 mm in length were compressed using a unique tensile/compression rig at STRESS-SPEC. Peak position and intensity variation with the compression strain were analyzed since they can indicate the evolution of lattice strain and preferred orientation, respectively. This will be related to the effect of Ca addition on the deformation modes of Mg alloys including basal slip, {10.2} twinning, prismatic slip and <c+a> pyramidal slip.

Results showed that the addition of Ca strengthened all the deformation modes at room and elevated temperature. However, the hardening effect of Ca on prismatic slip was more significant than that on the other deformation modes at room temperature. All the deformation modes were softened at 200 °C, where prismatic slip and <c+a> slip got easier to be activated and basal slip carried more internal strain than that as room temperature. The alloy with Ca addition showed a better thermal stability at 200 °C due to the significantly strengthening effect of Ca solutes.

Two-directional stress-free comb sample for neutron stress diffractometry.

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Neutron diffraction is a powerful instrument for residual stress investigations in bulk crystalline samples. This is the only method, which allows direct measurements of three mutually perpendicular strain components inside the specimen, which are necessary for correct stress calculation. The method is based on measuring relative change in stressed lattice spacing, d, with respect to the reference, or stress-free spacing d0. Therefore, the accuracy of stress measurement strongly depends on the measurement accuracy of d0. If the sample is inhomogeneous (e.g. weld), d0 depends on location in the specimen and should be measured for each experimental point in the sample.

Conventional stress-free comb sample with teeth in normal direction considerably simplifies d0 measurement in the weld. However, it was shown that in a thick weld, a "too long tooth" could contain residual stress. We suggest making a set of slots perpendicular to the teeth of conventional comb sample to relieve stresses in long teeth, so that each long tooth becomes a comb with short teeth in longitudinal direction. Such "two-directional" and conventional comb samples were prepared using wire electric discharge machining (EDM) for stress measurement in 45 mm thick steel weld. Experiments, conducted at neutron diffractometer "STRESS" of NRC KI, showed the difference in d0 values, measured at the same locations in the comb samples, which indicates reduction of residual stress in two-directional comb compare to the conventional comb.

If the slit in a stress-free comb sample passes through the gauge volume (GV), it can lead to a shift in the diffraction peak due to incomplete filling of the GV with scattering material. To estimate the influence of slits on d0 measurement, a stress-free comb sample was prepared from annealed ferritic steel plate using 0.2mm cutting wire. Experiments with 2×2×2 mm3 GV showed that the maximum apparent strain due to slits is about ± 150×10-6.

This work was performed using the equipment of Unique Scientific Facility "NRC IR-8"

Neutron diffraction research of residual stress in thin 410 steel plate, deposited on rigid substrate by DLMD method

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The significant advantages of additive manufacturing over traditional technologies induced its rapid and sustainable development. High production speed and highest material savings promote the additive technologies widespread in industry.

One of the features of direct laser metal deposition (DLMD) method is presence of high residual stress in produced parts. The information about internal stress distribution is critically important for the competent organization of production processes.

To study residual stress distribution in large thin-walled parts a test sample was manufactured using DLMD method. The sample represents a 2.2 mm thick steel plate on rigid substrate. Each subsequent layer was deposited with dwell time to simulate the deposition of large component, in which a significant amount of time would pass before the laser reaches the same location again.

Experiments were carried out with neutron diffractometer "STRESS", installed at the research reactor IR-8 at NRC «Kurchatov Institute». Small thickness of the sample allowed using calculation technique that does not require measurement of lattice parameter of stress-free sample.

Experiments showed that maximum tensile stress in the plate is located at the plate's edge near the interface with substrate. Stress distribution along the height at the middle of the plate is very different from the distribution in the plate, deposited on flexible substrate.

This work was performed using the equipment of Unique Scientific Facility "NRC IR-8"

The order/disorder transformation of β phase in binary and ternary γ TiAl based alloys studied by synchrotron and neutron diffraction

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Due to their high melting point, low density, and good oxidation resistance, γ-TiAl based alloys have recently started to replace Ni-based superalloys as a material for turbine blades in aircraft engines [1]. Conventional γ -TiAl alloys usually contain the ordered phases γ-TiAl and α_2-Ti_3Al at lower temperatures and disordered α-Ti(Al) phase at higher temperatures. Additional alloying elements like Nb, Mo, Ta, Cr or Fe, can stabilize the disordered β-Ti(Al) phase (A2 structure), which could transform at lower temperatures to ordered β_O-TiAl (B2 structure) or sometimes to more complex phases [2].

The ductile body centered cubic (bcc) β phase is important for processing because it significantly improves the hot forming behaviour of the material. Otherwise, the ordered low temperature β_O phase is said to embrittle the material at service temperature. Unfortunately, little is known about the exact order/disorder transformation temperatures of β/β_O in ternary alloy systems and the influence of β stabilizing element content is still under research. Additionally, even for the binary TiAl phase diagram the existence of an ordered β_O phase field at high temperatures has yet not been finally proofed or rebutted [3].

In situ HEXRD could be used for determination of the $\beta_O \leftrightarrow \beta$ phase transformation temperature, if the superstructure reflex of the β_O phase is not too weak. Neutron diffraction (ND) is best suited to study order/disorder transformations in titanium aluminides [4]. The fundamental reflections in ordered and disordered β phase in neutron diffraction are very weak because of the opposite sign of the scattering lengths of Al sites and Ti sites which sum up to the overall signal. Otherwise, the superstructure reflections of the ordered TiAl crystal structures including the ordered β_O-phase become rather large, because they scale with the difference of the scattering lengths of each site. Thus, the application of in situ neutron diffraction is a powerful tool to determine the temperature of $\beta_O \leftrightarrow \beta$ order-disorder transformation. Nevertheless, it is found that a combination of in situ neutron and synchrotron diffraction is even more powerful as also the fundamental peaks can be monitored yielding additional information about the disordered phases. We have studied the order/disorder transformation of β phase in several binary and ternary γ TiAl based alloys with ND at the MLZ as well as with XRD at PETRA III. An neutron experiment with standart high temperature furnace at MLZ is described in [5]. Results of synchrotron and neutron diffraction particularly phase composition and phase transformation temperature differ from each other for some samples because of application of different heating ramps. A comparison of methods and results of neutron and synchrotron measurements is given during the talk.

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Investigation of textures of alpha zirconium and zirconium-alloy by neutron and X-ray diffraction

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The preferred orientations of zirconium-alloys tubes were experimentally investigated using a quantitative texture analysis. Obtained results were compared with the textures of alpha zirconium samples deformed by uniaxial tension from strain 5% to strain 30% (strain step 5%).
The neutronographic texture measurements were performed on the KSN-2 neutron diffractometer located at the research reactor LVR-15 in the Nuclear Research Institute, plc. Rez, Czech Republic. The X-ray measurements were performed at theta/theta X'Pert PRO diffractometer with Cr X-ray tube. Observed data were processed by software packages GSAS and X'Pert Texture.
The (100) and (110) plane are oriented perpendicular to the rolling direction for both types of samples. The (102) and (103) plane poles are oriented parallel to normal direction. More significant tilt of basal poles from the normal direction toward the transverse direction is observed for alpha zirconium. Consequently, alloying of zirconium create ideal texture with respect to creation of zirconium hydride. The alloying of zirconium is reflected in decreasing the overall texture sharpness. The obtained results are characteristic for zirconium.

The comparison of neutron pole figure extraction methods

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Crystallographic texture is a set of preferred grains orientation in polycrystal. It is common in the quantitative texture analysis to draw conclusions based on pole figures (PFs) and orientation distribution function (ODF). Pole figures can be extracted from diffraction patterns measured by X-rays or thermal neutrons.

The objective of the present work is to compare two different methods of the pole figures (PFs) extraction from the neutron diffraction patterns. The neutron diffraction time-of-flight patterns were measured with SKAT diffractometer situated at 7A-2 channel of pulsed nuclear reactor IBR-2 (JINR, Dubna, Russia). The first method uses the sum of the total neutron intensity recoded by the detector. Herein a part of a measured pattern is divided into three regions. The side regions are used for background estimation whereas the central region is used for the peak intensity estimation. The second method is based on the profile analysis of each individual peak from each measured pattern (the local peak fit). So, the peaks are approximated by a bell-shaped function and a linear background. The difference between measured PFs and ones recalculated using an ODF are the measure of the method accuracy. Besides, the texture similarity parameter RP [1] was used for validation of both methods compared. The pole figures extraction was carried out by the computer program “Pole Figure Extractor” described in [2]. The ODFs computation, pole figure reconstruction, calculation of RP factors and differences between measured and reconstructed PFs were made by using the MTEX software [3].

The frictions stir welded aluminum alloys were selected for this experiment because accurate texture knowledge is critical to many practical applications of such materials in critical constructions. The materials used in the present study were in detail characterized elsewhere [4].

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A STUDY OF THE ACOUSTIC PROPERTIES OF ROCK MASSIF AND CONCRETE LINING UNDER NATURAL CONDITIONS

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A study was focused onto the experimental research of the propagation of acoustic signal (AS) in rock masses and concrete stratum with specified structural and mechanical characteristics. The measured parameters were the AC velocity detected by the first contact with a piezo-transducer and the spectrum in a broad frequency range. The measured value of the acoustic wave velocity for the rock mass and concrete well coincided with those calculated by elastic theory formula (with taking into account the stratum geometry in the latter case).

In addition, the photoelastic method was applied for measuring the acoustic wave stress, which allowed us to evaluate the mechanical energy of the wave. The energy balance in the process “AS source” – “transmitting media” – “AS receiver” was analyzed using a spectral analysis device. In laboratory investigations, the elastic collision of a steel ball (as AS source) with the sample surface served as wave radiation source. To exclude non-elastic processes at the instant of collision, a metal laying was applied. The spectral composition of the wave energy was also determined.

The obtained results could be used in the development of methods of the determination of AS source parameters (including its energy and location) as well as the structure of the transmitting media. Thereby, the information capacity of the acoustic emission method would be significantly increased.

Towards a correct interpretation of the results of the detecting of elastic waves signals from the rock massive in the system A-Line DDM, the study of the acoustic properties of the rock mass and concrete lining was needed. For this purpose, a film-type piezo-transducer with a linear amplitude-frequency response in the range of 20 kHz was designed, fabricated, and calibrated for measuring the elastic wave stress. The measurements of elastic waves were carried out by detecting a response of concrete lining and rock mass on the impact action. Impact was performed by a steel ball of 4.68 kg in mass through a steel plate attached to a concrete wall as well as over a laying imbedded in the concrete wall. The performed measurements of the elastic wave velocity in concrete stratum, triggered by the ball impact, were found to be of 3920 m/s. The wave velocity value in concrete estimated from the calculation of the elastic modulus for a plane wave appeared to be of 4343 m/s. It has been shown using the dispersion curves for symmetric Lamb mode S_1 and symmetric zero mode S_0 that in the case of the elastic wave source activity just in the concrete lining of mine roadway, the energy of impact action upon the rock massif transforms into the propagating normal waves S_0 and S_1 conditioned by the properties of concrete and lining thickness. The controlled rock massif was aggregated by biotite gneisses. The measurements of elastic waves velocity in the rock massive showed the value of 5318 m/s. The spectral composition of the rock mass response on the ball impact was measured, and the elastic wave energy was estimated (0.3 J). The spectral density of the impact-induced massif excitation was concentrated in the range of 0.7 – 3.2 kHz.

In the process of full-scale experiments investigated the acoustic properties of concrete lining and an array of heterogeneous rocks underground facilities FSUE "GHK" ("Mining and Chemical Plant" Rosatom " Russia, Zheleznogorsk, Krasnoyarsk region), near the well number 5. Tested the developed sensor check pulses AE for installation in wells with a diameter of 76 mm. the results of these experiments from the organization of the FSUE "GHK", "Rosatom" received the certificate (No. 212-25-60-01/2379 from 15.05.2018 G.) on the implementation (use) of the results of the work of H. F. Makhmudov.

PRINTED TECHNOLOGIES FOR SUPERCONDENSATORS - ONE OF THE APPLICATIONS OF GRAPHEN-LIKE MATERIALS

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Direct printing technologies are particularly attractive for the manufacture of portable storage devices and the conversion of energy. The undoubted strength of these technologies is the natural involvement of nanoscale objects in the technological process. The company Graphene 3D Lab showed the world's first battery based on graphene, printed on a 3D printer. A very important detail: batteries printed on a 3D printer can take on virtually any shape the customer needs. When mastering print technologies, interesting scientific problems also arise. This is evidenced by the appeal to the printing technologies of such major scientists as Nobel Prize winners Geim and Novoselov, who, together with co-authors, established that the conductivity of an electrode printed using “graphene” ink increases significantly if the electrode is mechanically compacted. The works cited also indicate that printing technology requires an exploratory work to create ink corresponding to emerging problems. In this report, we present the results of our research in this area. One of the most promising options for autonomous energy storage devices are supercapacitors (SC). Currently, they are used in a number of electrical appliances as primary and backup power sources. In addition, due to its properties, SCs are ideal storage of electricity for heat recovery systems. It was first shown that a film of deeply oxidized graphene oxide (OG) can be used as a supercapacitor separator. Further, data on the operation of the SC with the electrodes of graphite oxide, reduced during microwave exfoliation (MVE-OG), and a graphene oxide separator were published. Next came the task of manufacturing a current collector from a material that would not corrode in the acid electrolyte. An analysis of the literature has shown that this problem can be solved through the use of polymer composites with carbon nanomaterials. In this report, we demonstrate the possibility of producing an IC current collector by layer-by-layer welding using a 3D printer from an industrially produced filament containing a graphene component. Current collectors are studied by IR spectroscopy. Electrodes were also made from exhaust gas reconstructed by microwave radiation, and a micro-supercapacitors was assembled which did not contain metal components. Electrochemical tests were carried out for the manufactured SC, including its cyclic stability tested up to 1000 cycles. The method of obtaining a dry powder consisting of a reduced composite of graphene oxide and humic acids was developed and described. This powder is suitable for storage and easily turns into ink for the 2D printer by adding ammonia water. The composition of the dry powder was determined by X-ray photoelectron spectroscopy and its structure by IR and Raman spectroscopy. The specific surface area of dry powder was measured by Brunauer-Emmett-Teller (BET) and standard contact porosimetry (SCP) methods, with using of octane as wetting liquid. Surprisingly, the specific surface area, measured by BET method, was equal only 6.5 m2/g, while value measured by the SCP method was 200 m2/g. The reason for such behaviour is that working fluid driving carbon layers, making accessible pores, which remain closed for gaseous nitrogen molecules. The obtained ink was used for printing of films with various thickness and supercapacitor electrodes. It was shown that thin films formed upon ink drying have islands type. The dependence of the surface conductivity of such films on their relative thickness (the number of printer nozzle passes) was measured. The electrodes were fabricated on the basis of such ink were used in the assembly of micro-supercapacitor with sulfuric acid electrolyte. The shape of the cyclic voltammogram curves of the SC is quasi-rectangular which is typical for carbon materials. The specific capacitance of assembled supercapacitors decreases somewhat up to 350 cycles but remains above 82 F/g. Characteristics (features) of this supercapacitors certainly are not very high (record). They are obtained only as an example of a possible application of the developed ink.

The method for neutron imaging of components with lattice structure, produced by additive manufacturing

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Additive manufacturing, or layer-by-layer synthesis, are currently one of the most dynamically developing areas of modern industry. This is due to the fact that they allow to get cheaper and faster parts of complex shape that are difficult or impossible to obtain using traditional metalworking methods, for example, lattice structures. In materials produced by additive manufactoring, as a rule, large internal stresses arise, which can lead to deformation of the form and the occurrence of defects in finished products. Therefore, it is important to diagnose the internal structure of complex parts using non-destructive methods. One of such methods is neutron tomography. The maximum sample thickness for this method is determined by the total cross section for the interaction of neutrons with the sample material. The total cross section for a given material depends on the neutron wavelength.

For neutron tomography at the DRAKON station of the IR-8 reactor of the NRC KI the monochromatic neutron beam with variable wavelength is used. In order to achieve the maximum thickness, it is necessary to select the wavelength corresponding to the minimum neutron total cross section in sample material.

Another way to optimize tomographic imaging of large thickness samples is to find the shooting geometry, which minimizes the maximum thickness of the sample on the neutron beam path. In the case of lattice structures, the technique consists in choosing the proper angle of inclination of the object relative to the axis of rotation.

The proposed method consists in choosing the optimal neutron wavelength and the geometry of tomographic imaging. The technique was tested on samples with a lattice structure prepared by the selective laser melting method.

New small-angle scattering beamlines for MAX IV and SIRIUS synchrotrons

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In the first half of 2019, ADDED VALUE SOLUTIONS (AVS) finalized the installation of two relevant small-angle scattering instruments: CoSAXS beamline at MAX IV Synchrotron (Lund, Sweden) and CATERETÊ beamline at SIRIUS Synchrotron (Campinas, Brasil).

The CoSAXS beamline will be a state-of-the-art X-Ray small-angle instrument which takes advantage of the high coherence of the MAX IV machine and offers several modular techniques like time-resolved SAXS, SAXS/WAXS, protein solution SAXS, microfocusing SAXS, anomalous X-Ray scattering and X-Ray Photon Correlation Spectroscopy (XPCS). CATERETÊ beamline design is focused onto Coherent X-Ray Diffraction Imaging (CXDI) an XPCS.

This contribution presents both designs focusing onto their key-component: the detector tube. Both are stainless steel vacuum vessels with an in-vacuum precise Z axis. The state-of-the-art of X-Ray detectors has allowed the removal of an in-air wagon inside of the vessel, being the current design is more compact. The main difference between both instruments is the tube size, which has several implications on the design strategy: need for a stiff lower structure optimized for low vibration, accessibility for maintenance, etc. Both instruments include a robust personnel safety system to prevent from risks linked to vacuum and automatized motion. A key design parameter has been the parasitic errors (circle of confusion) induced by the rails misalignment and vacuum action, which thanks to an optimal design and alignment has been reduced below +/-0.5mm in the whole stroke.

Boosting charge transport in Poly(ethylene-oxide) comb polymers for applications in Li-ion batteries

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In our daily life the storage of energy is crucial. Among the many forms of energy, electric energy is the most versatile due to its rich variety of applications. Modern rechargeable ion-batteries are commonly used for the storage of electric energy. These batteries will play a major role, e.g., in the future of electromobility or the storage of energy from renewable sources. The rate of charging and discharging those batteries is crucial for applications, beside other requirements. Lately researchers are focusing on polymer-based Li-ion batteries as they have various advantages over their inorganic counterparts. However, to perform adequately they require high Li-ion conductivities and for this the right choice of the electrolyte plays an important role in the optimization process. Poly(ethylene-oxide) (PEO) with added Li-ions is the most common combination in polymer-based electrolytes. We studied just this PEO/Li-ion combination employing quasi-elastic neutron scattering and dielectric spectroscopy, amongst others.

Based on our results, we develop a microscopic picture of the conductivity process. We show that about 5 – 6 EO monomer units form so-called cages which entrap the Li-ion until it finds another cage and “jumps” into this new one while the pre-existing cage decays. We determined the characteristic lengths and times scales for this process. The jump lengths are around 30 Å and the retention time is in the range of 5 ns. In addition, we show that not only the local/segmental dynamics of the polymer chain plays a major role, but, in addition, the backbone seems to limit the cage forming and decay process in a similar way. Consequently and to further improve the Li-ion conductivity process, we disentangled the two contributors, the backbone and the side chain of PEO. In a second step, we added EO side groups to the PEO main chain polymer which appeared to be more flexible to form cages and thus led to an even higher conductivity. We developed a relaxation map for PEO and PEO side chain polymers with and without Li-ions and found 4 relaxations for each of these materials, namely the normal mode, α, β and γ–relaxations. It can be shown that ions in PEO side chain polymers are generally more mobile than in the pure main chain PEO. This directly results in an increased ion conductivity and, as a consequence, in faster chargeable and dischargeable batteries.

QEXAFS methods development using X-ray adaptive bending piezo-actuator

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At the “Langmuir” station of the Kurchatov Synchrotron-Neutron Research Complex, a single-crystal monochromator based on adaptive bending X-ray acoustic element [1] was implemented for X-ray beam energy fast tuning and for rapid recording K-edge absorption spectra (XANES-spectrum) of Bromine.

To control beam parameters and record the absorption spectrum, ultrasonic vibrations excitation and monitoring system was used, synchrotron beam diffracted on X-ray bending element and collimated by slits was recorded using a scintillation detector, connected with multi-channel analyzer. X-ray acoustic element was excited via the inverse piezoelectric effect by applying a AC electronic signal with first harmonic resonance frequency f_{rez} = 239 Hz. During the experiments, the beam intensity was recorded in relation to control signal phase, further converted into an absorption spectrum.

It has been established that the measured absorption edge oscillations positions agreed well with both the calculated values and the results of a traditional mechanical scan. Achieved energy scan range was 13.25–13.65 keV (400 eV). Maximum time resolution available using the x-ray acoustic method is 2.1 ms, and actual time required to record qualitative spectrum, achieved in this experiment, was about 30 seconds and can be reduced by using detector with a higher dynamic range and counting rate, as well as optimizing X-ray optical scheme.

The developed scheme is promising for QEXAFS methods implementation, useful for chemical reactions kinetics study, for example, the Belousov-Zhabotinsky cyclic reaction [2], as well as the deformation processes kinetics research under external influences.

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Visualisation of the catalysed nuclear-spin conversion of molecular hydrogen using energy-selective neutron imaging

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Molecular hydrogen (H_2) can be found in two nuclear-spin isomers, or modifications, depending on the relative orientation of the two proton nuclear spins: ortho-hydrogen (oH_2), and para-hydrogen (pH_2). At ambient conditions, hydrogen is found in the gas phase with a composition of 75% oH_2 and 25% pH_2, yet, at cryogenic temperatures and in the liquid phase, a slow natural conversion from oH_2 to pH_2 occurs. The amount of energy released in the conversion of one oH_2 molecule, corresponding to a local temperature increase of about 170 K, causes the evaporation of the neighbouring molecules in a process referred to as H_2 boil-off, causing a practical limitation to the efficiency of low-temperature hydrogen storage. Moreover, a fast conversion to pH_2 is crucial in the performance of spallation neutron sources, where pH_2 is used as a moderating material to optimise the neutron pulse time profile at short-pulse spallation sources, and maximize cold neutron brightness at long-pulse spallation sources.

Previously [1], we showed how neutron transmission can be exploited to determine the amount of pH_2 in an unknown mixture of hydrogen modifications, taking advantage of the dramatic change in neutron scattering cross section of pH_2 and oH_2 below ca. 15 meV. This procedure was used to determine the composition of the hydrogen moderators at the ISIS pulsed neutron and muon source in the UK. Here [2], we present time-resolved neutron imaging results on the molecular-hydrogen conversion in the presence of a nanoparticle powder of the ferromagnetic catalyst γ-Fe_2O_2. In particular, we were able to characterise the conversion rate as a function of time and position of molecular hydrogen with respect to the catalyst. Experiments were performed on the IMAT and VESUVIO instruments at the ISIS Facility, UK. Results are reported for liquid and solid molecular hydrogen at 15 K and 10 K, respectively. We discuss how newly generated para-hydrogen poisons the catalyst, thus slowing the process and preventing the full conversion of large quantities of condensed molecular hydrogen, and we underline how the performance of the conversion critically depends on the loading procedure. Moreover, we suggest how a hive-like distribution of the catalyst in a vessel can boost the conversion rates while minimising the amount of material needed.

Two main conclusions can be drawn from our study that are of relevance for the neutron scattering community. First, we show how state-of- the-art energy-selective imaging using pulsed neutrons can be used to provide molecular specificity beyond what is currently possible for in-situ and operando kinetic studies. Second, we provide a much-needed procedure to characterise hydrogen moderators at neutron sources that can be used to monitor the amount of pH_2 and optimise the conversion process.

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Residual stress investigation by neutron diffraction in a 7.4 mm thick Inconel 625 plate produced by direct metal laser deposition (DLMD) on rigid substrate

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Additive technologies represents a highly promising production method for the aerospace, automotive, medical and other industries due to its capability to manufacture complex shape components, which production with machine method is extremely difficult.

Complicated residual stress distribution in produced parts is one of the main problems in additive manufacturing. Appropriate heat treatment, mechanical and chemical post-processing strongly depend on inner stress values.

For the investigation of residual stress in DLMD parts, 7.4 mm thick Inconel 625 plate was produced on rigid substrate. The experiments were carried out with neutron diffractometer "STRESS" at the research reactor IR-8, Kurchatov Institute.

The measurements were conducted along horizontal line, 2 mm above the substrate edge, and along vertical line at the center of the plate. The maximum tensile stress was detected near the edge of the plate close to junction with the substrate.

This work was performed using the equipment of Unique Scientific Facility "NRC IR-8"

High-temperature studies on a new Ni-based superalloy VDM 780 Premium using neutron diffraction and small-angle neutron scattering

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Ni-based superalloys are used for high temperature (T) applications that require good mechanical properties, as for example gas turbines. Among these alloy 718 is the most widely used with operation T up to 650 °C. In this alloy the austenitic matrix is strengthened γ'-Ni_3Al and γ''-Ni_3Nb precipitates. Other phases that can be formed are δ-Ni_3Nb and η-Ni_3Ti. The existence of the different phases, quantity and shape of the precipitates depend on composition, heat treatment and processing conditions. It is crucial to control their evolution at high T in order to tailor the mechanical properties. The aim of increasing the operation T forces the development of materials stable at higher T. Waspaloy has higher amount of γ' phase which allows its use at higher T but has a poor hot formability. The alloy 718Plus improves the performance at high T and it is expected easier processing.

A new alloy called VDM 780 Premium, which was developed in a cooperation between Technical University Braunschweig and VDM Metals GmbH [1,2],] with good formability and the potential for high operation temperatures, was selected for this investigation due to its direct industrial application. Measurements have been performed on this alloy to determine its structure after different aging conditions. In-situ neutron diffraction (ND) and small-angle neutron scattering (SANS) experiments were carried out up to the dissolution temperature of all precipitates in the alloy [3,4]. We studied the amount of the phases present in the material and their stability with temperature as well as the evolution of cell parameters, grain sizes and morphologies as function of temperature.

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Quantification of phases by strain-induced martensitic transformation in Austempered Ductile Iron (ADI) using neutron transmision

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Austempered ductile iron (ADI) is a cast iron with high potential to substitute cast steel due to the lighter weight, higher tensile strength and significantly lower manufacturing cost [1]. This material has an ausferrite microstructure consist of acicular ferrite and high carbon enriched retained austenite which is the result of a dedicated heat treatment. Typically this process involves following steps to yield the characteristic ausferrite microstructure: austenitization (880~1000°), quenching to austempering temperature typically between 250°C and 450°C and isothermal austempering [2]. Moreover, for industrial applications in thicker cast pieces alloying elements such as Ni, Mn or Cu are generally used to delay the phase transition kinetics and improve the austemperability of such geometries.

Martensitic transformation was observed in ADI due to the carbon enriched austenite being metastable and being able to partially transform to martensite under plastic deformation. This behaviour is known in steels as Transformation-Induced Plasticity (TRIP). The influence of heat treatments conditions and Ni contents on the martensitic transformation as well as the texture formation was studied using neutron diffraction under the application of tensile or compression tests to different plastic strains [3]. Combining these results quantitative phase analysis and extraction of martensite phase fractions were performed and good agreement with a model originally development for TRIP steels was found for ADI materials.

The elastic coherent scattering cross section of neutrons in crystalline materials has sudden changes (Bragg edges) at well-defined wavelengths, which can be determined by the Bragg’s law. The relative intensity of the Bragg edges in the neutron transmission spectra are related to the volume fraction of the different phases present in the material. Therefore, the analysis of the Bragg edge transmission spectrum can in principle be used to study the martensitic transformation. The applicability of the method has been shown quite early already in a study of the evolution of martensite transformation and the quantification of the phases in globulitic grey iron (GGI) using the Bragg edges in the transmission spectra of thermal neutrons [4].

In the present study, the phase analysis in ADI deformed to different plastic strains was performed using energy selective neutron imaging at the instrument ANTARES at FRM II. These results are compared and discussed to previously obtained results by neutron diffraction.

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Evaluation of anisotropic small-angle neutron scattering data from metastable β-Ti alloy

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Metastable β-Ti alloys are technologically important materials used in automotive, aerospace and biomedical industries. They have outstanding mechanical properties (high strength, low density, corrosion resistance, toughness and good hardenability, low elastic modulus). However, the mechanisms producing high level of strength are still not fully understood. Therefore, these alloys are widely studied. One of the microstructural features contributing largely to strengthening for some alloy compositions is metastable ω phase (non-close-packed hexagonal phase) which forms on quenching from β-matrix and grows during subsequent ageing [1].

Small-angle neutron scattering (SANS) is well suited for investigation of microstructure and precipitates in alloys, both ex situ or in situ at various external conditions (e.g. at elevated temperatures or under stress).

SANS data from single-crystal metastable β-Ti alloys exhibit an anisotropic character with interparticle interference maxima due to ordering of the dense system of ω particles. For an evaluation of such data, the program NOC [2] (previously used for evaluation of data from dense ordered γ′ precipitate system in single-crystal nickel-based superalloys) was well suited. Nevertheless, an improvement of this evaluation program was necessary in its model-forming part [3]. Another change of the evaluation program related to the mode in which the size distribution was calculated. This upgrade is presented.

The improved NOC program was employed for the evaluation of SANS data of annealed metastable single-crystal β-Ti alloy containing ω particles. 3D fit in reciprocal space was successfully used. A model of ellipsoids did not lead to a better fit than a model of particles with the spherical shape. The microstructural parameters of ω particles were determined.

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Neutron diffraction study of Ti-Zr alloy microstructure evolution during annealing after severe plastic deformation

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TiZr alloys are technologically important material, which can, for example, be used as a high strength, yet biocompatible alternative to pure titanium for dental implants [1]. Processing via severe plastic deformation introduces crystallographic defects to the alloy, which results in changes in its mechanical, as well as other properties. The changes in yield strength and ductility are the most important ones.

Post-process or inter-pass heat treatment can reduce the residual stresses developed during fabrication through introduction of softening processes (recovery). Annealing can thus be an effective means to optimize the microstructure of the final component to achieve an optimum combination of ductility, machinability, dimensional stability and structural stability for the particular application.

The strength of neutron diffraction lies in the possibility to carry out investigations of bulk materials, i.e. large volume of materials in depth, not only at its surface or sections or in near surface region. Therefore, the results are free of local artefacts and, to a large extent, are independent of grain size, which could become very large after some annealing procedures, and thus not suitable to be investigated by X-ray powder diffraction. Moreover, in-situ test at elevated temperatures can be easily carried out by neutron diffraction techniques. It enables to avoid material changes during quenching for investigation by ex-situ techniques, and also to avoid possible variations between samples in a series being investigated e.g. by heating up to various temperatures.

Neutron diffraction study of a Ti-Zr alloy microstructure evolution during annealing after severe plastic deformation was performed. The aim of the presented study was to observe (i) relaxation of elastic stresses within the component during annealing, and (ii) changes of microstresses due to occurring recovery or recrystalization, and/or grain size evolution. The experiment was carried out at TKSN-400 diffractometer [2,3] of NPL laboratory (CANAM infrastructure, NPI Řež, Czech Republic) equipped with high-temperature vacuum furnace for in-situ heating. The sample bar was heated step by step ($\Delta T=10°$) from room temperature (RT) up to 600° and then cooled down to RT in a similar way.

The evolution of peak positions of 002 and 101 diffraction peaks on heating and on cooling was used for determination of macroscopic elastic lattice strain. According to the results, the residual macro-stresses relaxation starts at the temperature of 530-540°C. The steep decrease of the macrostrain continues up to 600°C.

The evolution of peak widths of 002 and 101 diffraction peaks on heating and on cooling provides information on microstructural changes during annealing. The peak width starts to decrease at 300°C, which indicates the start of dislocation density decrease. This decrease accelerates at 550°C and is finished at 570°C (2 hours hold). The particular microstructural cause (recovery/recrystallization) of this evolution is discussed.

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Correlation of Microstructural Damage to Functional Properties of Irradiated Carbon Fibre Based Composites Used in Neutron Chopper Discs

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By 2025 the European Spallation Source in Sweden will be operating ca 50 high speed neutron chopper systems operating under radiation levels exceeding 1 MGy per year. ESS is currently undertaking an extensive neutron irradiation campaign to examine the potential effect of the harsh ESS radiation environment on the most fundamental component of high-performance choppers: the carbon fibre reinforced polymer (CFRP) based disc.

The central aim of this work is to understand the microstructural mechanism of radiation damage on CFRP based discs that are used in neutron choppers and whether this mechanism is universal between CFRP composites made with different types of bonding materials. CFRP samples were irradiated with 3, 10 and 30 MGy to simulate conditions at the ESS and analyse how the microstructure and mechanical properties of the CFRP are affected by increasing radiation dose.

The mechanical properties were evaluated using three-point bending. No significant difference between the mechanical properties of the samples was found. The microstructure was analysed using neutron and x-ray tomography in combination with an image analysis program to quantify the defects. The number, size and shape of defects in some samples of one bonding type clearly increased with the radiation dose, although the effect was not seen in different types of bonding materials.

These results illustrate how the microstructure of the CFRP are greatly affected by the radiation dose and act a precursor to mechanical failure although differences exist between different types of bonding materials. This research enhances the ability to select the correct bonding material and allows for estimation of CFRP disc lifetime at ESS at a given irradiation environment.

Enhanced radiation and corrosion resistance of 316LN stainless steel with high densities of dislocations and twins

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316LN austenitic stainless steel containing 0.12 wt.% nitrogen has excellent mechanical and corrosion properties, making it ideal for making the pipelines of nuclear reactors. The performance of the steel would be typically degraded dramatically when exposed to the aggressive environment of a nuclear reactor. Particularly, neutron irradiation produces hydrogen and helium atoms in the steel, which results in significant reduction of strength. It has been reported that dislocations and interfaces such as grain boundaries, phase boundaries can act as effective ‘traps’ for point defects in metallic materials, which deters the accumulation of interstitial atoms and vacancies, and thus improves the material’s ability to resist radiation damage. Particularly, nanoscale twin boundaries (NTBs) and dislocations can provide for the fast diffusion routes to the interface, which hinders the formation of defect clusters. Another issue for nuclear reactors is their highly corrosive environment, which could limit the service life of the reactor components. Here we introduce high densities of dislocations and NTBs by rotationally accelerated shot peening (RASP) on the surface of 316LN and investigate their effect on radiation and corrosion resistance. The dislocations and NTBs not only impeded the formation of helium bubbles and unstable shear bands during irradiation, but also facilitated the formation of a super passivation film, which significantly improved its corrosion performance. These observations provide for an effective approach for designing radiation- and corrosion-resistant nuclear materials.

Zoom, a polarised small angle neutron scattering diffractometer at ISIS target station II

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Small angle scattering (SAS) is a very powerful for characterising the shape, size and interactions in systems such as like nanoparticles, precipitates, micelles or proteins [1]. Using neutrons (SANS) as the probe gives insight into the magnetic properties of the sample within a length scale of tens to hundreds of nanometers [2]. Additional information, such as the orientation of the moments inside the nanoparticles, or the magnetic correlations between the nanoparticle can be gained) if the incoming beam is polarised and/or the scattered beam analysed [3].

The Isis TS2 phase two project called for the construction of an additional small-angle instrument, to compliment SANS2d, Loq, and Larmor, and enable new areas of science for the user community. The first operational phase of Zoom offers a flexible, high count rate instrument with 4m and 8m detector and collimation positions, which will allow access to Q-ranges between 0.003 and 0.8 $Å^{-1}$ together with beam polarisation. The polarisation of the incoming beam is produced by a supermirror cavity, with a Drabkin spin flipper to select incident polarisation. The Zoom instrument will also have the ability to accommodate outsize sample environments, being ideal for fitting a ^{3}He cell for allow polarization analysis of the scattered beam. The use of the time of flight technique will allow a broader Q-range than in monochromatic sources, since the use of short wavelength neutrons will help to counterbalance the reduced exit angle of the ^{3}He analyser.

The second phase of the ZOOM instrument has been designed to enable access to the VSANS q-range, within an instrument of similar physical length to SANS2d (around 30 m). This will be achieved through the use of focussing devices. It is envisaged that this will take the form of refractive lenses[4], which will be cryo-cooled for increased transmission [5] allowing wavelengths >10Å to be focussed onto a high resolution detector bank at focal spot sizes of 1-2mm. This design will offer substantial gains over pinhole collimation and avoids the frame overlap issues that would plague a longer instrument on a pulsed source.

In this talk we will present the current status of Zoom as it is moving into the science program. It will be discussed as well the scheduled upgrades to the instrument.

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Cryo-TEM – A Complementary Technique for Neutron Scattering

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The neutron instrumentation at the MLZ, in particular Small Angle Neutron Scattering, reflectometry and macromolecular crystallography allow to investigate structures in the range from 1 nm up to several hundred nm in reciprocal space. In soft matter and biology the contrast between hydrogen and deuterium is used to gain deep and quantitative insights about the shape and interactions of the objects forming the investigated structure.

Transmission electron microscopy may yield real space pictures of soft matter systems; virtually it may complete and enhance any SANS investigation on soft matter investigation.

A transmission electron microscope (TEM) is available at the Jülich Center for Neutron Sciences at MLZ in the JCNS building.

In one hand, with TEM, we are able to extract information in the real space about size measurements and distribution of particles, shape, self-assembly systems and aggregates. SANS on the other hand is a non-destructive method providing structural information in the reciprocal space averaged over all grains of different sizes with high statistical accuracy. Transmission electron microscope allows to get quantitative information about roughness and intermolecular distances can be extracted and indirect information concerning average radius and periodical distances by performing a Fourier transform in TEM image. Additionally, diffraction patterns can be obtained. Hydrogen, which is mainly present in soft matters, can be highly distinguished from its isotope i.e. deuterium by neutrons whereas both of those light elements remain invisible in TEM and x-ray small angle scattering. Both techniques allow to detect structural changes occurring in the relatively large scale structures on the nano-scale. One main advantage in SANS is the contrast variation technique which allow, by using specific ratio of D2O/H2O for solution sample, to study multi-component system. With TEM, the energy filter and the energy loss method allows to get information about atomic composition of the observed system. The energy filter is an additional way to enhance contrast in complementary to thickness dependent amplitude contrast, the small angle phase contrast and the diffraction contrast for crystalline structure investigation.

The instrument is a 200 kV JEM-FS2200 from JEOL with a field emission gun (FEG) and an on-line Omega Energy Filter allowing measurements at magnification from x 50 to x 1 M with a resolution of 0,2 nm in point and 0,1 nm in lattice. The Microscope is equipped with a Tietz CMOS camera with 2048 x 2048 pixels square area. Unlike for neutron experiments the soft matter samples have to be investigated either in dried or frozen state (Cryo-TEM) to be able to work in the necessary vacuum and to suppress blurring motion of the object as well as radiation damage. Also the samples have to be very thin (max~100nm). TEM investigations require sophisticated sample preparation different from the needs for e.g. a SANS experiment, the TEM laboratory comprises an extended suite of preparation equipment. Users will be supported by JCNS scientists (M.S. Appavou) to conduct the suitable preparation and TEM investigation.

Characterization of the boron-based Multi-Grid detector on the thermal neutron spectrometer SEQUOIA at the SNS

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In Lund, Sweden, the European Spallation Source (ESS) is currently under construction. In order to increase performance at high neutron flux and remove the dependence on the expensive ^{3}He gas, alternatives to traditional ^{3}He-detectors have been developed. Here we present the MG.SEQ, the latest iteration of the Multi-Grid, a boron-based neutron detector developed for Time-of-Flight neutron spectroscopy. The detector, introduced by the ILL and developed in a collaboration between ILL and ESS, is currently advancing through the final characterization phase. The Multi-Grid is the baseline detector for the CSPEC (Cold Neutron Spectroscopy) and T-REX (Thermal Neutron Spectroscopy) instruments at ESS, and may be of interest for other facilities. In this paper, the latest results concerning the characterization of the Multi-Grid are presented. While the detector has previously been tested at cold energies, the current study presents results reaching into thermal and epithermal energies, with a range from 2 meV to 3500 meV. The main measurements were performed on V-metal samples, were the efficiency, energy resolution and line shape could be extracted from the elastic peak. Other important measurements were performed on water, Si-powder, and Si- and US-crystals, as well as $C_4H_2I_2S$, to study Bragg reflections and non-elastic scattering. The detector was also tested in Rate Repetition Mode (RRM). These measurements were performed using the Fine-Resolution Fermi Chopper Spectrometer SEQUOIA, at the Spallation Neutron Source (SNS). At the facility, the MG.SEQ was installed in the time-of-flight vacuum tank of SEQUOIA. This prototype consisted of three separate detectors, installed adjacent to each other, and together covering about 1 m^2 active area. These detectors differed in certain key aspects, such as the aluminum type used, grid size, and the extent of internal boron coating. The first detector was built at ILL, while the remaining two were constructed at ESS. The purpose of the measurements was twofold. First, it was to evaluate any differences between the three detectors, while at the same time characterize the overall performance of the MG.SEQ. This was done by using data collected from the same measurements with the permanent array of ^{3}He-tubes in SEQUOIA, and perform a direct performance comparison. Second, it was to test the vacuum vessel design concept for CSPEC, and demonstrate the detector operation in vacuum. The test has helped to further refine the vacuum vessel design. It was also clearly observed that the Multi-Grid matches the momentum- and energy-resolution of the ^{3}He-detector over the entire measured energy range, and compares well in terms of energy-dependent efficiency. Additionally, all non-elastic features observed from the ^{3}He-tubes were well reproduced from the Multi-Grid data. The details of the data analysis and results are presented in this paper.

In-situ, bellow-driven pressure cell for neutron scattering investigations in hydrostatic conditions

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In condensed matter physics the study of quantum critical phenomena amount to a significant part of today's research effort. The quantum fluctuations required by Heisenberg's uncertainty principle not only drive the phase transition at T = 0 K, but also influence the systems behavior for T ≥ 0 K in the quantum critical regime.

Especially neutron scattering methods, contribute in this field providing unique insight in magnetic critical phenomena in a wide range of crystalline bulk materials. Hereby, key is a versatile sample environment to tune the system to the quantum critical point.

In this context, we present a newly developed *quasi in-situ* pressure cell for neutron scattering investigations in a hydrostatic environment. The bellow-driven pressure cell is laid out to be compatible with standard cryogenic sample environment, having a tail diameter of $d_i \geq 80$ mm. A maximum axial force of F = 15 kN can be exerted on the pressure medium. Utilizing a sample space with diameter of $d_s = 5$ mm the system translates the force to a hydrostatic pressure of $p \approx 0.5$ GPa. Furthermore, the setup is designed in a modular fashion and provides adaptability to different requirements of a specific experiment with regard to sample size, pressure and neutron attenuation. This is possible by choosing the sample space material from Al, CuBe, TiZr or steel and

adjusting the inner diameter, which makes pressure $p \geq 2.0$ GPa accessible. During an experiment, the pressure cell remains inside the cryostat while heating the cell above the melting point of the fluorocarbon-based pressure medium to change the pressurewithout causing axial pressure comp onents. The procedure enables significant saving of time compared to the removal of a cell and the pressure adjustment in ambient environment.

Our poster contribution presents the initial material simulation with COMSOL and design considerations. Furthermore, an in-depth explanation of the individual components is given to emphasize the modularity and functionality of the setup. First calibration measurements, background evaluation as well as neutron scattering data will be presented.

Study of LiInSe2 single crystals for the thermal neutron detection

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Lithium-indium di-selenide ($LiInSe_2$) is the new semiconductor material, sensitive to the thermal neutrons. It allows obtaining fast signals readout, good spatial resolution and a large dynamic range for neutron detection. $LiInSe_2$ compound was synthesized from Li (99.99%), In (99.999%), Se (99.999%). $LiInSe_2$ (LISe) single crystals growth was performed using the vertical option of Bridgeman-Stockbarger method.

To prevent the deviations from the stoichiometric crystal composition, the melt of the initial materials was overheated by less than 50 degrees. Excess pressure of Ar gas was kept inside the ampule.

Crystal structure of LISe belongs to the β -$NaFeO_2$ type (sp.gr. $Pna2_1$ or C_{2v}^9). It was observed that Li ions can occupy two inequivalent crystallographic positions, one in the $LiSe_4$ tetrahedra center, while the other is in the octahedral structure pore. Stoichiometric composition of the $LiInSe_2$ was confirmed by the high precision chemical analysis as well as by X-ray diffraction.

To test the neutron detection characteristics of the $LiInSe_2$ crystal the sample 5x5x1,5mm^3 was used. ^{252}Cf – with the activity 6,3 x 10^5 n/s allowed to measure amplitude characteristics and to define the optimal operating voltage for neutron detection. Time-of-flight neutron spectra were measured at the fast pulsed research reactor IBR-2 at JINR. Future for the construction of working prototype of the neutron detector based on this semiconductor material is discussed.

Latest Developments in McStas for Polarized Neutron Experiment Simulation.

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We present the newest developments in the McStas[1,2] subsystem for simulation of polarized neutron scattering experiments.

McStas itself is a world leading neutron ray tracing software package for simulations of all and any neutron scattering experiments. A later addition to its original design is the polarization subsystem, which aims to support the ever growing pool of instruments with polarization analysis capabilities.

The new capabilities include a revamped set of components for describing Magnetic fields, which can now be nested by geometric shapes such as blocks and cylinders. Also it is now possible to handle tabled magnetic fields in a flexible manner allowing for free placement and orientation. Secondly, spin-flipper components have been developed; An idealized model for fast computations, as well as a more accurate model, at the expense of more computational power. Thirdly, the interface has been enriched to allow finer grained control of the precession computation.

In addition, we will present some newly performed simulations with the aim of a full virtual model of the Raden instrument at J-PARC[3].

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McStas Union components and python interface

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Monte Carlo simulations have become a crucial tool for designing, optimizing and understanding instruments, for instance for the construction of instruments at the European Spallation Source. For this reason, it is vital that the fidelity of these simulations becomes as adequate as possible such that important design decisions can be properly assessed.

Equally important is the accessibility of these simulations, as intuitive tools reduce the barrier to entry and allow researchers to reach important conclusions faster and easier.

The McStas Union components is an expansion of the popular Monte Carlo ray-tracing package McStas that aim to improve the fidelity and usability when simulating complex systems, such as the sample environment, where multiple scattering is important. The user builds the geometry with simple geometries (e.g. spheres, cylinders, boxes) that can be overlapped to create hollow constructs in many layers and thus to create systems of high complexity. Scattering physics is applied to these geometries in a modular fashion, allowing to add e.g., incoherent, powder and single crystal scattering. Mixtures of materials and twinned crystals can be easily described by using this modularity. The simulated neutrons can interact with every defined geometry and the scattering in each geometry is balanced appropriately between the selected scattering processes. This creates natural multiple scattering effects such as spurions that contaminate the detected signal. Helper tools are available to track and understand such issues so that these can be understood and prevented.

To describe real sample environments and instruments, a great number of geometries can often be required, which presents a challenge both to usability and simulation performance. The simulation performance is preserved by analysis of the given geometry ensemble, where unnecessary intersection calculations are removed without additional input from the user. In many cases an instrument has repeating sections that are naturally described using for-loops or other flow control. The PaNOSC EU project contains a work package that aims to facilitate online use of simulation codes such as McStas through modern Jupyter Notebooks. Here the Python scripting interface has the necessary flow control to produce repeating structures such as the filter/collimator shown in figure 1. The presentation will demonstrate what can be achieved with the McStas Union components, and how the Python scripting interface simplifies the task of creating complex geometries with the McStas Union components.

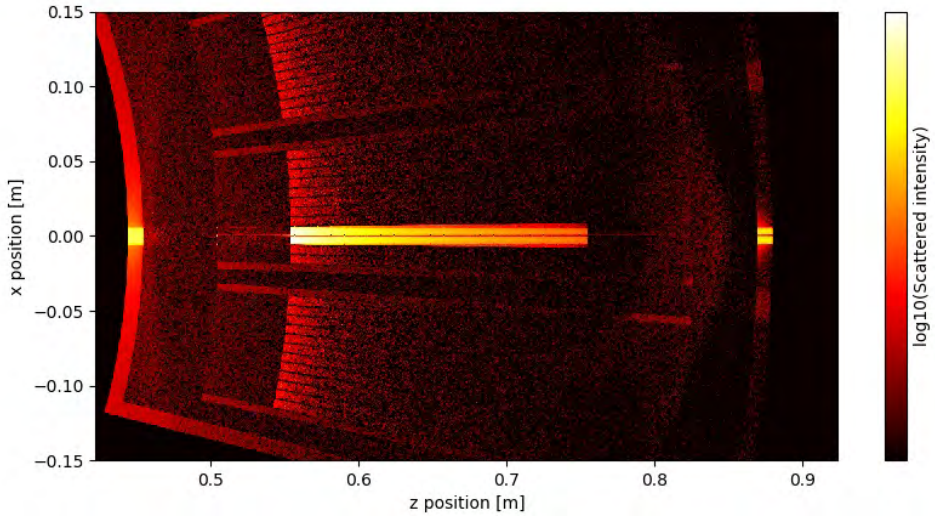

Figure 1: Simulation of filter under consideration for BIFROST extreme environment spectrometer at ESS. Spatial distribution of scattered intensity is shown on log scale.

Neutron detection by using Water Cherenkov Detectors

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In this work we show the neutron detection capabilities of a water Cherenkov detector (WCD). The experiments presented here were performed using a simple WCD with a single photomultiplier tube (PMT) and a ^{252}Cf neutron source. We compared the use of pure water and water with a non contaminant additive as the detection volume. We show that fast neutrons from the ^{252}Cf source can be detected over the flux of atmospheric particles background. Our first estimation for the neutron detection efficiency is at the level of (19)% for pure water and (44)% for the water with the additive. We also present the simulation of the response of the WCD to neutrons using a simulated ^{252}Cf source. We implemented a detailed model of the WCD and of the neutron source spectra using Geant 4. The results of our simulations show the detailed mechanism for the detection of neutrons using a WCD and support the experimental evidences presented. Since both active volumes studied, H_2O pure and with additive, are cheap, non-toxic and easily accessible materials, the results obtained are of interest for the development of large neutron detectors for different applications. Of special importance are those related with space weather phenomena as well as those for the detection of special nuclear materials. We conclude that WCD used as neutron detectors can be a complementary tool for standard neutron monitors based on ^{3}He.

High-resolution Fourier diffractometer at the IBR-2 pulsed neutron source

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The high-resolution Fourier diffractometer (HRFD) is installed at the IBR-2 pulsed reactor at the FLNP, JINR (Dubna) [1]. HRFD is a neutron time-of-flight spectrometer with a fast Fourier chopper and a correlation mode of data acquisition designed to study atomic and magnetic structures of crystalline materials with high resolution in reciprocal space. If correlation analysis is used, the HRFD $\Delta d/d$ resolution is determined by the maximum rotational speed of the Fourier chopper. For $V_{\max}$ = 6000 rpm, "high-resolution" patterns are measured by backscattering detectors with $\Delta d/d \approx 0.0015$ despite a very short flight path ($L \approx 20$ m) between chopper and sample. Switching to a conventional TOF-mode (without Fourier chopper) makes HRFD one of the world's best high-intensity diffractometers, capable of measuring diffraction patterns in the range of ~1 min and less. The data collected with HRFD are analyzed in the same manner as those from a conventional TOF-machine.

At present, the HRFD is mainly used for refinements of atomic and magnetic structures of polycrystalline materials (including material microstructure), sometimes for experiments with single crystals if a very high *d*-spacing resolution is needed, as well as for *in situ* real-time studies of transition processes in functional materials with good ($\Delta t_S \leq 1$ min) temporal resolution [2].

In this report the HRFD design is presented and examples of its application for studying various materials are given. New possibilities appearing after the recent substantial HRFD upgrade [3] and further perspectives of the method are also presented.

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Fourier diffractometer FSS at the IBR-2 pulsed reactor

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FSS is a Fourier RTOF diffractometer, optimised for residual stress studies and successfully operated at the FRG-1 steady state reactor in Helmholtz-Zentrum Geesthacht (Germany) since about 1990. After final shutdown of the FRG-1 reactor in 2010, the FSS diffractometer was transported to FLNP JINR (Dubna, Russia) for further use on the IBR-2 pulsed reactor. The FSS instrument is planned to be used for further development of Fourier correlation technique, for testing new detectors and advanced electronics, and for residual stress studies in materials.

The neutron beam at the sample position is formed with a new supermirror neutron guide (m=2) with curvature radius of 1900 m and characteristic wavelength λ_c=0.95 Å. The neutron guide is vertically convergent with beam apertures of 10×126 mm at the entrance and 10×50 mm at the exit part. The Fourier chopper modulates the primary neutron beam intensity with the rotation speed ranging from 0 to 2000 rpm. Two detectors comprising 12 (det. Ost) and 15 (det. West) geometrically focused ^{6}Li-glass scintillators are placed at scattering angles of 2θ=±90°. A set of radial collimators in front of the 90°-detectors makes possible to select gauge volume of 1 or 2 mm in the sample during strain scanning experiments. The sample positioning is provided by 4-axis HUBER goniometer. The FSS operation is controlled by SONIX software package that provides raw data acquisition in ***List-mode*** and full experiment automation.

Recently first high-resolution RTOF spectra from several typical structural materials and residual stress distribution in welded steel plate sample have been measured on FSS. The resolution functions of both detectors evaluated from neutron diffraction data confirmed the planned resolution level of the instrument: $\Delta d/d \approx 5.5 \cdot 10^{-3}$ for d_{hkl} = 2 Å.

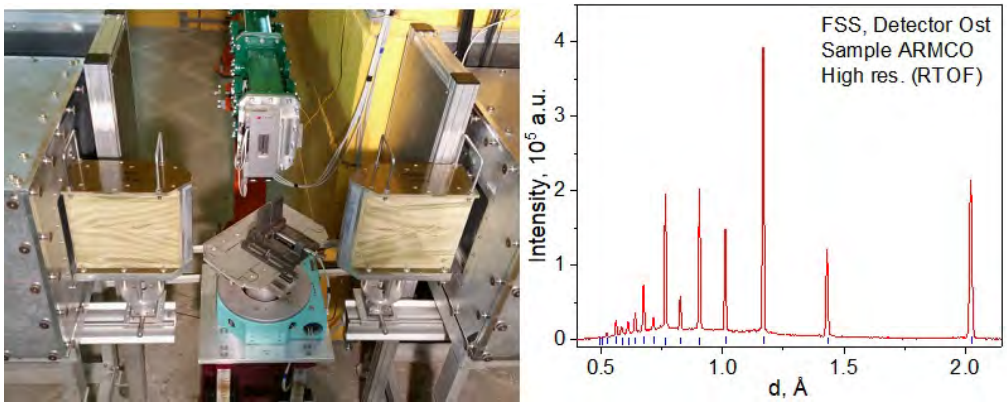

Fig. 1. Left: Sample place at the FSS diffractometer. Right: The high-resolution RTOF diffraction spectrum from ARMCO iron sample.

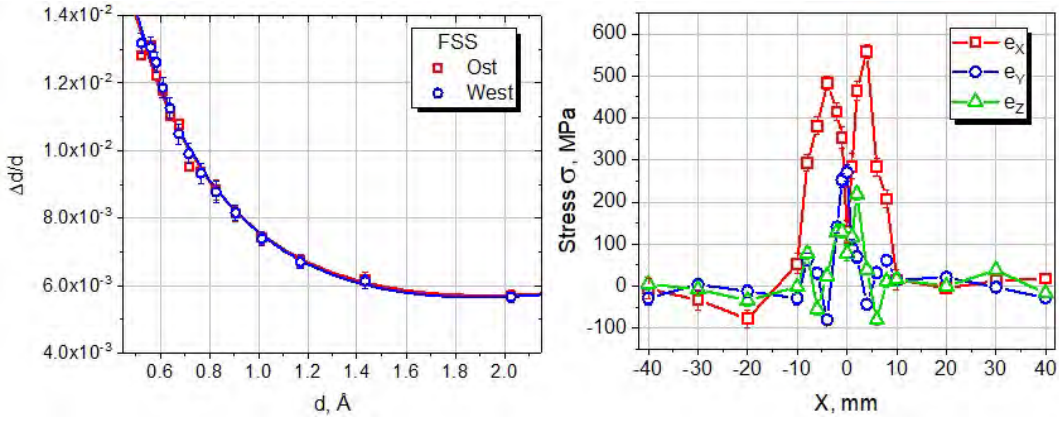

Fig. 2. Left: The FSS resolution function measured at the max. chopper speed Ω_{max}=2000 rpm. Right: Measured residual stress distribution in steel plate welded by electron beam.

Development of a sample environment for the study of mechanically confined and sheared geometries

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The study of soft materials confined between surfaces is central to the understanding of interactions that lead to adhesion, lubrication and colloidal stability. Force measurements have long been able to describe the potential that exists between various coated surfaces, but it is only more recently that scattering techniques, particularly reflectometry, have permitted the detailed study of surface layers under confinement. Specifically, the recent development of a confinement cell that consists of a solid surface confined by an expanding flexible film has been able to address key factors that have hampered these investigations for a long time by achieving parallelism and good contact over a large area. These advances have enabled new fields of research for studying surfaces under confinement using neutron reflectometry [1].

Within the framework of a project recently funded by the Swedish Research Council, researchers from Malmö University and the collaborative team behind the development of this cell will work with researchers at both ESS and ISIS to build on this success towards a next-generation surface confinement apparatus. Specifically, the key deliverable will be to develop a sample environment capable of applying shear under confinement which can be integrated with GI-SANS and reflectometry geometries to provide information on the structural changes in all dimensions. To achieve this goal, the cell will be designed and manufactured in collaboration with ISIS and fully optimized for full integration on to the beamlines at ESS. There is significant private and public sector interest in understanding lubrication and developing nanomaterials to mimic nature. Thus, the huge potential of this project to significantly expand the research field accessible with neutrons will be demonstrated by employing it to investigate the mechanism underlying the outstanding performance of biological lubricants, in particular, salivary pellicles and mucus blankets [2].

In this communication, we provide an overall presentation of the planned implementation and goals of this project.

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3He linear PSD for SANS, reflectometry, and TOF instruments: Two decades of development at the ILL

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^{3}He linear Position-Sensitive Detectors (PSDs) are nowadays used on several types of instruments. They usually consist of ^{3}He-filled tubes which are positioned side by side in flat or curved geometries to cover the detection area required by the instrument. They provide a high counting rate, and 2D localisation at medium spatial resolution, making them the gold standard for SANS. Reflectometers also benefit from their high counting rate capability, combined with the good spatial resolution achieved along the tubes. ^{3}He linear PSDs have proven to be an excellent choice to cover the large detection area of TOF instruments, even if this solution has become less affordable due to the worldwide shortage of ^{3}He. Three types of ^{3}He linear PSD configurations have been developed and installed on ILL instruments over the past two decades: independent aluminium tubes, stainless steel Multi-Tubes, and Monoblock Aluminium Multitubes (MAMs). The mechanical design and principle of operation of these various implementations of the ^{3}He linear PSD concept will be presented. The benefits and technical limitations of each mechanical configuration will be discussed, in relation with the performance achieved on each type of neutron scattering instrument. We shall focus more particularly on D22 and D33 for SANS instruments, FIGARO and PLATYPUS for reflectometers, IN5 and PANTHER for TOF instruments.

Study of periodic density modulation in holographic diffraction gratings

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In modern optics (UV, visible and IR spectral range 200 nm - 3 μm) various diffraction elements play a significant role. However, for the problems in which the radiation wavelength is on the scale of dozens of nanometers and less, at present there are no acceptable analogues. Natural crystals have a substantially lower lattice constant and are not suitable for such purposes, and artificial gratings are limited by the resolution of the materials on which they are created and/or by the method of manufacture. The main idea of this study is to use diffraction gratings created in the bulk photo-thermo-refractive (PTR) glass with a period of 200 nm or less for neutron optics. This glass provides ion concentration modulation during the process of grating manufacture, which creates a contrast density of neutron scattering.

It is proposed to study the submicron structure of low-periodic diffraction gratings recorded on PTR glass with a scope to a novel approach for neutron diffraction element production. Nowadays, the development of diffractive elements for neutron optics is focused on polymeric materials and composites, whereas glass materials are not considered. The main reason for that is the insensitivity of neutrons to the modulation of the optical refractive index, whilst volume holographic materials rely on this. In this case PTR glass is quite unique volume holographic material. Modulation of the refractive index in this glass is provided by crystalline phase (NaF) volume fraction modulation, which leads to a modulation of its components concentration along the grating vector (sodium and fluorine). Thus, the ion concentration modulation which naturally occurs during the grating preparation process, opens possibility of the neutron diffraction gratings manufacture on PTR glass. Another advantage of the glass in the framework of the problem is high spatial resolution. This is due to the fact, that the center of crystallization is silver nanoparticles with diameter of about 2 nm and the size of the crystals is determined by the concentration of nanoparticles and processing regime and lies within the range of 10-100 nm. In the recent experiments, we managed to record gratings on PTR glass with a period of 211 nm.

New TOF INS spectrometer at FLNP JINR

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The inverse-geometry inelastic neutron spectrometer NERA is optimized for high-resolution vibrational spectroscopy in the energy transfer range up to 150meV. The instrument has been operational for more than two decades and during that time has proven as a very successful and productive machine for broadband chemical spectroscopy with neutrons. Although NERA still showing very impressive scientific achievements, many components of the spectrometer getting obsolete with time and required modernization or exchange.

About two years ago we also began the last modernization process on NERA and as a first a step we have recently replaced the last 25 meters of the 100 meters long NERA m=1 guide with the vertically focusing supermirror guide that gave the density of flux increase by a factor 3.5. This major upgrade of the primary spectrometer needs to be complemented by a further upgrade of the secondary spectrometer in order to make use of the enhanced neutron density of flux.

Therefore, we have proposed to perform the feasibility study of a new secondary spectrometer replacing the existing one. The main characterization, geometry and potential gains in instrument luminosity and energy resolution will be discussed.

CSPEC : Development of the cold chopper spectrometer of the ESS.

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The European Spallation Source (ESS), expected to be the world's most powerful neutron source, will begin operations in 2022. Among the endorsed instruments foreseen for day one instrumentation at ESS, is the cold time-of-flight spectrometer CSPEC [1]. CSPEC is a joint proposal from the Technische Universität München, Germany, and the Laboratoire Léon Brillouin, Saclay, France. Experiments in an electric field, or laser excited light harvesting proteins, are still in an exploration stage, mainly due to the lack of flux at the instruments available today. CSPEC will benefit from the high brilliance of the ESS spallation in addition to the cumulative flux provided by repetition rate multiplication (RRM) that results in large flux gains making it possible to probe time-dependent phenomena with millisecond to second time resolution.

The unique pulse structure of the ESS with its long pulse duration (2.86 ms) and a repetition rate of 14 Hz requires new concepts for the instrumentation to make optimum use of the available source time frame. With an instrument length of ~160 m, moderator to sample, a wavelength range of $\Delta \leq 1.8$ Å can be probed within each ESS time period via RRM. The energy resolution can be tuned in the range of

$\Delta E/E = 6 - 1\%$, and CSPEC will utilize cold neutrons in the range from = 2 - 20 Å with the focus on the cold part of the spectrum. The guide is optimised to enhance signal to noise and will be able to focus on samples ranging from several mm2 to several cm2 in area. The large detector area, with a radius of 3.5 m, -30^{o} : 140^{o} and 3.5 m in height. In addition the sample chamber will, via the use of a gate valve, enable experiments under real and transient conditions. CSPEC is in the detailed engineering phase and we will present the current design layout and the expected performance.

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International Society of Neutron Instrument Engineers (ISNIE)

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The International Society of Neutron Instrument Engineers has been created in September 2017. It is an international platform for neutron instrument engineers to share general advancement of neutron instrument engineering and its applications in order to foster innovation, excellence and best practices within worldwide neutron scattering facilities.

ILL Modernisation Programme: Endurance. The ambitious renewal of the H15 cold neutron guide and instrumentation

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The ILL has begun a second phase of ambitious upgrades to scientific instruments and infrastructure under the Endurance programme. Endurance 2 (2019 - 2023) will involve the upgrade of many instruments including a number of large detector projects and with a main focus on the upgrade and re-modelling of instruments on the Vercors side of ILL 7, including a complete renewal of the H15 cold neutron guide. The massive scope of the H15 project aims to provide dedicated beam positions for the new or upgraded SHARP/RAMSES time-of-flight spectrometer, the polarised diffuse scattering instrument D7+, an upgraded D11 small-angle scattering (SANS) instrument as well as positions for additional instruments, GAPS (cold triple-axis spectrometer) and SAM (SANS). The conceptual design of the renewed H15 guide is highly complex, both in terms of its novel curved diverging trumpet expansion and the engineering constraints in the separation of six independent neutron guides and placement of instrumentation. Phase-space analysis shows how the diverging curved trumpet best allows for an optimal expansion of the initial high-m neutron guide and provides additional angular separation for the down-stream instrument branches. The Endurance programme, with a particular emphasis on the H15 guide project, will be presented.

Complex Geant4 Simulation Study for Background Suppression in the Multi-Grid Detector

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The European Spallation Source (ESS) aspires to be the world's leading neutron source of the upcoming decades. The required high performance and the recent restructuring of the ^{3}He market opened a new frontier for neutron detector development. A potent new solution for the large area detectors is the Multi-Grid thermal neutron detector [1], an Ar/CO_2 gas filled detector with solid $^{10}B_4C$ converter that will serve the chopper spectrometers at the ESS. Since the inelastic signals are orders of magnitude smaller than the elastic ones, for these instruments a high Signal-to-Background Ratio (SBR) is a key requirement.

Thanks to the recently developed neutron simulation tools [2], a detailed and realistic Geant4 Monte Carlo simulation study is performed on the intrinsic scattered neutron background, sourced by the complex geometry of the detector. The simulations are performed on the realistic and parameterised model of the Multi-Grid detector module designed for the CSPEC [3] instrument of the ESS.

In the built model different detector components, e.g. the entrance window and the detector vessel are studied as sources of scattered neutron background, and their impact on the SBR is determined in a detailed simulation of detector response. On the basis of the obtained results the background reduction potential of a combined, internal detector shielding is also studied: common shielding materials e.g. B_4C, Cd, Gd_2O_3 and LiF are applied in different shielding geometries, e.g. as end-shielding, and their impact on the SBR is compared to that of the ideal black absorber. The presented realistic simulations and the scattering study give a novel approach on how shielding optimisation as part the optimisation process can lead to instruments with higher SBR by design.

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New Aspects of Ultracold Neutron Scattering in Condensed Deuterium and on Material Surfaces

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Ultracold neutrons (UCNs) are a versatile tool for fundamental physics experiments, such as the determination of the lifetime of the free neutron and the search for a possible non-zero neutron electric dipole moment.

The precise knowledge of UCN cross sections of solid deuterium is pivotal to the design and improvement of new UCN sources throughout the world, which promise to provide significantly higher UCN densities than the UCN facility PF2 called "Turbine" at Institut Laue-Langevin (ILL) in Grenoble, France.

A novel sample container for cryogenic liquids and solids featuring highly polished transparent silica windows is presented. Using this sample container, the total UCN cross sections of liquid and solid deuterium for UCNs were measured in transmission geometry with a time-of-flight (TOF) setup at the PF2-EDM beamline at ILL. The talk will feature velocity-dependent cross section data for UCN scattering in liquid and solid deuterium. It will also discuss the importance of UCN scattering from rough surfaces and from deuterium crystal defects, the concentrations and scattering cross sections of which were determined quantitatively for the first time.

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Universal library of models for Quasi Elastic Neutron Scattering

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We report on a universal library of models for Quasi Elastic Neutron Scattering (QENS) data.

This QENS library was developed as part of SINE2020 Workpackage 10 on Data Treatment to develop an exhaustive library of dynamical models to increase interoperability and modularity for a rapid prototyping. It provides different building blocks that users can combine, convolute and plug in different frameworks for visualizing or fitting. A similar approach was used for Small Angle Scattering with SasView, SasModels and its marketplace[1].

The library is stored in a GitHub repository available at https://github.com/QENSlibrary/QENSmodels; it has been developed under an open-source license (GPL-3.0).

The models are written in Python for easy integration in workflows. In order to help users, a few examples of data analyses using different standard fitting engines (lmfit[2], scipy[3], bumps[4]) are provided as Jupyter notebooks[5]. Tools are also provided to help those interested in contributing to the project by adding models or sharing examples of data treatment.

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Correction of the Fermi pseudopotential conception in the theory of dynamic scattering of thermal neutrons

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The propagation of thermal neutrons through media with different degrees of ordering is considered. The necessity of changing the standard concept of the Fermi pseudopotential to obtain general description of the interference effects in crystalline and amorphous media is revealed. It is shown that satisfactory results can be obtained with the pseudopotential, which produces correct one center scattering amplitude in the second Born order, contrary to standard definition. General relations are obtained that describe the propagation of a neutron wave through a substance with an arbitrary degree of order [1].

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Study of through-thickness stress distribution in steel double-V butt weld

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Residual stresses in a weld occur as a result of uneven volumetric changes in the solidified molten weld metal and base metal during cooling and can reach yield stress and even exceed it. These stresses can greatly degrade the performance characteristics of welded structures. Therefore, quantitative measurement of residual stresses is necessary for more accurate calculation of structural strength characteristics, optimization of welding parameters and post-weld heat treatment, to verify existing computational models and develop new ones.

At present, the neutron diffraction (ND) is the only non-destructive method that allows measuring all three components of the strain / stress tensor in bulk materials.

This work presents the results of a study of the through-thickness stress distribution in ~45mm thick steel double-V butt weld using neutron diffraction (ND) and finite element (FE) methods. Experiments were conducted using diffractometer STRESS, installed at the reactor IR-8 at NRC "Kurchatov Institute".

Influence of constraints and post-weld heat treatment on distribution of stresses has been studied.

It is shown that tensile stresses in a sample, obtained by welding fixed plates with strong-backs are noticeably higher than those not fixed. Longitudinal stresses along the weld are greater than transverse. Normal stresses are small. The maximum longitudinal stress in the plate with strong-backs is greater than without strong-backs and close to the yield stress (820 MPa) of the weld metal. Stress distribution is very different from reported in literature distribution, obtained by destructive method.

Post-weld heat treatment at 600°C significantly reduces residual stresses. However, after annealing, the residual stresses are quite high (~ 250 MPa).

It is shown that the distribution of residual stresses obtained by the FE method, in general, is in qualitative agreement with the experimental results. However, the numerical values of the stresses obtained by the FE method are, as a rule, higher than those obtained by the ND method. Possible reasons for this discrepancy are considered.

This work was performed using the equipment of Unique Scientific Facility "NRC IR-8"

FREYJA – a new multipurpose time-of-flight neutron reflectometer at the JEEP II reactor in Norway

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FREYJA is a time-of-flight neutron reflectometer with vertical sample geometry. This new instrument will be part of the Norwegian Center for Neutron Research (NcNeutron) [1] and its construction will be finished by the end of 2020.

The reflectometer will offer the possibility to use polarized neutrons. Its main application will be the characterization of materials developed for energy (hydrogen storage, battery applications, solar cell components), nanomagnetism (magnetic thin films and multilayers) and biological membranes (interaction of natural and artificial membranes with surrounding media).

FREYJA neutron reflectometer (Fig.1) is developed using the following key parameters:

- Cold-neutron TOF reflectometer with horizontal scattering geometry (sample surface vertical);

- Instrument length/TOF length: 8.31 meters (source-detector), 4.00 meters (chopper-detector), 2.40 meters (sample-detector);

- Wavelength range: Unpolarized: 2 – 15 Å; upper limit set by FOM* Polarized: 2.5 -10 Å; set by polarizing SM**, (*FOM = frame-overlap mirror; **SM = supermirror);

- Maximum flux at sample position: $5*10^5$ n/s/cm^2;

- Typical Resolution settings: (ΔQ/Q) = 3%, 6% and 12%;

- Limiting Reflectivity: ~10^{-5}; Q-range: 0.004 – 0.22 Å^{-1} (Θ = 0.3° and 2.0°); up to 0.35 Å^{-1} (Θ = 3.5°) for solid-air and solid-solid interfaces;

- Neutron optics: In-pile 4-channel collimator-guide assembly (l = 1 meter, m = 5 top/bottom) plus neutron guide (l =1 meter, m = 5 top/bottom) with integrated V-shaped cavity acting as FOM* (λ_{max} = 15 Å);

- Chopper: Van-Well type double-disk chopper; radius: 157 mm; frequency: 35 Hz; 2 slots per disk; 3 resolution settings: Δλ/λ = 2.5%, 5% and 10%;

- Slit system/Slit separation: 4.20 m; slit opening adjustable between 0.5 mm and 8.0 mm;

- Detector system: State-of-the-art ^{10}B Multi-blade detector; 200x260 mm^2 active area; 640 wires and 1280 strips; possibility to operate 100x130 mm^2 area as 2D-detector; spatial resolution: 0.5 mm (wires) and 3.5 mm (strips); Digitizer and readout system: Athena + CAEN V1740D + JADAQ.

The Research Council of Norway is acknowledged for providing the financial support.

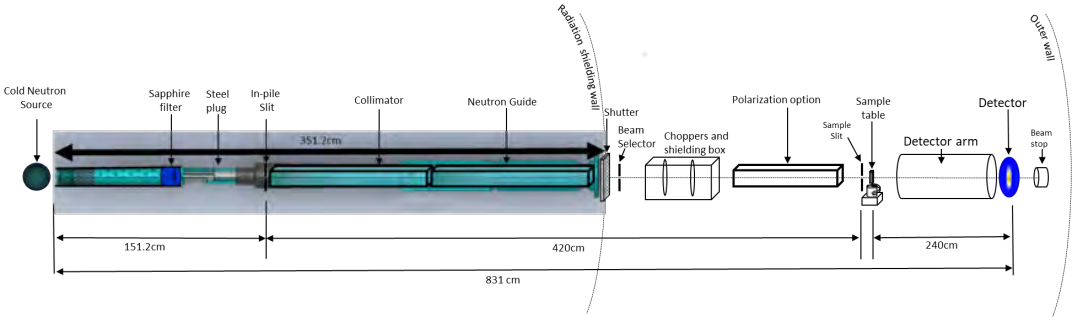

Fig. 1. Design concept for the neutron reflectometer FREYJA.

[1] www.ncneutron.no

Studies of the d-spacing distribution in powder alpha-Fe2O3 and CaCO3 by Larmor diffraction

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The neutron Larmor diffraction gives a possibility to measure the d-spacing distribution for a given (hkl) Bragg peak [1-3] with a resolution (Delta d)/d approximately 10^{-6}, i.e. better than with conventional X-ray or neutron diffraction. The d-spacing distributions in powder samples of alpha-Fe_2O_3 and calcite, $CaCO_3$ were studied with the Larmor diffraction method by using the triple axis spectrometer TRISP at Garching [4,5]. The measurements were performed with powder samples placed in cylindrical and rectangular-flat containers. The resulting d-spacing distributions are compared with the results of earlier synchrotron radiation (SR) powder diffraction studies of alpha-Fe_2O_3 [6,7] and $CaCO_3$ [8]. The d-spacing distributions obtained with neutron Larmor diffraction are broader than those obtained with SR diffraction [6-8]. One of the possible reasons of this broadening are spin-echo small angle neutron scattering (SESANS) effects [9]. This hypothesis is in agreement with Larmor diffraction results measured in containers with different shape. For this reason additional SESANS measurements in transmission geometry were performed. The Larmor diffraction data properly corrected for SESANS gives d-spacing distributions in agreement with those obtained from SR powder diffraction [6-8]. Larmor diffraction data shows that in both alpha-Fe_2O_3 and $CaCO_3$, the d-spacing distribution is described with a pseudo-Voigt function much better than with a Gaussian function.

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Design and features of the Engineering Diffractometer BEER at ESS

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The neutron time-of-flight engineering diffractometer BEER (Beamline for European Materials Engineering Research) is currently under construction at the European Spallation Source (ESS). The main tasks of BEER are to enable fast *in situ* and *in operando* characterization of materials and their microstructure during processing conditions close to real ones and to provide state-of-the-art and fast analysis of residual stresses, microstructure/crystallographic texture characterization and phase analysis. These tasks are supported by the instrument design. It enables, for example, to choose between a standard pulse shaping chopper technique or a newly developed technique called pulse modulation. The latter extracts several short pulses out of the long ESS pulse. Thus leading to a multiplexing of Bragg reflections and to substantial intensity gain for high symmetric materials while preserving the resolution. By the combination of both chopper techniques, BEER is a versatile engineering diffractometer providing easy tuneable resolution/flux ratios across wide wavelength and resolution ranges. Together with a large detector coverage, BEER enables sub-second *in situ* measurements for fast residual strain scans; texture analysis as well as phase analysis of complex composite systems where high resolution is needed. Advanced sample environments dedicated to thermo-mechanical processing, e.g. a quenching and deformation dilatometer, support these measurements. Here, we present the current BEER instrument design and its features, in particular the modulation technique.

The project of the spectrometer BRISPX

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BRISPX is a project for a Time-of-Flight (ToF) instrument to perform inelastic neutron scattering with thermal neutrons, aiming to access a wide (Q,E) region. The conception of BRISPX combines the experience gained with BRISP and an innovative low-divergence implementation of the time- focusing technique based on a double crystal monochromator scheme that will allow investigating low-Q dynamics in materials with higher flux, more flexibility and a reduced background compared to BRISP.
The Italian (CNR) and German (University of Marburg) spectrometer BRISP has operated at the ILL between 2007 and 2017, and it has been especially dedicated to the study of collective dynamics in disorderedand magnetic systems. It has been the first instrument worldwide fully devoted to the Neutron Brillouin Scattering technique, and is the state-of-the-art of neutron Brillouin scattering.

We present here the status of BRISPX, the upgrade project aiming at overcoming BRISP limitations, thus offering to the scientific community an instrument able to perform neutron Brillouin scattering in a more extended family of materials.

Observation of TOF-MIEZE signals with focusing mirrors at BL06 at J-PARC MLF

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In the study of condensed and soft matter, probing both spatial and dynamical properties of the sample is important. Neutron spin echo (NSE) measures intermediate functions of quasi-elastic scattering with the energy resolution that is independent of the beam monochromatization [1]. Neutron resonance spin echo (NRSE) is also a method for measuring the intermediate functions of a sample using resonance flippers and neutron-polarizing devices [2]. MIEZE (Modulated Intensity by Zero Effort) spectroscopy which has the two resonance coils with different frequencies uses intensity modulations in time for observing the quasi-elastic scattering from a sample [3]. This intensity modulation is unaffected by the depolarization at the sample position. No optical component are required between the sample and detectors. These characteristics makes the set-up and the sample environment more flexible. MIEZE spectroscopy has been testing for small angle neutron scattering and neutron reflection geometry [4, 5]. However, the energy resolution can be limited because of the sensitivity of the neutron path.

Recently, ellipsoidal neutron focusing supermirros, which enable the neutron path length distribution to be negligible small between the ellipsoidal foci, have been developed [6]. By using the focusing supermirrors in MIEZE spectroscopy, high energy resolution and better signal-to-noise ratio neutron-spin-echo experiments can be achieved. Focused neutron beam at the sample position can then be utilized to analyze very small samples. Polarization analysis can also be easily applied using well controlled scattered neutrons. In this instrument, the advantage of the MIEZE spectroscopy with time of flight (TOF) measurement at short pulse neutron source (TOF-MIEZE) is used [7]. The contrast of a TOF-MIEZE signal is robust against the misalignment of optical component.

In this presentation, we will report concept of focusing TOF-MIEZE spectroscopy and current status of the development at BL06 at J-PARC MLF. We also show the TOF-MIEZE signals with the ellipsoidal neutron focusing mirrors.

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Neutron Beam Tests of ESS Test Beamline Components

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Key components of the ESS Test Beam Line prototype equipment, developed in the frame of the Moderator workpackage of the EU-H2020 BrightnESS project have been tested on the Time of Flight Diffractometer Beam of the Budapest Research Reactor.

The instrument has been designed to perform energy selective imaging and brightness measurement of the low dimensional cold neutron moderator of the ESS long pulse neutron source [1]. A double disc chopper running at up to three times the source frequency serves for time structure investigations of the cold neutron pulses. Time stamped data acquisition of TBL chopper signals and neutron detection events allow sweeping through the pulse duration with free running chopper disks (phased only against each other) [2].

A beam with direct view of the BRR reactor core has been selected for the tests in order to verify the beam shaping efficiency against higher energy neutrons of the gross pinhole mask, attenuator and adjustable pinhole changer. The chopper system of the chosen beamline has been used to emulate the ESS long pulse operation. The continuous high energy component is subtracted during data processing.

A four-layer, double readout solid boron converter neutron detector with delay-line position encoding has also been developed and tested with the aim to achieve high neutron intensity tolerance, high count rate and reasonably good resolution. This detector is less sensitive for faster neutrons, hence more tolerant to high intensity T0 pulse (faster recovery than 3He).

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Development of a Miniture Polarisation Analysis Device

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Spherical neutron polarimetry (SNP) has been systematically developed and applied over the last decades since the cryogenic polarisation analysis device (CryoPAD) presented by Tasset et al. in 1989. This technique allows to determine all the nine components in the polarisation matrix at once and therefore to solve the Blume-Maleyev equations. The biggest advantage of SNP over conventional polarisation analysis methods is the ability to separate nuclear and magnetic contributions in the scattering processes even with finite nuclear-magnetic interference terms. Hence the magnetic properties, e.g. magnetoelectricity, non-collinear magnetic structures, different types of magnetic domain in antiferromagnetic structures, and commensurate and in- commensurate structures, can be finely determined. Inspired by the CryoPAD, the Mu-metal Polarisation Analysis Device (MuPAD) presented by Janoschek et al., and the following Mini MuPAD, introduced by Haslbeck and Kindervater et al., with a more compact form, we want to report on the currently being developed cylindrical Mini PAD. In comparison to the existing Mini MuPAD, the precession coils are bent into cylindrical shape around the sample, and the scattering angles are hence no longer restricted to be smaller than 10 ◦ . Furthermore, thanks to its size, it is simple to handle and can be combined with a cryostat.

Gd-loaded scintillation ceramics - a flexible detector material for neutrons

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Scintillators have several advantages as neutron detection material. They have high volumetric concentration of neutron absorber allowing compact and effective detectors. There are materials with fast kinetics among the modern scintillators, which allow detectors with high count rates. Finally, scintillation detectors are relatively cheap solutions, compared to alternatives. It was shown recently, that Gd-based scintillators of garnet family are efficient neutron detectors [1]. Ce-doped garnets demonstrate fast scintillation response with coincidence time resolution down to 165 ps, which make them perfect choice for time-of-flight applications. These compositions could be obtained either as single crystals or polycrystalline ceramics. The latter form gives additional advantages: ceramic materials could be cheaper than single crystals due to lower formation temperature; ceramics could be easier obtained in thin plates or complex shapes, which is beneficial for some applications, e.g. beam monitors; ceramics allows wider composition range within cubic solid solutions area, and so – wider possibilities for tuning of properties. This work deals with (Gd,Y)3Al2Ga3O12:Ce (GYAGG) ceramics. The powders were obtained using coprecipitation approach, compacted and sintered up to densities 98-99% in air or oxygen. Composition, microstructure and luminescent properties of the ceramics were studied. Both scintillation light yield and decay kinetics were found to depend on host composition – Gd-Y variation as well as (Gd+Y)-(Al+Ga) ratio deviation from the stoichiometric composition. Local optimum compositions are proposed. Scintillation properties of the obtained ceramics of different thickness were probed under gammas of 60, 511 and 662 keV and under 5,5 MeV alpha-particles. These are compared to previously obtained data on detection of neutrons from Am-Be source.

KOMPASS – the polarized cold neutron triple-axis spectrometer at the FRM II

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KOMPASS is a polarized cold-neutron three axes spectrometer (TAS) currently undergoing its final construction phase at the MLZ in Garching, Germany. The instrument is designed to exclusively work with polarized neutrons and optimized for zero-field spherical neutron polarization analysis for measuring all elements of the polarization matrix. In contrast to other TASs, KOMPASS is equipped with a unique polarizing guide system. The static part of the guide system hosts a series of three polarizing V-cavities providing a highly polarized beam with expected polarization about 98%. The exchangeable straight and parabolic front-end sections of the guide system allow adapting the instrument resolution for any particular experiment and provide superior energy- and ***Q***-resolution values when compared with the existing conventional guide and instrument concepts [1, 2]. In combination with the end position of the cold neutron guide NL-1, the large doubly focusing monochromator and analyzer using highly oriented pyrolytic graphite, the cavity of trapezoidal geometry for analysis of polarization of scattering beam, the KOMPASS TAS will be very well suited to study various types of weak magnetic order and excitations in variety of complex magnetic structures and indeed first successful experiments on chiral magnets or very small crystals could already be performed. Special emphasis was put on a compact design of the instrument in order to maximize intensity.

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SCATTERING KERNEL AND NEUTRON TRANSPORT PROPERTIES OF NANODIAMOND AT COLD AND THERMAL ENERGIES

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Nanoparticles are of great interest nowadays for science and technology. In particular, it has been shown that nanodiamonds could be efficient reflectors for very cold and ultra cold neutrons [1]. However, it is not clear what could be this material efficiency as reflector for neutron energies above 10^{-4} eV, although it was estimated that a high purity material (free from hydrogen contamination) could be of interest even beyond that energy [2]. We developed a scattering kernel and generated cross section libraries for bulk diamond and powders of nanodiamond, over the thermal and cold neutron energy ranges. The calculated cross sections are in very good agreement with recent experimental data [3]. The scattering kernel, including small angle scattering effects, was implemented in the Monte Carlo program OpenMC [4], and this tool was used to study the reflective properties of nanodiamond layers.

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Implementation of polarized neutron spectroscopy on TOF spectrometer NEAT at Helmholtz-Zentrum Berlin

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Time-of-flight spectroscopy with polarized neutrons is still not very common today, mostly because of the large reduction in flux caused by polarizing the beam. A substantial increase of the incoming neutron flux has been recently achieved at the time-of-flight (TOF) cold neutron spectrometer NEAT at Helmholtz-Zentrum Berlin as the result of a large scale technical upgrade [1]. The upgrade yields 75 – 300 fold gain in detected neutron count rate compared to the predecessor and opened up the opportunity for the polarized neutron spectroscopy implementation. The optional availability of polarized neutrons substantially expands research capabilities of a TOF spectrometer, e.g. in the investigation of magnetic excitations or cooperative phenomena in material science or soft matter.

In the implemented setup the polarization of the incoming neutrons is realized using a specially designed transmission polarizer with eight ‘V cavity’ channels. The channels have non-polarizing supermirror-coated, opaque side walls and neutron-transparent Si cavity plates, coated by m=3 polarizing supermirrors on both sides. The nominal operational wavelength band width of the polarizer is 2.5 – 8 Å, with measured polarization efficiency between 92 and 96 % for well collimated beam. The beam transmission efficiency for the preferred neutron spin state is about 65%. The neutron beam polarizer is placed inside a 3.8 m long evacuated neutron 'guide changer', which allows us to move into the beam delivery guide one of 3 alternative straight neutron guide sections mounted in parallel on a linear translation stage [2]. Polarization analysis is realized using 3He analyzer and system of coils in PASTIS like setup developed originally for TOF spectrometer TOPAZ at MLZ [3]. The setup has been successfully tested and applied for the investigation of bulk and confined water.

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Neutron Reflectometry at ILL on D17 and FIGARO: Recent Developments

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In this contribution we will show recent developments on the ILL neutron reflectometers D17 and FIGARO. We will start with recent upgrades on the vertical sample plane reflectometer D17 including the time-of-flight (ToF) polarized neutron reflectometry (PNR) option [1] and the installation of a new focusing guide allowing the more efficient use of a divergent beam for specular reflectometry [1,2]. Next we will show recent developments in using the large wavelength band on the horizontal sample plane reflectometer FIGARO for fast surface excess measurements on free liquids [3]. Finally we will present new sample environment capabilities like the liquid/liquid interface cells [4].

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Recent development of multilayer neutron mirror at KURNS

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Progress of neutron optical devices is very significant for neutron science and multilayer mirror is one of the most important devices for neutron beam handling.The Institute for Integrated Radiation and Nuclear Science, Kyoto University (KURNS) has a history of development of multilayer mirrors. There are an ion beam sputtering machine (KUR-IBS) for coating of advanced neutron optical device [1]. Recently we found promising fabrication method for aspherical focusing supermirror with metal substrate [2-4]. The metallic substrate is robust and ductile, to which able to fabricate steeply curved surface with high form accuracy. It is also applicable to use under high radiation irradiation and high-temperature filed, even at a place close to the neutron target and moderator. Furthermore, it is possible to fabricate a large focusing mirror by combining multiple segmented mirrors with mechanical fastening entailing the usage of screw holes and fixture tabs. The big problem was required surface roughness for neutron mirror. The roughness should be smaller than 0.3 nm for high-m supermirror coating. Here m is the maximum critical angle of the mirror in units of critical angle of natural nickel. By using electroless nickel-phosphorus (Ni-P) plating, we overcame the problem and are establishing fabrication process for aspherical focusing supermirror. We fabricated ellipsoidal metallic substrates with the Ni-P plating, based on the technology using ultrahigh precision cutting with correction processing, followed by mechanical precision polishing.

We fabricated several couples of NiC/Ti ellipsoidal supermirrors in which length of 900mm. The semi-major and semi-minor axes of the ellipsoidal supermirror were 1250 mm and 65.4 mm, respectively. The acceptable angle of the minor axis arc of the ellipsoidal supermirror is 20 degree [5].These ellipsoidal supermirrors were installed to neutron resonance spin echo spectrometers (VIN ROSE) at BL06 at J-PARC MLF [6,7].We also fabricated flexible self-standing multilayer sheets. We will show these recent developments and perspective of multilayer neutron mirrors at the KURNS.

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HUGINN: PELTIER-BASED TEMPERATURE CONTROLLED SAMPLE PLATFORMS FOR NEUTRON SCATTERING

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The RUC/ESS Huginn project uses Peltier elements to improve temperature stability and decrease thermalization time compared to conventional sample environments used in neutron scattering. The ability to change temperature fast becomes increasingly important at ESS, with greater neutron brightness and therefore shorter measurement time. Furthermore, the ability to rapidly change temperature of the sample will open new possibilities such as:

Studies involving time resolved measurements which are performed on processes that start when the sample is moved to a given temperature, i.e. physical aging, crystallization, water uptake or chemical reactions. It also becomes possible to access new meta-stable phases of the investigated substances. Finally, studies of glass-forming liquids and other system with strong temperature dependence will benefit greatly by the increased stability and precision of the sample temperature.

We present design and prototype tests of two Peltier element based sample holders:

- A sub-cryostat insert for top loading cryostats, for use with general purpose sample cells.
- A multiple temperature SANS sample environment based on individually controlled Peltier elements.

The sub-cryostat insert has the following key performance parameters:

- Very fast temperature changes, typically a few minutes for 10-20K temperature changes.
- The possibility to change the sample temperature by at least 10K from the main-cryostat (at overall temperatures down to 150 K).
- An improved temperature stability compared to the main-cryostat by at least an order of magnitude (in most cases two orders of magnitude).
- A working temperature range from 100K to 370 K.

The multiple temperature SANS sample environment has the following performance parameters:

- Individual cuvettes can have a temperature difference from the base temperature of at least 30 K.
- Temperature changes of up to 30K can be achieved within a few minutes.
- The temperature is stabilized within 10-100 mK.

Altogether we demonstrate that Peltier element based sample environments is able to decreases thermalization time and improve temperature stability. The two sample environments presented will be available at the ESS, and can easily be adopted to other facilities. We are particularly interested in finding collaborators to use this equipment for experiments at existing facilities.

Developping a High Resolution Focussing Configuration for the Pitesti TRIGA Reactor Neutron Diffractometer

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A Q-space focussing configuration is characterized by high-resolution even when no spatial focussing exists at sample position or anywhere else or is used quite open beam without any Soller collimators; only coarse collimators should be used to reduce the background level. This is possible just by decreasing the scan variable variances.

The following steps should be followed: to define the scan variable / to define the significant spacial variables as are the monochromator and sample with for example / to express the scan variable, using specific geometry characteristics and existing correlation between variables, through the spatial variables / to cancel the significant contributions to the scans variable variances by cancelling the important variables coefficients, from the scan variable expression; *when correlation between variable exists*, as is the case for these kinds of experimental configurations, such a coefficient has more than one term, not all of the same sign, appearing the possibility to be cancelled and therefore to cancel entirely the corresponding contribution of this spatial variable to the line-width

The Crystal Diffractometry . One Crystal monochromator

For this geometry, following the above-described procedure and canceling the l_m coefficient, one obtains:

$$R_m=(2a)/(2a-1)[L\,sign(\Theta_m+x_{sm})]/[\sin(\Theta_m-x_{sm})] \quad \text{where} \quad a=-\tan\theta_s/\tan\theta_m \text{ and } sign\alpha=abs\alpha/\alpha \qquad (1)$$

Cancelling the "l_s" coefficient one obtains:

$$\tan x_s=\cot\Theta_s\{1-2/[1+(2a-1)L_2/L_1]\},\quad \cot\dot{\alpha}_s[\cos2\Theta_s-(2a-1)L_2/L_1]/\sin2\Theta_s],\quad \alpha_s=\chi_s+\theta_s+\pi/2 \qquad (2)$$

where α_s as the inclination angle measured from the monochromatic beam direction.

The (2) condition is fulfilled if the sample is rotated during the experimental diffraction pattern raising. The (1) relation is the condition to cancel the monochromator width contribution to the line-width. But as the crystal reflectivity is strongly dependent on the radius of curvature, is not possible to be changed during the diffraction pattern raising; this would lead to a significant variation of the incident beam intensity and no data processing is possible in this situation. It is convenient to keep the monochromator radius of curvature constant, at a value corresponding to that given by (4) for a scattering angle 2q, in the range 90-110 degrees, where the overlapping problems are the mosnt significant and therefore the line-width should be minimum. A value of around 10m for the monochromator radius of curvature is quite convenient, giving a minimum line-width of 12-15 minuted and not more than 25 minutes for the rest of the scattering values.

But is not necessary that the sample to be rotated for every scattering angle, at the position given by (1) , the resolution is still very good even for a range of 20^0 around the scattering angle for which the sample is in the optimum position; if still a better resolution is desired, the detector angular width can be lowered at 15^0; that means that the diffraction pattern can be got from 5-7 steps. With such an approach, a position sensitive detector can be used.

New Rietveld program suited for processing patterns recorded with a inverse-space focusing neutron diffractometer equipped with position sensitive detector

The program is divided in six modules that can be run independently. These have their own input file and provide output files that could be input files for other modules. Five modules prepare a lot of input files for the main module. Besides these files the main module reads its own input file containing the fitting parameters and the file containing the measured diffraction pattern which is further processed by the Rietveld method. The main module provides an output file with the refined parameters and various quantities of interest (sample transmission, texture pole figures, peak shifts, peak FWHM, amplitude of structure factor) and a number (at choice) of files for graphical representation. In order for the instrument to become functional, a suited position Sensitive detector and the corresponding soft, should be procured

From IN8 to THERMES – development of the thermal three-axis spectrometer at ILL

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The three-axis spectrometer IN8 offers to ILL users advanced conditions for studies of thermal excitations in single crystals and liquids. The instrument performance and flexibility are ensured by the use of large double-focusing monochromators and analysers providing high counting rate even for small and low-scattering samples. The new monochromator unit has been recently commissioned. The device is the fruit of the experience accumulated in the former TAS-group at ILL in using Bragg-focusing beam optics with independently variable and remotely controlled horizontal and vertical focusing (bending) of the crystal reflecting planes. The new monochromator for the thermal neutron beam considerably outperforms the previously used one. It consists of 4 different exchangeable crystal planes. The two planes are built from mosaic crystals of pyrolytic graphite and copper with the principal reflections *PG002* and *Cu200* chosen to provide a broad range of monochromatic neutron wave vectors and energy resolution of the incident beam. The other two planes are assembled with elastically bent perfect silicon crystals set to make use of the reflections *Si111* and *Si311* with prohibited second-order diffraction harmonics. The mosaic crystal planes are used in experiments requesting maximum monochromatic intensity at the sample position and variable resolution. The silicon crystal planes, with similar to mosaic crystals available resolution range, provide particularly “clean” conditions for experiments with multi-analyser configurations (such as *FlatCone*, for instance) at the expense of marginally lower monochromatic flux. The following step in renovation of the spectrometer is the ongoing construction of the classical single-detector secondary spectrometer set-up called *THERMES* (*THERM*al *E*xcitations *S*pectrometer). The new instrument benefits from a compact design that permits a larger accessible dynamic range (wider available angular ranges in the existing experimental zone) with particular attention paid to neutron shielding including special construction of the detector diaphragm. The manufacturing of the instrument mechanics is actually finished. We hope to assemble and make first tests of the new equipment in the coming months. Further development of specific sample environment for this spectrometer is under way.

The SoNDe high-flux neutron detector

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The Small-K Advanced DIffractometer (SKADI) is a joint in-kind project of French and German partners to deliver a SANS instrument to the ESS.[1] This contribution will detail the current development status of SKADI, highlighting the final changes before the construction phase. In addition, further practical requirements for performing experiments, such as sample area and environment will be considered. The SKADI is designed to deliver

- Flexibility (sample area is approx. 3x3 m2, and versatile collimation)
- Very small Q accessible through VSANS (using focusing collimation elements)
- Polarization for magnetic samples and incoherent background subtraction
- Good wavelength resolution, being the longest SANS instrument at ESS
- High dynamic Q-range over three orders of magnitude (using two detectors).

This will be combined with a neutron flux of 8E8 neutrons/s cm^2 at sample position, which will make it the world's brightest SANS instrument.

SKADI is a versatile SANS instrument, which will enable scientists to perform a wide range of investigations on topics requiring small scattering angles to access long length scales. The scientific areas targeted by SKADI include investigations of **smart materials**, **biological** and **medical research**, **magnetic materials** and **materials for energy storage**, as well as experiments on **nanomaterials and nanocomposites or colloidal systems**. These experiments promise a high potential impact on science and society. To maximize the societal applicability of these studies SKADI is designed to accommodate **in-situ measurements** with custom made sample environments to provide **"real-world" conditions**.

In addition to being uniquely accommodated to complex sample environments SKADI will also feature a newly developed detector system, **SoNDe[2]**, which is developed within the EU Horizon2020 framework (funding reference No. 654124). This detector system will enable to use the hitherto unachieved flux of the ESS to capacity. While still being in the development stage, the current versions already outperform current detector technologies by a factor of four in terms of usable neutron flux.

This will be combined with a new resolution selection system that will allow SKADI to achieve high-resolutions, which could not be used before in SANS, as well as tune the resolution to the experiment at hand.

These features, **accommodation of a wide range of custom sample environments, full use of the neutron flux available at the ESS using a newly developed detector system and versatility in terms of resolution selection**, put **SKADI** in a position **on-par or better than any current world class SANS instruments** from the first day of operation. They will allow SKADI to cater for the needs of a wide range of scientists, making it an ideal choice to support the early success strategy of the ESS in order to achieve a high publication record during early operation.

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Design of the new guide for the time-of-flight spectrometer Focus at SINQ

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Focus is a direct geometry cold neutron time-of-flight spectrometer at SINQ [1]. Within the present SINQ Upgrade project, Focus will get a new guide, while the rest of the instrument remain unchanged. The new guide will provide significant intensity increase across the whole spectrum (e.g. gain factor increasing from 2 to 6 at 6 to 2Å, respectively). The main benefit comes at 2Å from the increased m value of the coating, whereas at 6Å from the new ballistic shape. Guidebot has been used for a rough survey, whereas final optimization has been performed by mcoptimize, a particle swarm optimization routine on top of mcstas, which was kindly provided by Markus Appel, ILL. The challenging part is the “potato shape” of the curved section in the horizontal plane, which obeys an analytical restriction to avoid direct line-of-sight. The coating was optimized by the same routine aiming for the best cost-performance ratio. The upgraded instrument will start operation in 2020.

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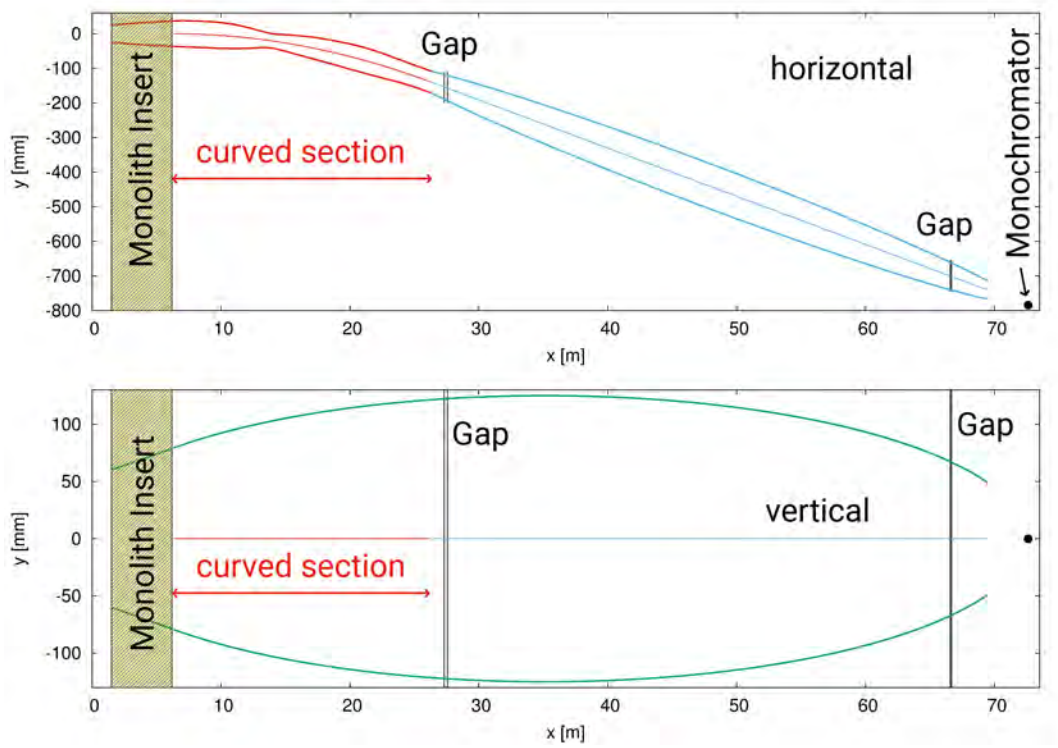

Visualization of the boron distribution in simulated melted core material by neutron energy resolving method

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The energy resolved neutron imaging system RADEN, installed at the Japan Proton Accelerator Complex (J-PARC), utilizes short-pulsed neutrons in the energy range from meV to keV by means of the time-of-flight method. The wide neutron energy range makes it possible to adjust neutron attenuation of a sample to suit a particular measurement by selecting the neutron energy range. Especially, this adjustability is attractive for visualizing such nuclides as boron-10 and lithium-6 owing to the fact that their cross sections decrease with the inverse square root of the neutron energy up to higher than keV. The authors expected that such a feature would be one of the advantages of RADEN, and have started developing a method to visualize boron distribution using energy-resolved neutrons.

The Core Material Melting and Relocation (CMMR) experiments have been performed to investigate core melt accidents in the Fukushima-Daiich (1F) nuclear power plant. Some amount of boride was found to be contained in simulated melted core material [1]. This led to a concern that the hardness of the boride compounds would present difficulties for cutting the fuel debris in decommissioning of 1F. The high neutron absorption of boron also raised a concern of recriticality after separating boride from the debris. The estimation of these effects from boride in the real debris is of great importance to develop safe debris removal plans. A method to measure the boron distribution in simulated melted core materials, to be brought about by RADEN, is essential to improve the reliability of the estimation of boride content in the real debris.

In this presentation the authors show the status of the development of a method utilizing energy-resolved neutrons and demonstrate some measurements of boron-containing samples, including simulated melted core material.

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New control system for single crystal diffractometer MOND at reactor IR-8.

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The diffractometer MOND is installed at the thermal neutron beamline at research reactor IR-8 at NRC “Kurchatov Institute”. MOND had been designed for the study of single crystals using a 5-circle goniometer and a double monochromator, which provides monochromatic neutrons with variable wavelength. The old instrument control system limited the ability of MOND for solving chemical and crystallographic tasks that require fast scanning of a large number of Bragg reflections.

The control system hardware is based on ONITEX step motor controllers and LIR916 absolute encoder controllersfor new step motors and 16-bit encoders.

Indexing of a unit cell, calculation of the UB matrix, angular coordinates and interval of scanning of Bragg reflections in the new control system are based on the mathematics of the SAD-5 software complex for the X-ray diffractometer RED. This software complex was modified for neutron diffraction and successfully exploited in the neutron single-crystal diffractometer at the WWR-c reactor of Karpov Institute. Maths has been integrated into a new software package written in LabView. It provides motion control of the goniometer axes and data collection by detectors. The interface has also been written in LabView.

A new control system of the diffractometer MOND has successfully passed the commissioning phase.

This work was performed using the equipment of Unique Scientific Facility "NRC IR-8" and was supported by grant RFBR 18-32-20050.

Large Phase Space Extraction with High Time Resolution at ESS

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At the European Spallation Source (ESS) a low-dimensional so-called butterfly moderator will be installed (see Fig. 1) [1]. The paths of the cold neutrons with high divergence cross each other inside the monolith. Looking from the direction perpendicular to the axis of the cold moderator both sides of the cold moderator are visible. We optimized a guide system accepting the neutrons from both moderator (see Fig.2.) by extracting two separate beams, and later merge the beams together with little loss in intensity and little decrease of the brilliance during the neutron transport. Another advantage of this guide geometry is the possibility to improve the time resolution of the pulse-shaping chopper due to the reduced guide width – like the so-called Bewley splitter [2] at LET and NEAT chopper spectrometers. Furthermore, the narrower neutron guide implies a shorter length of the guide through which there is no line of sight. The neutron guide geometry used to stitch the neutron beams [3] substitutes for the linearly diverging section of a ballistic guide. The neutron guide system described above is useful for high resolution instruments at long-pulse neutron sources where a pulse-shaping chopper is needed to provide high time resolution like MIRACLES at ESS [4]. In my presentation the newly developed guide system with the existing guide of MIRACLES instrument will be compared.

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Fig.1. The geometry of butterfly moderator

Fig.2. The geometry of the guide system

Unconventional neutron guides for horizontal sample reflectometers

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Using horizontal focusing can significantly increase the flux on the reflectometer with a vertical plane scattering. Usually one tries to use a guide as wide as possible. Unfortunately, in practice, extracting wide beam from the reactor is difficult, given the lack of space at the face of a beam tube.

A valuable option could be to take the full-height beam (which is usually several times larger than maximal possible width) and then to rotate it by 90 degrees in the lateral plane. This transformation could become possible using inclined reflecting surfaces in the neutron guide and different approaches can be realized. We considered the two particular cases to achieve that: twisted guide and octagonal one.

Twisted guide was earlier developed for REFSANS instrument at the FRM-II facility in Munich[1,2]. Octagonal guides were mainly used for homogenization of beam divergence[3,4] or kind of beam shaper[5]. In our case, following the earlier proposal by Gaehler, such geometry is used to change adiabatically the shape of the guide and tilt it towards the end.

We have made a detailed mesh grid to describe geometry and made McStas calculations using guide-anyshape component. Optical properties and best configurations were determined for each type of guides.

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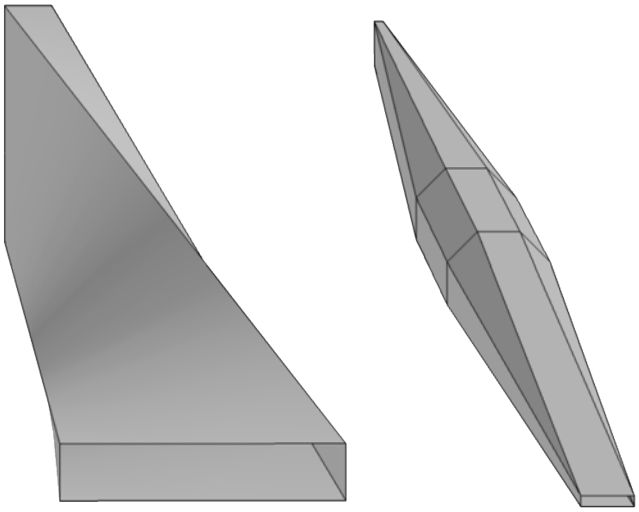

NCrystal : a library for thermal neutron transport

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An open source software package, NCrystal[1,2], for modelling thermal neutron transport is presented. Originally developed to support instrument simulations at the European Spallation Source, the code facilitates Monte Carlo-based transport simulations and focuses in the initial release on interactions in both mosaic single crystals as well as polycrystalline materials and powders. Both coherent elastic (Bragg diffraction) and incoherent or inelastic (phonon) scattering are modelled, using basic parameters of the crystal unit cell as input.

Included is a data library of validated crystal definitions, standalone tools and interfaces for C++, C and Python programming languages. Interfaces for two popular simulation packages, Geant4 and McStas, are provided, enabling highly realistic simulations of typical components at neutron scattering instruments, including beam filters, monochromators, analysers, samples and detectors.

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The MEPHISTO beam port for nuclear and particle physics at FRM II

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The beam port MEPHISTO at the FRM II is dedicated for mostly long term experiments in the field of nuclear and particle physics. The first planned instrument at MEPHISTO is PERC, an intense source of free neutron decay products. The author will present an overview of the parameters of the cold white neutron beam and its experimental area in the new east hall. The values are based on the already existing neutron optics components, including the neutron guide. The existing additional equipment (as shielding) awaiting the installation at the reactor within the next year. A first light at the instrument is awaited soon.

Observation of Slow-Neutron Diffraction from Holographic Nanodiamond Composite Gratings

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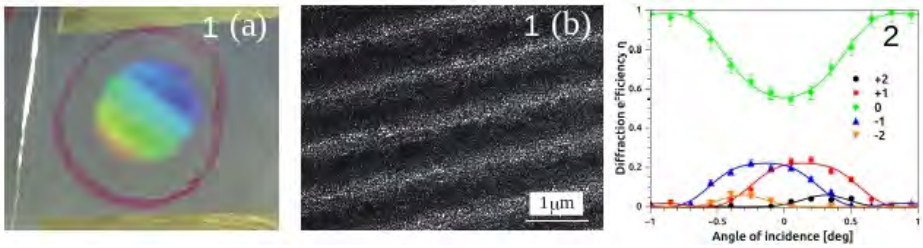
Photopolymerizable nanoparticle-polymer composite (NPC) is a photonic nanocomposite material consisting of photopolymer dispersed with nanoparticles (*e.g.*, SiO_2 and ZrO_2) [1]. The distribution of dispersed nanoparticles can be manipulated holographically by light. This technique, the so-called holographic assembly of nanoparticles in polymer [2], enables us to perform the single step formation of large area photonic lattice structures for photonic applications such as holographic data storage, holographic diffractive elements and nonlinear optics [1]. Previous experiments have shown that holographic NPC gratings can control slow-neutron (cold and very cold neutron) beams as well [3]. In principle, the diffraction efficiency (DE) can be readily increased by increasing the grating thickness. However, this -- in turn -- also decreases the rocking curve width. The resulting high angular selectivity is detrimental to the use of holographic gratings for slow neutrons for low-flux applications like interferometry. A possible solution is to maximize the DE by using nanoparticles with suitable neutron optical properties (large coherent scattering length density, low incoherent scattering cross section, low absorption), like nanodiamonds (NDs) [4], at moderate grating thickness. Here we report for the first time on slow-neutron diffraction from ND-dispersed holographic NPC gratings [5] with very large neutron-refractive index modulation amplitudes. Their properties can provide for an increase of the DE with relatively thin gratings, at desired low angular selectivity. Figure 1(a) illustrates a photograph of an ND composite grating (approximately 1 cm in diameter) recorded in an NPC film sample dispersed with 19 vol.% NDs. Figure 1(b) shows a transmission-electron microscope image of the cross section of the corresponding grating. The dark (bright) banded areas correspond to high concentration portions of NDs (the formed polymer), confirming holographic assembly of NDs in the formed polymer. Figure 2 shows a rocking curve exhibiting up to the 2nd diffraction orders measured at a mean wavelength of about 4.5 nm. Curve fitting by the rigorous coupled-wave analysis (RCWA) [6] is also shown (solid lines). We find that the DE can reach ~22 % from an NPC grating of only ~73 microns effective thickness.



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Interfacing multiple simulations using Monte Carlo Particle Lists, MCPL

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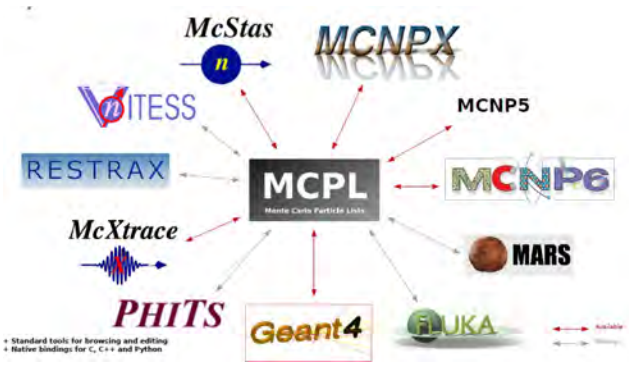
Simulations of neutron scattering instruments entail a wide range of different software suites, each with its own strengths and tailored to specific domains. For example, MCNP is conventionally used to describe the liberation of neutrons through spallation and their moderation, ray-tracing codes such as McStas model the transport of neutrons through optics while Geant4 models the neutron detectors. Using different tools in different facility domains generally tend to degrade the simulation accuracy, since details are lost at each transition. To resolve this the Monte Carlo Particle List (MCPL) toolkit [1] was developed. MCPL allows for the individual neutron state parameters to be transferred in-between codes, hereby facilitating the use of multiple software without loss of accuracy. MCPL thus has the potential to replace the multitude of ad-hoc interface solutions which exist throughout the neutron scattering community.

The basic idea is that users of the various frameworks can simply use those pre-existing and validated converters in order to carry out their work. Once a converter to/from a given code to MCPL has been prepared, any user can transfer neutrons (or any other particle) to/from any other software equipped with MCPL converters.



Overview of existing and (some) foreseen converters.
Vitess support available from version 3.4 (Nov 2018).
Support will be included in upcoming RESTRAX/SIMRES release (2019).

During the presentation, the structure of the software framework will be outlined and several examples of the use of MCPL in data analysis will be shown.

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Control of thermal neutron and hard X-ray beam parameters under external influences

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The development of new methods for the generation of monochromatic beams of thermal neutrons and hard X-rays with controllable in space and time parameters, e.g. angular divergence and monochromaticity, is stimulated by the requirement of creation of more sensitive and universal methods for the research in different areas of science and technology.

One of these methods is the diffractometry of radiation of angstrom order wavelengths formed under the presence of external influences. The presence of external acoustic fields or temperature gradient in the crystal monochromators enable to control the parameters of diffracted neutrons and X-ray radiation in space and time. It was experimentally shown that under the influence of temperature gradient the angular width of fully pumped X-rays is directly proportional to the thickness of the quartz single crystal. As the thermal neutrons (the absorption length ~50 cm) are absorbed much less as compared with X-rays, one can separate from a primary beam a neutron beam with large spectral and angular width used quartz crystal of several centimetres thickness with a temperature gradient or acoustic field. Taking into account the fact that a neutron De Broglie wavelength is comparable with the wavelength of electromagnetic radiation in the X-ray range, the expected effects for neutrons should be the same as for hard X-rays, for which absorption is also small.

In this work, aiming to obtain basic elements of hard X-ray and neutron optics with controllable parameters, we consider the principles and features of the reflection of hard X-rays from quartz single crystal in Laue geometry under the influence of temperature gradient. It is experimentally proved that, depending on the value of the temperature gradient, the intensity of the reflected beam can be increased up to several orders for reflecting atomic planes (10-11). We show that with an increase of the temperature gradient the focus becomes closer to the crystal, the focal spot becomes narrower in the diffraction plane and the integral intensity increases tenfold. Reflection of thermal neutrons beam from the Quartz single crystal in the Laue geometry under the external influences was investigated theoretically. The possibilities and estimation of the time-spatial control of neutrons beam parameters (relative maximum intensity, angular and energy distributions of receiving beams, etc.) are analyzed.

This work was supported by the RA MES State Committee of Science and Russian Foundation for Basic Research (RF) in the frames of the joint research project SCS 18RF-142 *and RFBR* 18-52-05024 Arm_a *accordingly.*

URANOS - a voxel engine Neutron Transport Monte Carlo Simulation

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URANOS (Ultra RApid Neutron-Only Simulation) is a newly developed 3D neutron transport Monte Carlo for the thermal to fast regime. Emerging from a problem solver for detector development [1] in collaboration with environmental physics [2] the project aims towards providing a fast computational workflow and an intuitive graphical user interface (GUI) for small to medium sized projects. It features a ray-casting algorithm based on a voxel engine. The simulation domain is defined layerwise, whereas the geometry is extruded from a pixel matrix of materials, identified by specific numbers. Therefore, input files are solely a stack of pictures, all other settings, including the configuration of predefined sources, can be adjusted by the GUI.

The scattering kernel features the treatment of elastic and inelastic collisions, absorption and absorption-like processes like evaporation. Cross sections, energy distributions and angular distributions are taken from the data bases ENDF/B-VII.1 and JENDL/HE-2007. In order to simulate multi-layer boron detectors it also models the charged particle transport following the conversion by computing the energy loss in the boron and its consecutive layer. The electron track is then projected onto a readout unit by longitudinal and transversal diffusion.

URANOS is freely available and can be used to simulate the response function of boron-lined or epithermal neutron detectors, small-scale laboratory setups (both shown below) and especially transport studies of cosmic-ray induced environmental neutrons.

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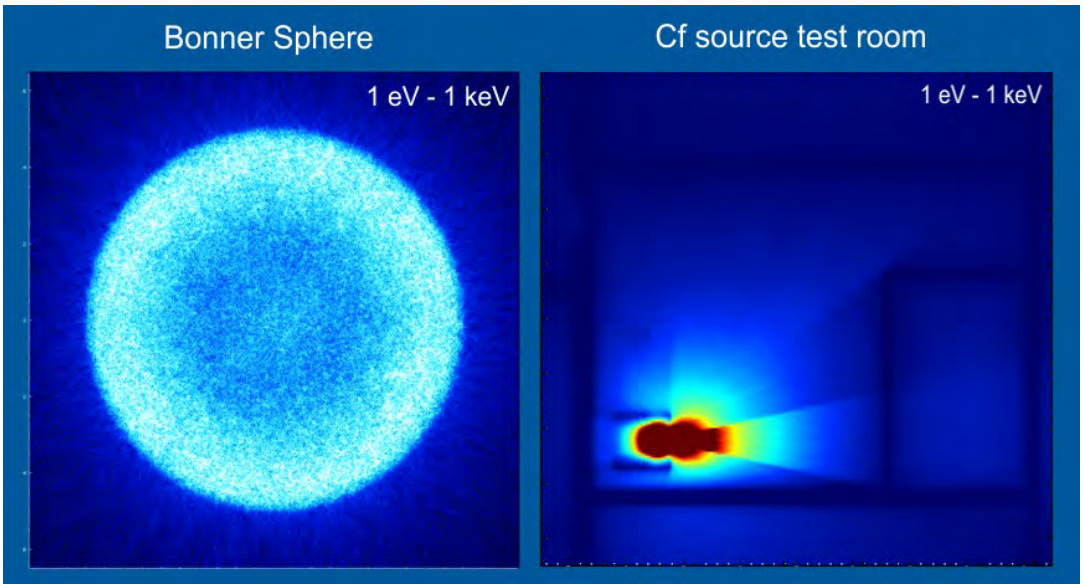

Prompt gamma shielding of neutron guides from ray-tracing Monte-Carlo simulations

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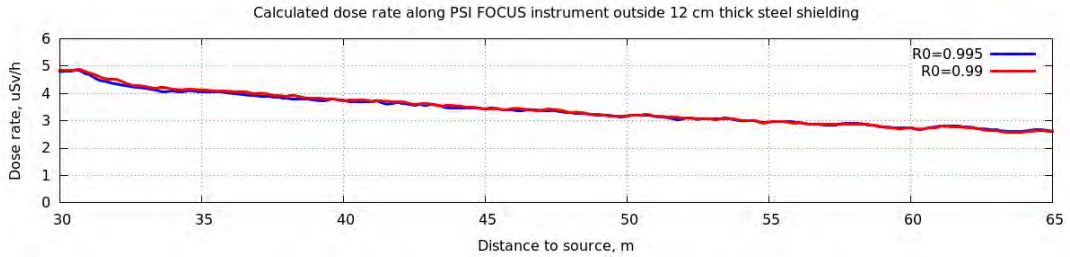
Use of neutron guides with multilayer supermirror coatings nowadays becomes common at most neutron scattering facilities. They provide a significant gain in neutron transport compared to the nickel coated guides due to *m*-fold increase in the angle of total reflection from the guide walls. The guides currently designed for the instruments at the European Spallation Source have values up to $m = 5$.

Absorption in the guide coating upon specular reflection is one of the major loss mechanisms during the neutron transport. It releases photons with energies up to 9-10 MeV which make up one of the major sources of ionizing radiation around the neutron guides, especially those with high *m*-value coatings. An accurate evaluation of this contribution by pure means of transport Monte-Carlo codes commonly used for shielding applications is currently not possible as they are not capable of treating coherent scattering of thermal neutrons in the multilayers [1].

A novel approach to evaluating the dose rates around the neutron guides will be presented. It is based on results of a rigorous calculation of the neutron absorption probabilities in commercially produced supermirrors [1] with some further developments and makes use of Scatter Logger component collection for McStas ray-tracing simulation package [2]. The Scatter Logger was extended to incorporate neutron absorption probabilities and to record capture rates of neutrons in materials of the coating along the guide. The numbers can be used to construct a source description for a transport Monte-Carlo simulation. Equivalently, the dose rate outside the guide shielding can be evaluated analytically using data on prompt photon spectra, linear attenuation coefficients, flux to dose and build up factors available from literature. This possibility was realized in supplementary McStas components.

Calculated dose rates from prompt gamma radiation agree with measurements at the Paul Scherrer Institute (Switzerland) where the overall dose rate from gamma radiation reaches 5 μSv/h outside 12 cm steel shielding of the guides beyond 30 m from the source [3]. The approach is currently used in the design of neutron guide shielding at the European Spallation Source [4].



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Progress in simulating realisation SESANS at the reactor PIK

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SESANS is a Spin-Echo (SE) Small-Angle-Neutron-Scattering (SANS) method with wavevector transfer $\boldsymbol{Q}$ ~10^{-6}-10^{-3} nm^{-1}, in regions with magnetic field $\boldsymbol{B}$, shaped as *parallellograms* with ''top angle'' $\theta_0 < 90^o$. The depolarisation of the beam due to scattering in a sample with inhomogeneous density is measured as a function of the parameter *spin-echo-length* δ which is set by the ''technical'' parameters of the setup: neutron wavelength λ, magnetic field $\boldsymbol{B}$ and length. SESANS is applied in materials science in samples with inhomogeneities 10^2-10^4 nm. Examples are: phase transitions, defects, porosity, clusters, (biological) nanostructures, membranes, colloids, etc [1].

In the past 6 years we made software for calculating the precession and the ''collected precession phase'' along **one trajectory** through a SESANS setup (**prototype exists**) without sample, made up of 2 regions with 2 *adiabatic/ RF/ gradient flippers* each. Precession is written as a progressing product of (3´3) rotation matrices of the polarisation vector for successive steps along the trajectory. The software is **modular**: all flippers are treated similar (in the ''rotating frame''): the input is the end matrix of the preceding flipper; the input for flipper 1 is the (3´3) Identity matrix. A trajectory is defined by the parameters {direction [ψ,ζ], *vertical* start position z_0, and λ}. At given [ψ,ζ] the *horizontal* start position y_0 is irrelevant since the final precession phase hardly depends on y_0.

For a **beam** the final matrix of many trajectories is averaged, varying {[ψ,ζ],z_0} over the range imposed by lay-out. Due to inhomogeneity of the field $\boldsymbol{B}$ *measured* in our flippers, this matrix departs from unitary. One diagonal element (corresponding to an axis $\boldsymbol{B}$) is evaluated as a function of extra precession through a ''phase coil'' in one field region. The amplitude of this ''signal'' is the empty-beam polarisation $P_0(\lambda)$.

To transform $P_0(\lambda)$ to $P_0(\delta)$, we convert λ to spin-echo-length δ, using the relation $\boldsymbol{\delta = \Delta\varphi / Q \equiv \lambda\, \Delta\varphi/4\pi}$ between δ and the *precession-offset* Δφ from SE. Δφ is obtained from a simulation in which we assume scattering in a ''sample'' with *given* wave-vector transfer $\boldsymbol{Q}$ [2]. In our prototype with {cot θ_0=1.5, *net* length=4.5 m and RF=1.0 MHz ($\boldsymbol{B}$=0.034 T)}, wavelength λ=1.0 nm converts to δ=10.8 μm. With (10´10)mm^2 windows 4.5 m apart, we get $P_0(\delta=10) \sim 0.25$. For our prototype, when installed in a beam of PIK (λ certainly exceeding 1.4 nm) it implies that **we can access δ >20 μm**.

At present we are including a **polarisation rotator** ''installed'' in the stray field of a mirror polariser with vertical field, to get the polarisation vector $\boldsymbol{B}$ for any λ, as required for measuring SE. It results in an input matrix, different from the Identity matrix. A similar rotator must be ''installed'' at the analyzer side.

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In situ Thin Film Growth Capabilities for Polarized Neutron Reflectometry

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(The talk is based on the presenter's work at TU Munich before joining GTIIT)

Thin magnetic films and heterostructures thereof are the basic building blocks of a large number of magneto-electronic devices whose fabrication is almost exclusively based on thin film deposition techniques. Because sample structure, stoichiometry, and defect population are defined by and evolve with the deposition process, their precise control and optimization are of great importance. It is, hence, highly desirable to directly analyze the development of the physical properties of magnetic heterostructures, e.g. the magnetization, during the growth process and to correlate them with the structural parameters of the sample. While, the *in situ* characterization of thin films by electron- and photon-based probes as well as by scanning probe techniques is common practice, the *in situ* measurement of the magnetic properties of thin films using (polarized) neutron reflectometry ((P)NR) is an extremely challenging task. The collaborative effort between TUM, University Augsburg and MPI Stuttgart in constructing a mobile sputtering facility for the growth and *in situ* monitoring of magnetic multilayers, which can be installed at suitable neutron beamlines, will be presented: In particular, the current state in development will be shown, ranging from unpolarized and polarized proof of principle neutron reflectivity measurements on Ni/Cr and Fe thin films carried out at the ToF reflectometer REFSANS at the FRM II neutron source to the latest fast *in situ* PNR measurements at the AMOR beamline at PSI. For the latter, the "Selene" neutron optical concept, based on elliptic neutron mirrors is essential. An overview over the latest developments and future modifications as well as the completion work carried out to allow the setup to be applied for even broader scientific research will conclude the talk.

Development of a new wide-aperture backscattering detector (BSD) for the HRFD diffractometer on IBR-2 facility.

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The High-Resolution Fourier Diffractometer (HRFD) developed in the framework of collaboration between FLNP JINR (Dubna), PNPI (Gatchina) and VTT (Espoo, Finland) has been operating at the IBR-2 reactor since 1995. In the past few years, some of the key units that became morally obsolete or worn out, have been replaced. Specifically, in 2016 a new mirror neutron guide and fast Fourier chopper were put into operation and in the previous years there was a complete replacement in the data acquisition and experiment control electronics.

At present, the most important element of the program for further modernization of HRFD is the replacement of existing backscattering detectors with a new version.

The new detector has a ring structure reflecting the axial symmetry of neutron scattering by the sample. The detector comprises 6 rings of scintillation screens.

The detector rings provide $2\theta=133°–175°$ continuous coverage with a total solid angle of ~2.0 sr (12.5 times greater than the existing one). To increase the efficiency of neutron detection, two layered screens will be used. In this case, the average detector efficiency (for $\lambda=1.8$.) will be from 65 up to 96%, for the inner and outer rings, respectively. Calculations suggest that the detector contribution to the geometrical component of the resolution function will be around 0.0002 for all rings.

Current status of neutron reflectometer at HANARO

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The neutron reflectivity measurement and analysis technique is a method of studying the structure of the thin film in the vertical and horizontal directions by measuring and analyzing the neutron specular and off-specular reflection occurring at a low angle of incidence on the surface of the thin film sample. By using the strength of neutrons as a probe, it has been developed as one of the most powerful technologies for searching the surface and interfacial structure of thin films in various fields such as polymers, dielectrics, magnetic materials and semiconductors. The neutron reflectometers have been widely used for researching thin film structures in various fields as mentioned above as a means for implementing such technique. In Korea Atomic Energy Research Institute (KAERI), a REF-V which is a vertical type neutron reflectometer is currently operating on the CNLB(cold neutron laboratory building) in HANARO. In addition, commissioning work of a Bio-REF which is a horizontal type neutron reflectometer is underway. Both instruments have a wavelength of 0.475 nm and have a performance of Q_{max} = 3.0 nm^{-1}. On the other hand, the REF-V is equipped with the necessary equipment for measuring the polarized neutron reflectivity which can study the structural characteristics of the magnetic thin film. Also, since it has a liquid cell and a high-temperature vacuum chamber, it is possible to study in-situ phase transition phenomena for some various thin film.

Full field neutron microscopy based on refractive optics

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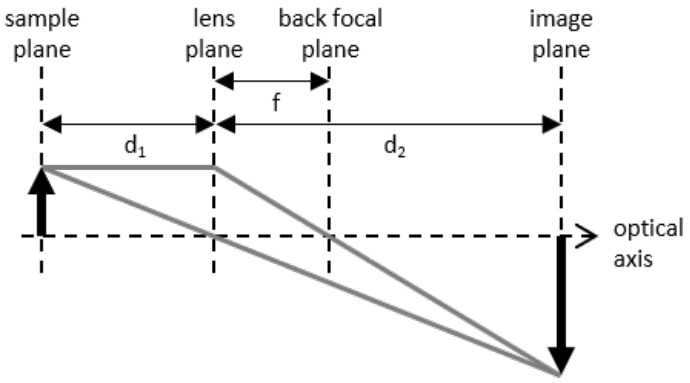
Neutron imaging is traditionally done by placing the detector in close proximity to the sample whereby a variety of contrast modes can be explored. Because of the high divergence of neutron beams, the resolution deteriorates with increasing sample volume-to-detector distance rendering it difficult to make high resolution images of e.g. a sample in a bulky sample environment or the scattered signal where a distance is required to gain angular resolution [1,2]. In these cases, spatial resolution can be obtained by reducing the beam dimensions (and hence the interaction volume) and scanning the sample through the beam. This approach is, however, tedious limiting the obtainable number of voxels and/or time resolution. An alternative approach is neutron full field microscopy [3]. Here the entire volume of interest is illuminated at once and spatial resolution is obtained by introducing an objective lens between the sample and detector. Like in classical microscopy an inverted and potentially magnified or de-magnified image is then formed at the image plane.

We here explore uses of a neutron full field microscope based on compound refractive lenses (CRL) as imaging optics. We provide analytical expressions for the resolution, field-of-view and other relevant optical parameters and discuss imaging configurations that optimize the throughput and reduce the chromatic aberration. Potential uses for 1) bright field imaging with polarized neutrons, 2) depth resolved imaging, 3) SANS microscopy, 4) phase and strain mapping and 5) mapping of individual grains are illustrated by comparing suggested approaches to state-of-the-art instrumentation.



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Neutron reflectometry at spallation neutron source IN-06 of INR RAS

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The time-of-flight neutron reflectometr HORISON at the spallation neutron source IN-06 of the INR RAS is designed to study two-dimensional nano-objects, such as multilayer nanofilms, using neutron reflectometry. Due to a vertical scattering plane the reflectomery of liquids samples is possible too. The instrument can also be used for small-angle neutron scattering studies [1]. The instrument consist of the 7 meter long curved neutron guide, two slit packages, the deflecting supermirror, the sample stage and the hand with a neutron detector. The measurements were performed in the mode of a neutron reflectometer with a test sample — a NiMo / Ti neutron supermirror (m = 2) with known characteristics. The Fig. 1 shows the neutron reflectivity R from this super mirror as a function of the neutron wavelength referred to the incidence angle λ/Θ. The measured value of the critical wavelength corresponds to the previously obtained with an accuracy of 5%. Also, using Monte-Carlo simulation, the dependencies of the resolution of the instrument for various collimations were obtained. One of the planned application of the instrument is testing of supermirrors, designed for various neutron optical devices of the reactor PIK (NRC Kurchatov Institute - PNPI). These measurements are required for the refinement and optimization of new methods of manufacturing super mirrors.

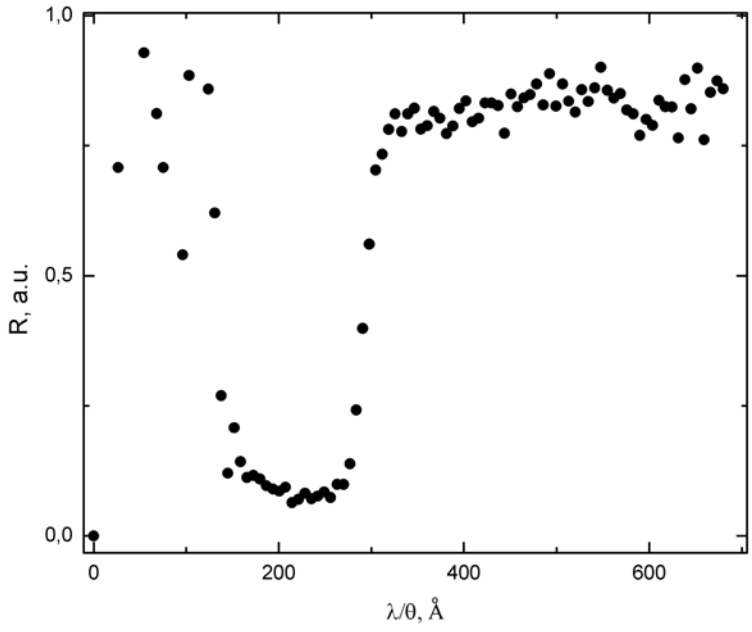

Fig. 1. Dependence of the neutron reflectivity on the test sample of the NiMo / Ti supermirror (m = 2) as a function λ/Θ. The measurements were obtaned at HORISON neutron reflectometer.

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Comparative study of the characteristics of the data acquisition systems for position-sensitive detectors with a delay line on the neutron instruments of the IBR-2 reactor

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Finding an optimal variant of electronics for neutron position-sensitive detectors with delay line readout is always an intricate task, and this is especially actual for time-of-flight instruments on high-flux beams of the IBR-2 reactor. The strong non-uniformities of the flow from the pulsed reactor create additional restrictions for the bandwidth of data acquisition systems. We carried out parallel measurements with the following three systems: DeLiDAQ-1, DeLiDAQ-2, and the system based on CAEN N6730 digitizer. We used two-dimensional 200x200 mm^2 He^3 position-sensitive detectors at the REFLEX and the GRAINS neutron instruments of IBR-2. The results of the study and the conclusions on the conditions of applicability of these data acquisition systems are presented in our report.

The Scalable Readout System: A generic readout system for next generation detectors

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In 2009, the RD51 collaboration introduced the multi-purpose Scalable Readout System (SRS). The architecture simplifies the implementation of different front-end ASICs due to a common hardware part. Examples are the Timepix and the most commonly used APV25.
The SRS became widely used for R&D on Micro-Pattern Gaseous Detectors (MPGDs) and found its application in other fields of research like muon tomography for geology. Due to the scalability, table-top systems for small test detectors as well as large readouts with several 10000 channels have been realised.
The analogue APV25 designed in 2001 has meanwhile been superseded by more advanced digital ASIC technologies and will not be produced any longer.
To provide the community with an adequate continuation of the SRS, the RD51 collaboration decided to implement the VMM ASIC developed in the scope of the ATLAS New Small Wheel upgrade in the SRS. The RD51 group at CERN carried out this task, which is now continued in our group. The project was part of prototyping for an instrument and its readout at the European Spallation Source in the framework of the Horizon2020 project BrightnESS. Additional funding was provided by AIDA2020.
FPGA firmware for the general-purpose SRS Front-End Concentrator (FEC) card has been developed. A new front-end board with VMM ASICs and a new digital adapter card were designed, built in several iterations, tested at CERNs SPS and neutron facilities as ILL in France, BNC in Hungary and IFE in Norway. Currently, the hardware is under final commissioning and first pilot system will be provided to the community within the coming months. The system will be applied as readout of a multi-stage boron-GEM detector. Other groups will apply the system to generic detector R&D as well as medical science, neutron scattering, cosmic ray detection and fundamental physics research. The SRS with VMM is expected to play a significant role in the next decade of detector R&D, but will also find its application in operational physics experiments.

The presentation will outline the implementation of the SRS with the VMM ASIC with related hardware, firmware and software followed by an overview of its application with a focus on neutron detectors.

GaAs-extension on IN16B for improved energy resolution in backscattering

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Since the invention of neutron backscattering 50 years ago, developments in instrumentation have focussed primarily on increasing the intensity, while little progress has been made in enhancing the energy resolution. We have built a demonstrator setup on IN16B at the ILL with a crystal surface of 1/10 of a full scale instrument using the GaAs 200 Bragg reflection to bring about a significant increase in resolution. This progress is offered by the narrow intrinsic Darwin width of GaAs 200, an order of magnitude smaller than the line width of the currently used Si 111. To retain this high resolution, other limiting parameters need to be controlled precisely. This includes variations of the lattice parameter $\Delta a/a < 10^{-6}$, the angular misalignment of crystals to $\Delta q < 0.1°$ or keeping mechanical strain to $\gamma < 10^{-6}$. In addition, a vertical temperature gradient of 3.3 K/m along the 3 m high analysers is required to compensate for the gravitational energy shift of the neutrons. Recent tests yielded an unprecedented energy resolution of E = (77 ± 3.) neV FWHM, about one order of magnitude narrower than the 750 neV measured with bent Si 111 under the same conditions.

This work was supported by the German Federal Ministry of Education and Research (BMBF) through grants no. 05K13WE1 and 05K16WEA.

REFSANS: The horizontal time-of-flight reflectometer with GISANS option at the Heinz Maier-Leibnitz Zentrum.

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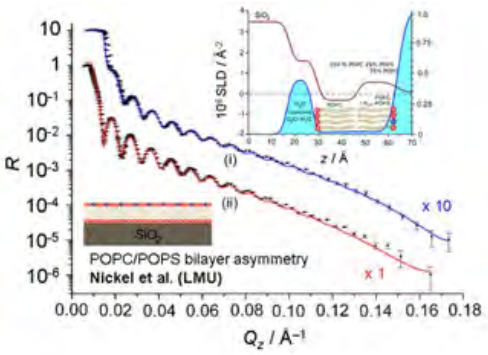
REFSANS is the horizontal time-of-flight reflectometer installed at the Heinz Maier-Leibnitz Zentrum in Garching. It is designed to enable reflectometry and grazing incidence neutron scattering studies of solid/liquid, solid/air and liquid/air interfaces. By using a white incident neutron beam and time-of-flight (TOF) analysis, REFSANS gives simultaneous access to a range of Q values, which is especially useful to study air-liquid interfaces or kinetic phenomena for covering a range of momentum transfer with only a few instrumental settings.

A three double-disc chopper system allows performing measurements with a tunable wavelength resolution, going from 0.2 % up to 10%. The neutron optics of REFSANS comprise neutron guide elements with different channels and special apertures to provide, on the one hand, slit smeared beams for conventional reflectometry and, on the other hand, point focused beams for GISANS measurements. Furthermore, it is possible to independently control the horizontal and vertical beam divergence, in dependence on the sample characteristics.

The provided sample environment allows investigations of all possible interface combinations. Furthermore, the realization of an electrochemical compact cell and the design of an humidity cell are in progress, in order to allow the investigations of electrode processes and of processes in a controlled atmosphere.

Given the TOF nature of REFSANS, the investigation of kinetic processes is possible thanks to the possibility to embrace a Q-range with a single instrumental setting. Time resolution can be pushed down to 30 s. Finally, neutron data are recorded in event-mode (*i.e.* each neutron arrival time and impact position is recorded). This feature makes possible to perform various time re-binnings in order to tune the resolution/ intensity trade-off after the experiment.

A view of the REFSANS sample area and of the detector tube



Specular reflectivities of phospholipid asymmetric bilayers of POPC/POPS.

Implementation of attenuation correction procedures for position resolved neutron powder diffraction studies

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Chemical phase quantification from neutron diffraction measurements relies on accurate Bragg peak intensities at all diffraction angles. Amongst others these intensities are influenced by the total distance that the neutron beam has traversed through the sample in reaching the contributing volume segment and the distance from this segment to the outer edge of the sample in the direction of the neutron detector. Since the total path length is dependent on the diffraction angle, gauge volume position inside the sample, as well as the sample dimensions and shape, the measured diffraction pattern should be corrected to account for this non-constant attenuation effect.

A new module was created using the Shapely Python library and integrated with the neutron diffraction data reduction system ScanManipulator. During configuration, variables (such as sample and detector position) can be linked to parameters present in the diffraction data file to simplify experiment geometry definitions. Once all the parameters are configured, the attenuation correction coefficients are automatically calculated and applied to all datasets in the data file. In addition, an illustration of the sample and instrument geometry for each dataset will be saved and converted to a movie file once all the datasets has been processed.

Results show that in highly attenuating materials sample shape and relative orientation can have a detrimental effect on untreated data which can lead to incorrect phase quantification. The correction technique can further be used to accurately determine diffraction patterns obtained form position resolved neutron diffraction experiments.

Time-focusing analyser for TOF quasy-backscattering spectrometers

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The main part of the secondary energy resolution of the time of flight backscattering spectrometer with silicon analyser is given by the sample height and the deviation from the exact backscattering geometry. The effect of the sample height is decreasing with the analyser take-off angle, however the decreasing of the analyser take-off angle results in increasing of the vertical coverage of the analyser - thus with the detected intensity. Here I propose a time-focusing toroidal analyser geometry together with position sensitive detectors which practically eliminates the effect of the sample size - comparing to the other parts of the resolution function. This geometry enables to use analysers farther from the exact backscattering which opens the way to increase both the analyser surface and the sample height i.e. higher detected intensity. The effect of the toroidal geometry on graphite analysers will also be discussed.

Software project for the texture diffractometer (TEX) as an element of the instrumental base of the PIK reactor

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Our major goal is a set of programs for the control of scientific experiments at the instrumental base of the PIK reactor. One of them, a program for texture diffractometer TEX should measure diffraction peaks by moving stepper motors and readings data from a monitor and detector. Main requirements from users and scientists are: complete functionality of the diffractometer, user-friendly interface, telemetry and data storage, primary processing of the experimental data.

There are many software products, for creating software for scientific instruments, each of which has its pros and cons. Arguments in this dispute can be: functionality, price, required amount of labor and developer level, support or number of community members, open source or not, compatibility with operation system and other software, etc.

After a detailed study of possible variants, we came to Tango Controls framework, which is a “free open source device-oriented controls toolkit for controlling any kind of hardware or software and building SCADA (supervisory control and data acquisition) systems” [1, 2]. It means, developer doesn’t need to write whole program code, but focus only at unique features of instrument. It reduces needed time and labor for developing. Other important idea, which was used at Tango, is distributed architecture – parts of program run as separate process independently from computer or operation systems. Tango framework is used about 50 mega science facility: DESY, ALBA, ESRF, SOLEIL and others.

We see the architecture of the program at the moment as:

1) hardware drivers for low-level communication.
2) Tango servers for forming packets of the bytes for hardware drivers.
3) Sardana servers for standardization of the functions of the Tango servers. This is needed to use the Taurus auto GUI.
4) Taurus auto GUI, maybe with specific widgets for TEX. They will be written with PyTango modules and Qt-designers by Taurus GUI.

Second and third paragraphs can be combined in case of using Python for hardware communication, but this decision does not seem obvious without testing. Now, two of the four Tango servers have been written, we also wrote one sardana server and the Taurus auto GUI.

1. http://www.tango-controls.org
2. https://sardana-controls.org/

Beam Monitors at ESS

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The main objective of the European Spallation Source [1] Lund, Sweden is to implement the highest integrated neutron brightness from the target. The design and deployment of 22 instruments spanning over 3 instrument halls requires more than 150 choppers and numerous guides to deliver the beam with the energy, intensity and spatial profile specified by the instrument. In order to continuously diagnose the delivered beam and to aid in carrying the scientific investigations, various neutron Beam Monitors are to be placed in different locations along the beam, namely in the bunker near the monolith, along the beam guides, in the close proximity of the choppers, before the sample and optionally after the sample.

Beam monitors Common Project was established in order to standardise the beam monitors for all ESS instruments, assure minimum operational monitoring requirements and provide monitoring needs for up to 2 MW source power. Here we present the current results of the project: we aim to deliver an overview of commercially available beam monitors that have been characterized [2] and determined as suitable to fulfill the requirements for various locations along the beam, as well as to introduce novel beam monitors, whose design is currently undergoing further optimization.

First, near the monolith, due to the complicated environment where fast, slow neutrons and -ray are present, the fission chambers from commercially available beam monitors are suggested as a suitable option.

Next, alongside the beamguides and to verify the functionality of choppers, novel approaches are presented. In particular parasitic beam monitors recording the -ray spectra from the borated parts of choppers. The main condition for the monitors to be placed alongside the beamguides is low attenuation: these parasitic monitors are using the advantage of the -rays induced by presence of boron without the need to place additional material in the beam. Furthermore a quasi-parasitic beam monitor based on a thin Vanadium foil, from which the neutrons scatter to be then detected by Helium proportional counters, is introduced here.

Last, the main performance requirements for the Beam Monitors that are to be placed before and after the sample is for the absolute flux and time resolution. Existing multiwire proportional chambers, are suggested as candidates.

As a first result of the Common Beam Monitor Project, this study briefly summarizes the tests performed on commercial available beam monitors, describes the design and principle of the novel parasitic beam monitors and presents the results of the initial characterisation of the Vanadium beam monitors.

[1] European Spallation Source ERIC. *europeanspallationsource.se*.

[2] F. Issa, A. Khaplanov, R. Hall-Wilton, I. Llamas, M. Dalseth Riktor, S. R. Brattheim, and H. Perrey. Characterization of thermal neutron beam monitors. *Phys. Rev. Accel. Beams*, 20:092801, Sep 2017.

Neutron reflectometry with the Multi-Blade detector, correlation between detector performance and scientific output.

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Neutron reflectometry is a powerful technique to study surfaces and interfaces on typical length-scales on the order of nano-meters. At current instruments, a typical dynamic range for reflectivity measurements is about 10^{-6}. Strong limitations are set by the available flux, hence, in the past few years, several methods have been proposed to improve the performance of reflectometry instrument [1].

The European Spallation Source (ESS), presently under construction in Sweden, will ensure an intensity increase of at least one order of magnitude [2]. The two reflectometers foreseen at the ESS, FREIA and ESTIA have an innovative design to exploit the higher incoming flux. From the detector point of view, the demanding requirements set by the instruments concern in particular the counting rate capability and position resolution. The Multi-Blade [3,4] is a Boron-10-based detector conceived to face the challenges arising from the neutron reflectometers at the European Spallation Source (ESS).

A prototype has been installed and tested on the CRISP reflectometer at the ISIS neutron and muon source in UK [4,5], and on the AMOR reflectometer at PSI in CH. The latter allows high flux measurements, exploiting the refocus mode by using an elliptical neutron guide. This concept will be adopted for the ESTIA reflectometer at ESS.

From previous characterizations, it has been shown that the spatial resolution is improved by approximately a factor three over state-of-the-art Helium-3-based reflectometer detectors. For the first time this has been used to improve the q-resolution in the data analysis. Moreover, from the rate measurements performed on AMOR, a lower limit for the counting rate capability has been set with the Multi-Blade. This value is already above the maximum rate detectable by the state-of-the-art detector technology employed in neutron reflectometers, and close to the work operation needed at ESTIA.

The difference between the measurements performed in a standard instrument configuration and in a setup reproducing the ESTIA operation modes will be presented, highlighting the correlation between the improvements in the data analysis and the detector performances.

[1] F. Ott et al., Eur.Phys. J. Spec. Top. 167, 93–99 (2009)
[2] R. Garoby et al., Physica Scripta 93(1), 014001 (2018)
[3] F. Piscitelli et al., Journal of Instrumentation, **12**(03), P03013 (2017)
[4] F. Piscitelli et al., Journal of Instrumentation, **13**(05), P05009 (2018)
[5] G. Mauri et al., PRSA: Mathematical, Physical and Engineering Sciences 474 2216 (2018)

Single Crystal Diffraction Experiments under Extreme Conditions with Hot Neutrons on HEiDi

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Diffraction techniques are one of the most versatile tools for detailed structure analysis. Due to their specific pecularities neutrons are a very useful probe for structural studies on various hot topics related to physics, chemistry and mineralogy. The single crystal diffractometer HEiDi (operated jointly by RWTH Aachen University and Forschungszentrum Jülich) at the research neutron source at the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching offers high flux, high resolution and wide range in reciprocal space, low absorption and high sensitivity for light elements.

In order to adapt this instrument to the most recent scientific topics its core features but also its sample environment have been continously extended and improved. For instance, at low temperatures various multiferroic compounds from the melilite family were studied not only in order to study their nuclear and magnetic features in detail (especially in combination with thorough magnetic measurements on the sister instrument POLI with polarized neutrons) but also to reveal the risks of misinterpretation of structural data due to multiple scattering [1].

At very high temperatures studies on $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$ brownmillerites concerning their oxygen diffusion pathways reveal anharmonic diplacements of the apical oxygens pointing towards the interstitial vacancy sites which create a quasicontinuous shallow energy diffusion pathway between apical and interstitial oxygen sites [2]. Recent studies use a special mirror furnace developped at MLZ which allows not only temperatures > 1300 K but also atmospheres with various oxygen content and pressure around the sample to study their influence to the evolution of the occupation of the interstitial sites.

In 2016 a project funded by the BMBF (German ministery for education and research) was launched in order to develop a set of new pressure cells for HEiDi. Some of them can be combined with HEiDi's low temperature equipment in order to study structural properties down to temperatures below 10 K, e.g. $MgFe_4Si_3$ compounds and their magnetic features [3], other cell designs allow combined measurements of the same sample with X-rays and with neutrons.

[1] A. Sazonov, M. Meven, G. Roth, R. Georgii, I. Kézsmárki, V. Kocsis, Y. Tokunaga, Y. Taguchi, Y. Tokura and V. Hutanu; Origin of forbidden reflections in multiferroic $Ba_2CoGe_2O_7$ by neutron diffraction: Symmetry lowering or Renninger effect?; J. App. Cryst. 49(2) (2016).

[2] M. Ceretti, Wahyudi, O.; Cousson, A.; Villesuzanne, A.; Meven, M.; Pedersen, B.; Bassat, J.-M.; Paulus, W.; Low temperature oxygen diffusion mechanisms in $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$ via large anharmonic displacements, explored by single crystal neutron diffraction; J. Mater. Chem. A 3, 21140-21148 (2015).

[3] A. Grzechnik, M. Meven and K. Friese; Single-Crystal Neutron Diffraction in Diamond Anvil Cells with Hot Neutrons; J. Appl. Cryst. 51, 351-356 (2018).

High resolution analysis with bent perfect crystal (BPC) in powder diffraction - I

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Unconvential triple axis set-up with bent perfect crystal monochromator and analyzer was tested in diffraction on *alpha*-Fe(211) polycrystalline pins of 8 mm and 2 mm diameters when situated between the crystals. After realization of optimum conditions at the scattering angle of $2\theta_S = 88^o$ and at the neutron wavelength of 0.162 nm, a high angular resolution down to *FWHM* (*delta d / d*) = 4.7×10^{-3} and *FWHM* (*delta d / d*) = 3.5×10^{-3} for 8 mm and 2 mm pins, respectively, was achieved; however, with opened beams i.e. without any Soller collimators. Such diffraction setting can be exploited in high-resolution powder diffraction, namely, in analysis of diffraction profiles with a small lattice parameter difference or a small change due to an application of an external load.

High resolution analysis with bent perfect crystal (BPC) in powder diffraction - Part II

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As a continuation of our previous studies carried out on α-Fe(211) samples (at the scattering angle of $2\theta_S=88^o$) and presented at this conference, the triple axis set-up with bent perfect crystal monochromator and several analyzers was tested in diffraction on α-Fe(110) polycrystalline pins of 8 mm and 2 mm diameters at the scattering angle of $2\theta_S=47.1^o$. After realization of focusing conditions in real and momentum space at the neutron wavelength of 0.162 nm, a higher angular resolution down to $FWHM(\Delta d/d) = 2.5\text{x}10^{-3}$ and $FWHM(\Delta d/d) = 1.4\text{x}10^{-3}$ for the diameter of the α-Fe-samples of 8 mm and 2 mm, respectively, was achieved with opened beams (without any Soller collimators) and within the range of used curvatures of the analyzers. Similarly to the previous setting tested on α-Fe(211) samples this one can be also exploited in the high-resolution powder diffraction, namely, for strain/stress measurements and the analysis of diffraction profiles responding to small lattice parameter changes e.g. due to an application of an external load on the samples.

Microstructured multicore SCIntillating FIber (SCIFI) for high resolution thermal neutron radiography

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The improvement of neutron imaging towards and beyond the microscale is a well-documented need for the iterative characterization and modeling of numerous microstructured X-ray opaque materials. This work presents the recent progress in evaluating a SCIntillating FIber (SCIFI) proof-of-concept towards micron-level thermal neutron radiography. These SCIFIs are composed of ^{6}Li-enriched silicate glass cores doped with a Ce activator. The cores possess ~8.5 µm diameters and ~10 µm pitch following fiber drawing with a cladding glass into an all-solid multicore fiber. A polished 5 x 5 mm array of 100 microstructured multicore SCIFI pixels was fabricated into a 1 mm thick faceplate. The neutron efficiency and light yield of the faceplate are characterized as functions of the 7.38 weight percent of Li_2O, thickness, and the 70% active volume. It was determined that approximately 39% of a thermal neutron (2 Å) beam can be absorbed by the faceplate. The ^{6}Li (n, α) t reaction is estimated to produce 7,700 ± 1,000 scintillation photons per event, referencing light collection from ^{241}Am irradiation of the faceplate. Simulations suggest that on average 17.5 ± 1.4% of these photons will be transported to an end of the fiber array for a thermal beam, with at least 7.2% of that total scintillation light being confined into the fiber cores in which it originated. The SCIFI faceplate was integrated into the Neutron Microscope at the Pulse OverLap DIffractometer beamline located at the Paul Scherrer Institut to image a Siemens star test object. Processed neutron radiographs acquired with the proof-of-concept faceplate resolved features at a state-of-the-art resolution of 16.1 ± 0.5 µm (see Figure 1). The potential for even high resolution designs having smaller pitch or different cladding material is discussed.

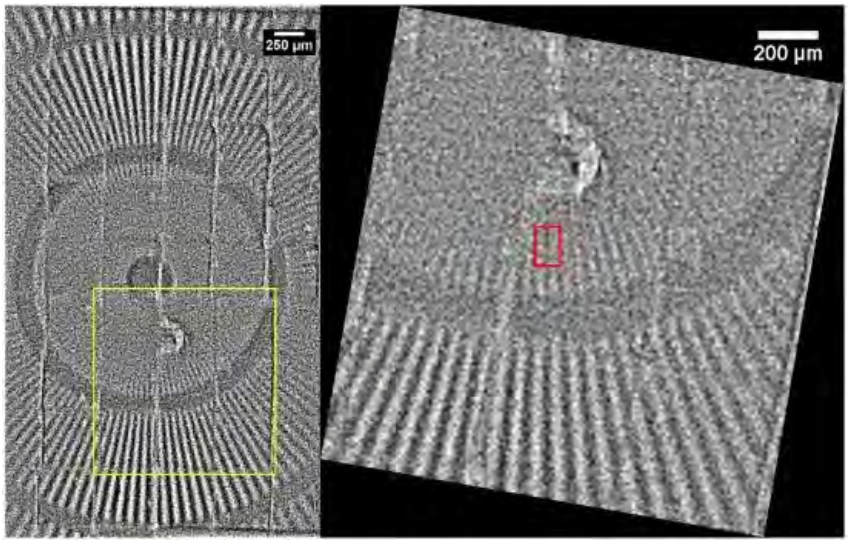

Figure 1. Neutron radiograph of PSI's gadolinium-based Siemens Star processed with a Fourier Filter (left), and an enlarged region of interest with ~16 µm feature highlighted (right).

The ODIN instrument at ESS

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The European Spallation Source is under construction in Lund (Sweden). It promises to be the world's most intense pulsed neutron source and the first beam on target is expected to be in 2022.

In the first suite of instrument to come online and begin hot commissioning at that point is the Optical and Diffraction Imaging with Neutron (ODIN) instrument, which is being designed as an in-kind collaboration between the Technical University of Munich and the Paul Scherrer Institut.

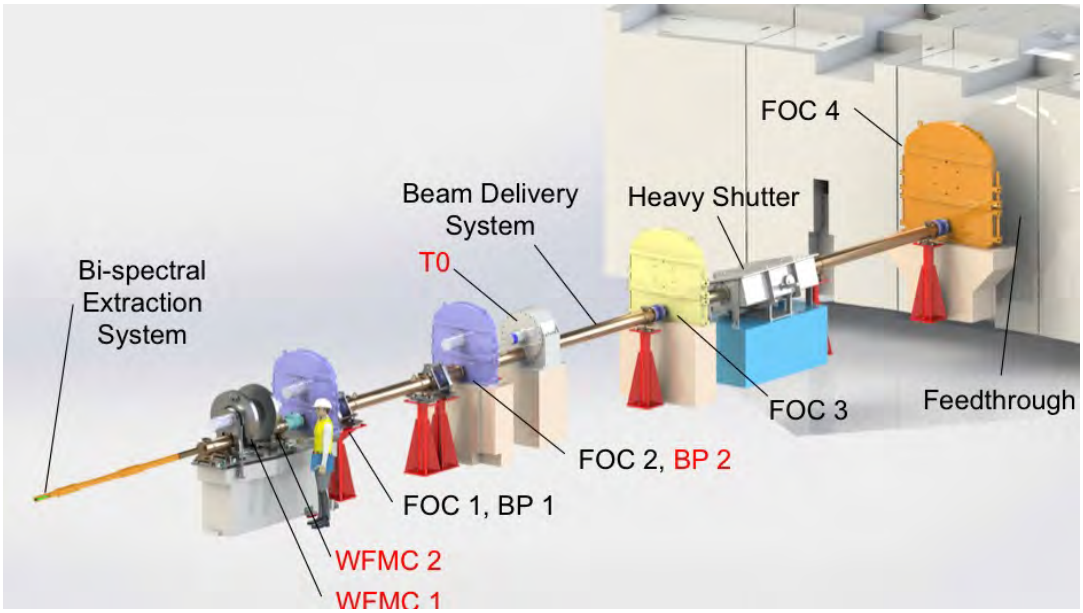
The aim of the ODIN consortium is to design and realize the next generation, state-of-the-art in neutron imaging instruments. Many new and upcoming techniques have been developed in recent years to complement the standard "white beam" imaging, and ODIN aims to accommodate all of them in the best possible ways by flexibly leveraging the characteristics of the long pulse of neutron provided by the ESS.

A cascade of 9 choppers (Fig. 1) will shape the beam in the time domain, allowing the flexible choice of neutron wavelength resolution from 10% (natural resolution) to 1% and down to 0.4%. This will allow to employ a wide array of techniques, each requiring a different wavelength resolution, with world-class performance by tailoring the chopper cascade to the most appropriate $\Delta\lambda/\lambda$.

The neutron delivery from source to sample area will be achieved with an optimized double ballistic guide with an elliptical and bi-spectral feeder, with a total length of 43m. The design of the guide has been driven by the requirements of a large (15x15 cm^2 at the standard measuring position and up to 25x25 cm^2) Field of View (FoV) measured at 75% of the maximum. On top of the spatial homogeneity, we aimed and achieved a spectral homogeneity across the entire usable FoV within 0.1Å from the desired wavelength.

In order to accommodate the wide variety of cutting-edge techniques that will be available with such a flexible system, a long and spacious cave will be designed which will also house all the relevant state-of-the-art sample environments.

The current status and the timeline of the project is discussed here, together with the foreseen parameters of the completed instrument and a brief description of the scope of the beamline.



Service for storage of measurement results from the spectrometers of the IBR-2 reactor.

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The poster is dedicated to the service developed for the storage and work with the results of experiments from all the FLNP spectrometers. The service consists of a fail-safe data storage with a package for automatic recording of experiment results. The service is integrated with the Journal, which organizes the search for data on the parameters of the experiment (user name or sample, date of measurement, etc.).

Novel sputtering facility at NRC KI - PNPI

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Petersburg Nuclear Physics Institute (PNPI) is among the known worldwide neutron optics supplier. PNPI sputtering lab was among the first who implements the supermirror multilayer coating for neutron optics devices. Sputtering facilities designed at PNPI 20-30 years ago, are now worn and obsolete. New high-flux reactor PIK requires about 1km of good quality neutron guides. On the other hand, neutron coatings with the required characteristics, which are produced by modern manufacturers (SwissNeutronics, Mirrotron etc.), are very expensive, and productivity is restricted. Therefore, there is an urgent need to create a new sputtering facility that meets the most modern requirements.

One of the main tasks of the developers of this project will be to master the technology of manufacturing neutron optics units with parameters corresponding to the world level. In particular, it is necessary to create super mirror coatings with *m*up to 5. This will allow us to perform the tasks in this project and continue to meet the needs of the neutron-optical elements for research neutron centers in Russia and, above all, in NRC KI PNPI, with a reactor PIK.

Technical design and performance of the novel multiplexing spectrometer CAMEA

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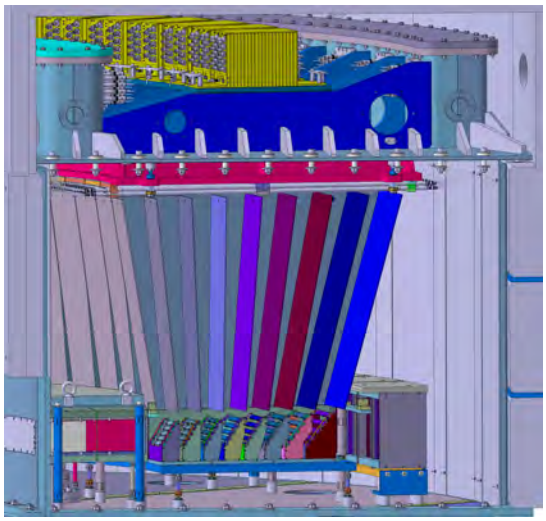
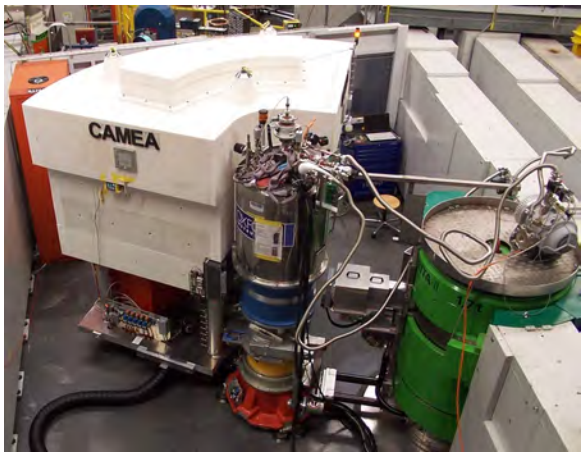
The multiplexing neutron spectrometer CAMEA (Continuous Angle Multiple Energy Analysis) was installed and commissioned at the cold neutron beam port RNR13 at the Swiss spallation neutron source SINQ. The spectrometer is optimized for efficient and rapid mapping of excitations in the horizontal scattering plane. The novel design comprises consecutive, upward scattering analyzer arcs and an array of position sensitive detector tubes, which are mounted in a stainless-steel vacuum vessel with low magnetic permeability. We will present a technical overview of the spectrometer, engineering solutions and in-house developments for the analyzer - detector system. First data taken during the commissioning demonstrate the tremendous gain in data collection rate with respect to a standard triple axis spectrometer.





Left: A sketch of the components of the CAMEA spectrometer inside the vacuum tank. The drawing shows from bottom to top the upward scattering analyzer arcs, the cross talk shielding, the position sensitive detector tubes and the detector electronics. **Right:** The new spectrometer CAMEA during commissioning at the cold neutron beam port RNR13 replacing the Rita-II back-end.

Upgrades at the high-resolution backscattering spectrometer SPHERES

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The SPectrometer for High Energy RESolution (SPHERES) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It provides high energy resolution with a good signal-to-noise ratio. Different components of the instrument have been upgraded to further improve the instrument performance.

Some recent years ago the PST chopper has been renewed. The new more compact one-wing chopper can be operated with the desired frequency with a crystal speed of 225m/s, close to the optimum velocity for the phase space transformation. Within this upgrade, also the graphite deflector crystals on the circumference of the PST chopper were replaced with ones of a higher reflectivity and mosaicity. The combination of the increased operation velocity and the better deflector crystals led to a doubled intensity in most detectors.

Just recently the focusing neutron guide has been replaced with an elliptic guide. It had been optimized based on McStas neutron ray-trace simulations, which also considered the new PST chopper. With the new elliptic guide another intensity gain at the sample position of about 30% was obtained. Together with the exchange of the focusing guide also a new background chopper has been installed about 2m upstream of the PST chopper to further reduce background. The background chopper can be operated in a “high intensity mode” (at the same frequency of the PST) or in “low backround mode” (at half the frequency of the PST). The latter setup allows a high signal-to-noise ratio by eliminating every second pulse, albeit at the cost of intensity.

Design study of a new 1m2-Multi-Wire-Proportional-Chamber Neutron detector

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Modern Neutron Multi-Wire-Proportional-Chambers operating with alternative solid-state converter as $^{10}B_4C$ coatings have the potential to surpass the position resolution and count rate capability of ^3He based detectors at comparable detection efficiency [1, 2]. The use of large area converter coatings on sub-mm substrates makes it essential to develop a mechanical concept to avoid their deformations in operation due to their own weight, pressure differences between stopping-gas and ambient gas and acting electrostatic forces resulting from the applied High Voltage for gas amplification. The Helmholtz-Zentrum Geesthacht had introduced and investigates currently the idea of stabilizing the converter elements by gas pressure gradient between both sides of the converter to counteract these forces [1]. A gas-vessel Position Sensitive Neutron detector consisting of 24× parallel stacked converters with a detection depth precision < 12 mm is designed at a position resolution of 2 mm. The deposition method of $^{10}B_4C$ coatings with thicknesses up to 10 µm on pretreated Al substrates was elaborated [2, 3]. A converter layer thickness-profile from 0.6 µm up to 1.2 µm is envisaged to gain an efficiency up to 60 % at reasonable coating costs. The delay-line read-out of the detector is designed for count rates up to > 200kc/s (global $2.4x10^6$ c/s) per detector plane. First neutron tests of the new read-out chain conducted at the ESS test beamline V20 operating at the Helmholtz-Zentrum Berlin using a small $^{10}B_4C$ neutron prototype detector verified the envisaged signal to noise ratio.

[1] European Patent: EP 17184906.0 (published 09.02.2019)

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Evaulation of beam diagnostic apparatus

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The development of advanced neutron sources and scattering techniques together with quality assessment of neutron delivery systems require detailed neutron beam diagnostic. The first test results on a compact, flexible, mobile and robust standalone neutron beam diagnostic apparatus are presented. The equipment comprises beam shapers, chopper, detection system, data acquisition and control software. Its operation is based on time stamped event recording, allowing time-of-flight measurement for the recorded neutrons. The narrow slit chopper together with a reduced size aperture defines the origin of the flight time. Corrections for the energy-dependent detector efficiency, included in the data processing software, allow absolute intensity measurement.

Reduced size and weight facilitate deployment in sample environment positions or gaps of existing neutron beamlines. A compromise between spectral accuracy and reduced neutron flight length is achieved. Wavelength distribution, neutron flux and neutron background are provided by measurements on continuous sources. In case of pulsed sources the equipment allows time structure investigation. The modular structure of the device ensures flexibility and adaptability to various requirements of beam characterization. A reduced size, high resolution position sensitive detector can be useful for energy sensitive divergence mapping of neutron beams, source imaging or quality assessment of beam delivery systems.

The test experiments have been carried out on a thermal and two cold neutron beams of the Budapest Research Reactor. High count rate capability and timing accuracy are demonstrated.

Development of a GEM-based neutron transmission detector for 2D-resolved TOF measurements

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Modern spallation neutron sources like ESS require the use of advanced thermal neutron detectors to be used either as beam monitors or transmission detectors for sample diagnosis. The requirements for these applications are 2D and energy resolution (the latter obtained through the Time-Of-Flight technique), ease of use and implementation on the beamlines, minimal influence on the transmitted beam, long-term stability. A small encumbrance is a plus especially when concerning use as a beam monitor.

Here we present a thermal neutron detector, developed by IFP-CNR in collaboration with Università degli Studi di Milano-Bicocca and Nuclear Instruments s.r.l. that has all the necessary and above mentioned requirements. The detector is based on the well-proven GEM (Gas Electron Multiplier) technique [1]: the GEM foils are coupled with a boron-coated, high-transmission cathode and a 2D-resolved (padded) anode. The pads are of 3 mm x 3 mm dimensions, and the total frontal sensitive area is of 90 x 90 mm^2. The collected signals are read by ASIC electronic cards based on GEMINI chips [2] and both the space-resolved images and TOF histograms are obtained through an FPGA. The novelty of the present instrument respect to previous use of GEMS as a neutron detector [3, 4] is the possibility to be used as a sealed detector, i. e. without the use of a continuous gas refill, with obvious advantages in terms of reliability and ease of use.

In this work we present the working procedure to obtain the sealed detector, the constructive details of the working prototype and the preliminary results obtained, especially discussed in terms of efficiency, energy (TOF) and spatial resolution.

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Neutron ray-tracing simulations for the upgrade of the OSIRIS spectrometer

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The OSIRIS spectrometer, located at the ISIS Neutron and Muon Source, is a cold-neutron time-of-flight inverted-geometry instrument optimised for quasielastic and low energy spectroscopy, with capabilities for long-wavelength diffraction. It consists of a 34 m long supermirror guide, band width choppers, a pyrolytic graphite (PG) crystal-analyser array for energy analysis of neutrons scattered by the sample, and a ^{3}He detector array. In its present configuration, with λ = 6.6 Å neutrons and using the (002) reflection of the PG analyser, it is characterised by an energy resolution of 25 μeV. [1,2]

The instrument upgrade of OSIRIS includes the addition of a silicon analyser (SA) array that will bring the energy resolution down to 10 μeV, for the same dynamical window as the concurrently operated PG analyser [3]. Relaxation times of up to 400 ps will be accessible. Here we present the optimised geometry and predicted performance of the silicon analyser, from neutron ray-tracing simulations performed with the McStas software [4]. Furthermore the primary spectrometer will be upgraded by a new supermirror guide with a geometry optimised for high transmission of cold neutrons. The simulation results for the new elliptically-tapered high-*m* supermirror guide predicts an estimated fourfold increase in neutron flux at sample position.

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In-situ calorimetry with Quasi-Elastic Neutron Spectroscopy: current developments realising a complimentary dynamic and thermodynamic sample description

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Differential Scanning Calorimetry (DSC) is an analytical technique commonly used to probe phase transitions and quantify enthalpy changes that occur in complex systems. Many of these transitions are accompanied by changes in dynamics at the molecular level, which are well characterised using Quasi Elastic Neutron Spectroscopy (QENS). Performing the two measurements simultaneously can be a powerful tool, ensuring that the experimental conditions remain the same - temperature equilibration, sample mass etc. Here we present the development and progress of the first working calorimeter for this purpose, designed and tested in a standard top-loading CCR on the IRIS spectrometer at the ISIS Neutron and Muon Source, UK. The calorimeter has an operating temperature range of 80K to 320K and is currently suitable for liquid samples. Its functionality is discussed in light of both *in-situ* and *ex-situ* experimental work, including details on design challenges; test results showcasing its sensitivity to both first order transitions and the glass transition, and its potential as a partner to both dynamic and structural information obtained from neutron measurements.

A novel transportable neutron spin filter based on dynamically polarized protons

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We present the status of development of a novel neutron spin filter based on the strong spin dependence of the neutron scattering on protons. It is compact and works in inhomogeneous fields. Using photo-excited triplet states for the dynamic nuclear polarization (DNP) process, proton polarization values of 80% can now be achieved in pentacene doped single crystals of naphthalene at a field of 0.36 T in a simple helium flow cryostat. Careful sample preparation lead to extremely long polarization decay times under moderate conditions that allowed us to develop a transportable device. The filter is polarized in the lab under well controlled conditions and is then transferred to the neutron beam line where it can be operated during several days with almost constant polarization while requiring only a minimum of equipment. Relaxation times of T1 ~ 800 h are achieved at a field of 20 mT and the polarization can be reversed by adiabatic fast passage with an efficiency of above 99% [1].

We describe the main features of the spin filter and its use as a spin analyzer in a small-angle neutron scattering (SANS) experiment probing the magnetic structure of a nanocrystalline soft magnetic material. The procedure for the background and spin leakage corrections of the neutron data is outlined. The next development steps to increase the filter performance are discussed.

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Response of a Li-glass/multi-anode photomultiplier detector to α-particles from Am-241

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The Solid-State Neutron Detector, SoNDe [1], is a position-sensitive thermal-neutron detector for high-flux sources currently being developed for the upcoming European Spallation Source (ESS). In this study, the response of the GS20 scintillator to alpha particles from a ^{241}Am source was studied using a multi-anode photomultiplier tube (MaPMT) from Hamamatsu. Using 3D-printed collimators and a motorised setup, alpha particles were scanned over the scintillator surface in controlled steps. The spread of scintillation light leaking into adjacent MaPMT pixels was mapped in relation to the position of the collimated alpha-particle beam. In general several pixels will register a signal (a hit) above a given threshold. The effect of this threshold on hit multiplicity has been studied, with a view to optimise the single-hit efficiency of the detector. Results are compared with Ray Optics simulations [2].

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url:http://www.fz-juelich.de/jcns/jcns-2/EN/Forschung/Instruments-for-ESS/SoNDe-Projekt/_node.html

[2] https://ricktu288.github.io/ray-optics/

First experimental test of the time-gradient magnetic field SESANS prototype

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The Q-resolution of the pinhole-type small angle neutron scattering (SANS) diffractometers is practically limited at $1x10^{-3}$ $Å^{-1}$, that doesn't allow for studies of large-scale structures. Focusing [1] and spin-echo based [2] SANS techniques developed to complement the conventional SANS are allowing to overcome this limit.

In this work we describe the implementation of a new spin-echo SANS technique based on the use of time-gradient magnetic fields (TGF NSE) [3] aiming to extend the possibilities of the REFLEX reflectometer [4] at the pulsed reactor IBR-2 (Dubna, Russia).

This technique requires the use of the linearly increasing magnetic field in the form of the sequence of sawtooth pulses, that suites very well to pulsed structure of neutron beam at IBR-2. A wide range of neutron wavelengths employed in the time-of-flight operation mode allows for the simultaneous coverage of a wide range of spin-echo lengths (corresponding to a wide Q-range in conventional SANS), as the latter is proportional to the cube of the neutron wavelength, and therefore for SANS studies over a wide length scale.

In this work, the last experimental results obtained using the prototype of the TGF-NSE setup at the pulsed beam of IBR-2 reactor are presented. Some technical problems and their solutions are discussed.

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Hemispherical high-pressure cells for inelastic neutron scattering studies of proton dynamics in materials

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A specific generation of hemispherical modification compact high-pressure cells is made for experiments on neutron inelastic scattering. The cells of a generic “piston-cylinder” type offer a pressure range up to 30 kbar with the sample volumes up to 100mm3. The cell body may be composed from different metallic alloys such as Cu-Be, Ti-Zr, Ni-Cr-Al or their combination. The energy of atomic vibrations of these materials do not exceed some 40-45 meV what permits studies of higher-energy excitations, including proton vibrations in different compounds, in relatively comfortable instrument background conditions. The cell design is particularly adapted for the neutron spectrometer IN1-Lagrange at ILL with large open solid angle for scattered neutrons. The performance of the first members of this high-pressure cell family is illustrated by the measured spectra at IN1.

High performance in-situ 3He-NSF polarizer for Thermal neutrons and analyzer for cold neutrons

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Over the past several The program for in-situ SEOP 3He NSF at the JCNS at the MLZ has made many advancements. Several systems are in construction and or testing phases. including PA for separation of incoherent from coherent scattering in soft matter studies (SANS), and online polarization for analysis for neutron reflectometry, SANS, GISANS and spectroscopy.

here we describe the neutron polarizer for a new time-of-flight neutron spectrometer with polarization analysis TOPAS. This instrument will use the convergent focused incoming beam of thermal neutrons with energies up to 150 meV (wavelength down to 0.74Å). The system was successfully prototyped, and tested. In the course of first experimental test at the polarized hot neutron diffractometer POLI at MLZ, neutron polarization of 97.6% was achieved for 0.895Å neutrons and kept constant during 30 days.

Neutron ray tracing: from modelling of instruments to analysis of experimental data

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Neutron ray-tracing simulations have become a standard method, which is widely used in all major neutron instrumentation projects nowadays. Significantly less frequent are the applications employing ray-tracing simulations to analyze experimental data. One of the reasons (apart of usually long computing times) is the missing interface to the large variety of specialized programs which are needed to solve particular problems, such as structure refinement, texture analysis, evaluation of residual strains or solving inverse problems in small-angle scattering and reflectometry. Although examples of such software exist (e.g. RESTRAX [1] for three-axis spectrometers), it is practically impossible to develop and maintain data analysis code for the growing variety of scattering models together with the instrument simulation package. The solution could be a standardized data exchange mechanism and interface allowing to pass the results of neutron ray tracing to the data analysis software. The recently introduced Monte Carlo Particle Lists library (MCPL) [2] offers a great opportunity for such development.

In this presentation, we demonstrate this approach on the example of fast modelling of synthetic data suitable for use in data fitting, namely for two types of strain diffractometers: monochromatic (STRESS-SPEC, FRM-II, Garching) and time-of-flight (BEER, under construction at ESS, Lund). In both cases, the instrument response is represented statistically as a list of scattering events: coordinates of the incident and scattered neutrons together with associated detector variable (in this case the lattice parameter, d_{hkl}). This list is produced by using the simulation programs RESTRAX and McStas [3], which can be combined via the MCPL data exchange. This event list is then used as an input to an independent code which can fit various models of strain distributions to the measured data. Since the list contains complete information about the instrument needed for data analysis, the user is freed from the laborious setting of instrumental parameters - often missing in the experimental logs - and running the simulation software. Only the event list needs to be provided by the instrument team together with experimental data. The results show that this method is fast enough for use even with standard office computers, while providing much more detailed and complete description of the instrument response than alternative analytical models.

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3. McStas, A ray-trace simulation package, http://mcstas.org

The neutron time-of-flight strain/stress diffractometer EPSILON with extended sample environment for investigations in material and geoscience

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The investigation of uniaxial and triaxial stress states in geological samples is a key to a better understanding of the behaviour of *e.g.* metals, alloys, ceramics and rocks. The neutron time-of-flight strain/stress diffractometer EPSILON at the pulsed neutron source IBR-2M is equipped with different sample environment techniques to allow *in situ* deformation experiments as well as at axial and triaxial deformation conditions.

The sample environment has been extended by a triaxial pressure device to generate the axial pressure, the confining pressure, and the pore pressure, independently. This sample environment allows *in situ* determination of intracrystalline strain of porous polycrystalline materials. We developed and used this pressure device for the investigation of porous sandstone to generate the conditions in geological samples, as they occur in upper crustal reservoirs, namely depth intervals from 3,000 to 5,000 m.

Lattice spacing up to d= 5.3 Å are achievable at the time-of-flight strain/stress diffractometer EPSILON, so that lower symmetrical crystal structures with large elementary cells can be investigated.

Neutronic calculations for shielding designing of the VESPA instrument at the European Spallation Source

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The VESPA (Vibrational Excitations Spectroscopy with Pyrolytic-graphite Analysers) instrument is the only inverse geometry, incoherent inelastic instrument fully dedicated to Neutron Vibrational Spectroscopy that will be built at the European Spallation Source (ESS. Lund, Sweden), fully devoted to in-situ research for chemical and material science applications. The beamline is composed of a straight guide about 60 meters long in direct line of sight of the thermal moderator. Its guide has an elliptical profile which is designed in order to transport neutrons of a broad range of energies (0÷500 meV) and to promote the neutron flux especially in the fingerprint region (60÷220 meV) of vibrational spectroscopy.

The direct line of sight between the moderator and the spectrometer represents a challenge for the shielding design of the VESPA instrument since undesired fast neutrons and gammas can find their way down the beamline.

A detailed neutronic calculation of VESPA using MCNP software has been performed. I will present a study of the optimization of the design of the heavy shutter, the guide shielding, as well as the experimental cave shielding.

Phase imaging using pulsed polarized neutrons with Talbot-Lau interferometer

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The Talbot-Lau interferometer with three gratings has become commonly used in the field of neutron phase imaging, owing to its simple structure and relatively relaxed conditions for beam coherence compered with crystal-based interferometry. Since the neutron possesses a magnetic moment and interacts with a magnetic field, a phase shift of the neutron wave is induced by not only nuclear potentials but also magnetic potentials in magnetized materials. Because the sign of the magnetic potential depends on the neutron spin polarity, we can achieve neutron phase imaging, which is sensitive to phase shifts due to both potentials, and distinguish contributions from nuclear and magnetic induction by applying polarized neutron beams to the Talbot-Lau interferometer.

We have demonstrated this approach at the Energy-Resolved Neutron Imaging System, RADEN [1] in the Materials and Life Science Experimental Facility (MLF) of J-PARC, where it is possible to analyze wavelength dependent phenomena precisely by taking advantage of short-pulsed neutrons. Three triangular-pyramid-shaped metal samples, nickel, iron, and aluminum, were prepared as samples. A magnetic field was applied to all samples using Nb-Fe-B permanent magnets with a permalloy yoke , and nickel and iron samples were magnetized. Incident beams were polarized with a neutron polarization apparatus of RADEN instrument, which consists of a magnetic supermirror cavity, a spin flipper to flip neutron spin polarity and guide fields. Moiré fringes were observed in the wavelength range of 2-8 Å using a counting-type neutron imaging detector "μNID" [2] . The fringe analysis yielded the differential-phase-contrast image of the samples as shown in Fig. 1(a). Switching the neutron spin polarity inverted the sign of the magnetic phase shifts (Fig.1(b)). By addition and subtraction of two images obtained with the spin-up and -down conditions, we successfully produced differential-phase-contrast images derived from only nuclear and magnetic potentials, as shown in Fig. 1(c) and (d), respectively. We also attempted the wavelength-resolved analysis of the differential-phase-contrast images [3] in order to evaluate nuclear and magnetic potentials of samples quantitatively.

In this presentation, we will give a detailed description of the measurement and analysis, and discuss future prospects.

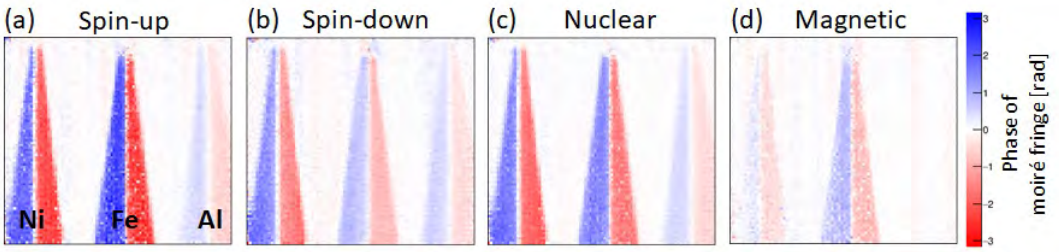

Fig. 1: Differential-phase-contrast images of metal samples in the magnetic field. (a) Spin-up condition. (b) Spin-down condition. (c) Nuclear components calculated from ((a)+(b))/2. (d) Magnetic components calculated from ((a)-(b))/2.

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Creation of a facility for radiography and tomography on channel 7B of the IR-8 reactor of the NRC “Kurchatov Institute”

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On the tangent channel 7B of the research reactor IR-8, the Kurchatov Institute research center a prototype experimental setup is created for conducting research using the method of high resolution neutron radiography and tomography. A polychromatic beam of thermal neutrons with a cross section of 50 x 40 mm is formed by a system of collimators, for which the value of the collimation parameter L / D = 625. The image is recorded by the mar345 detector and Imaging Plate plates. The report will present the results of the first radiographic experiments conducted on a new facility using neutron and reactor gamma radiation on samples representing various branches of science and technology (materials science, paleontology, archeology, additive technologies, etc.).

The study was supported by RFBR according to the research project № 18-32-00262

Neutronics and everyday life at a neutron source

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The role of neutronics expert (nuclear physicist) at spallation neutron source, or research reactor, or any similar neutron production “factory” is, typically, to: create and use the Monte Carlo model of the facility to help the instrument scientists to get maximum from their instrumentation [1]; calculate the build-up of radionuclide inventories in activated materials [2] and perform measurements of particle fluxes and radiation dose rates in operational environments [3].

While the results of these activities are very useful for a facility in question and the broader scientific community, the most interesting and challenging tasks in the life of a nuclear physicist at a neutron source are to use the simulation codes to solve some of the operational issues any of the facilities suffers from time to time.

Several examples from ISIS Neutron and Muon Source (United Kingdom) about the power of state-of-the-art Monte Carlo codes in resolving the operational issues or addressing the open questions about the neutron source performance will be presented.

Special attention will be paid to the attempt to characterize the ortho/para hydrogen ratio in the ISIS TS-1 hydrogen moderator. The main idea applied in this study was that wavelength dependence of the variations of count rates from corresponding neutron instruments, if combined with Monte Carlo simulation results, could give a reliable indication about the ortho/para conversion in the hydrogen moderator. The results of this analysis were later confirmed in the direct measurement of the neutron transmission through thin hydrogen samples (with different para-hydrogen fractions) using the VESUVIO instrument at ISIS [4].

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Relocation of the cold triple axis spectrometer FLEXX to MLZ, Munich: Larmor diffraction and more…

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The cold triple-axis spectrometer (TAS) FLEXX at HZB is a well-designed and recently upgraded instrument [1-4]. There is a strong wish that this excellent instrument should be preserved for the community after shutdown of the HZB neutron source. One attractive gap in the present instrumentation suite, which could be filled by FLEXX, is the Larmor-diffraction technique [5-6] (LD) and, as a natural extension, cold neutron NRSE. LD permits the exact measurement of lattice constants and their distribution: the latter arising, for example, from internal strain, from a small splitting of Bragg peaks due to structural distortions or magnetostriction. In addition, spin correlation lengths in antiferromagnets and antiferromagnetic domain sizes of up to 1 µm can be determined with high accuracy. For looking at time-dependent processes one needs to switch to the NRSE mode.

The instrument will be placed on a cold neutron source. This will allow for a four-fold increase in Q resolution, as well as most importantly access to the low Q region, as compared to the existing TRISP@MLZ. Further, new developments are under way to allow for application of magnetic fields at the sample, hitherto not possible [7-9]. This opens up new vistas in the exploration of materials, magnetic or not. A last attractive gap to be filled within MLZ, is the possibility to combine high magnetic fields together with cold TAS.

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MARMOT - New generation multiplexed analyser unit for cold Triple Axis Spectroscopy

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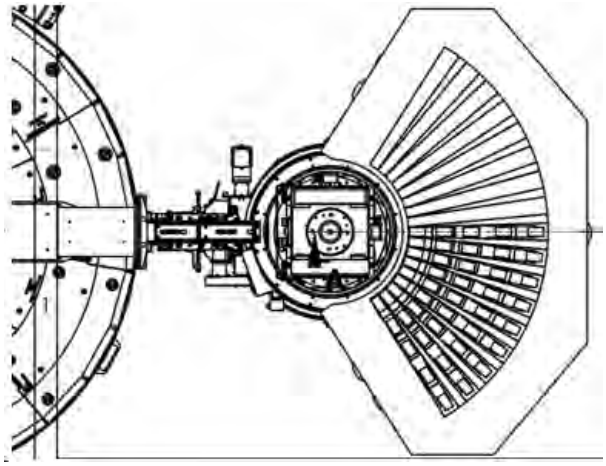
The Multiplexed array for mapping on ThALES (MARMOT) is a multiplexed analyser-detector stage for the cold three axis-spectrometer ThALES covering a scattering angle of maximum 100 degrees and multiple analysers in every channel. As its predecessor FlatCone it is foreseen as an interchangeable analyser-detector unit replacing the classical secondary spectrometer of ThALES for applications necessitating a coverage of the whole, or several Brillouin zones with data collection at a range of evergy transfers simultaneously.

By increasing the data acquisition rate by one or two orders of magnitude while maintaining the good energy and momentum resolution that makes the strength of cold triple axis spectroscopy, it will enable a rapid overview in the exploration of new systems and open new possibilities in particular for the study of the dynamics of materials with broad features in $S(Q,\omega)$ such as strongly frustrated, low dimensional or disordered systems.

In contrast to other spectrometers, we use silicon as analyser material, thereby optimizing the signal-to-noise ratio and the resolution.

Currently in its design phase, we expect MARMOT to be available in 2021 and, together with the worldwide unrivalled neutron flux of the ThALES spectrometer, open new horizons for cold Triple Axis Spectroscopy.



Hardware project for the texture diffractometer (TEX) as an element of the instrumental base of the PIK reactor

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The main goal of the project is to create an automated research system (ASRI) for the entire instrument base of the PIK reactor complex.

For this purpose, the first software and hardware complex for the specialized four-circle diffractometer (TEX), designed for texture investigations of various types of polycrystalline materials, has been created. The complex is based on the Tango Controls framework and programmable logic controllers (PLC).

The implemented system manages and controls the monochromator, the sample assembly, the monitor, the PSD using peripheral devices such as stepper motors, pneumatic valves, and relay switches. In turn, the system monitors the states of limit switches, position sensors (encoders), pressure in the pneumatic system, information processing from the monitor and the PSD.

This project was implemented using controllers manufactured at NRC «Kurchatov Institute» - PNPI and amplifiers manufactured by Phytron.. Due to this decision, it is possible to quickly switch to PLC systems of other manufacturers, changing only the logical and software part of the control without changing the power part. This feature ensures the operational reliability of the system as a whole.

Using a new type of chopper in neutron reflectometry

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The neutron chopper of a new type for time-of-flight (TOF) measurements is proposed in [1, 2]. This is neutron disc bandpass chopper. With the help of this chopper it is possible to form a neutron spectrum of the required width and range, reduce TOF measurement time, completely to eliminate the undesirable contribution of long-wave neutrons. Using the proposed chopper in a three-disk version will allow to the above-mentioned advantages is added possibility to carry out TOF measurements with a constant relative resolution over the wavelength in a wide range of wavelengths.

It is shown that with the help of the proposed chopper one can significantly to improve the resolution over the wavelength for neutron facilities on monochromatic beams (for instance, neutron reflectometer SuperAdam) by carrying out TOF measurements on these beams.

The report discusses the use of the proposed chopper in the polarized neutron TOF reflectometer LIRA (PIK reactor, PNPI) with a vertical scattering plane. There is no frame overlap mirrors in this reflectometer.

The all advantages of using the proposed chopper in neutron reflectometry compared to the well-known chopper [3] are shown.

The work was supported by the Ministry of Education and Science of the Russian Federation, Agreement No. 14.607.21.0194 of September 26, 2017 (project No. RFMEFI60717X0194).

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SEMSANS with RF flippers: calculation and realisation

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Spin Echo Modulated SANS (SEMSANS) is an alternative for SESANS where, in contrast to SESANS, all the spin manipulation is performed upstream of the sample and a modulated intensity beam is created on the detector plane. Scattering from a sample (USANS) will reduce the amplitude of this modulation, like in SESANS, and data analyses can be treated with the SESANS formalism.
To create this modulated intensity pattern on the detector plane a certain magnetic field arrangement needs to be constructed. So far this has been realised with triangular field coils [1], tilted foils in DC magnets [2] and super conduction Wollaston prims [3]. We would like to present calculations and measurements that show this can also be realised with RF flipper setup. The advantage of such an arrangement is that there is almost no material in the beam (no parasitic scattering) and the instrument is very stable as the echo is determined by the stability of the frequency and not DC fields (frequency generator versus DC-power supplies). Calculations also show that the instrument can be compacted to table top size making it suitable as an add-on component on a SANS or imagine instrument adding the SEMSANS, 20 nm 10 µm length scale in case of SANS instrument.

We would like to present an overview of the magnetic field calculations, performance calculations as well as experiments performed on the V20 ESS test beamline.

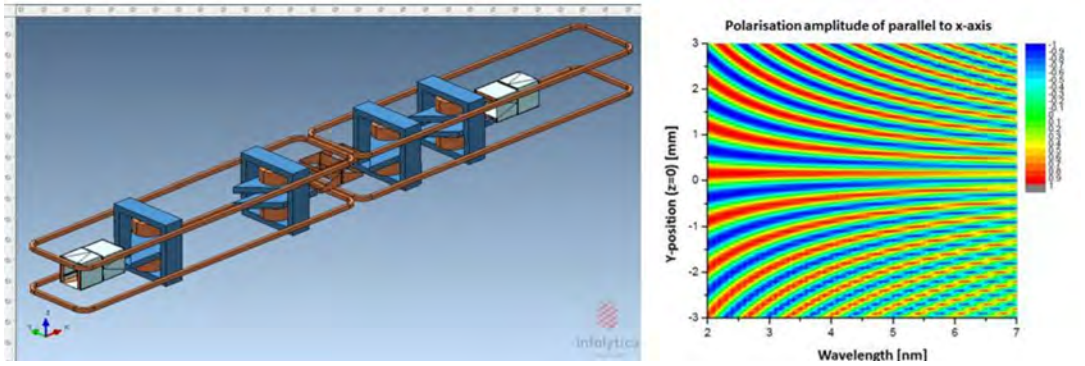

Fig. 1. On the left the model for field calculations of a RF based SEMSANS instrument and on the right the result of a line-integral calculation that creates a modulation pattern.

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Capabilities of applying neutron Laue diffraction

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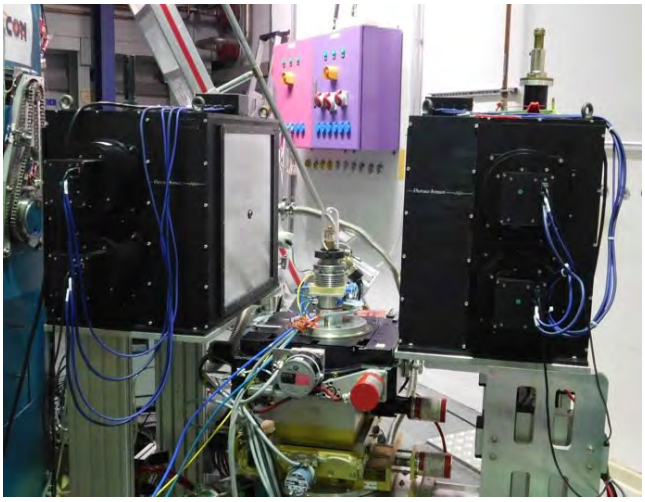
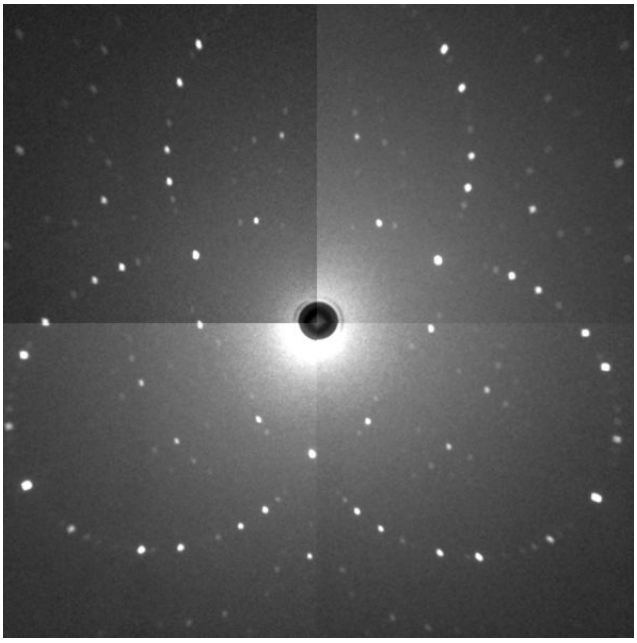
The FALCON Laue diffractometer at the Berlin neutron source BERII was developed in collaboration with the ILL, Grenoble. It is designed for fast neutron Laue data acquisition and makes use of a white (“pink”) neutron beam with wavelength band of 0.8-3.2 Å. Pattern acquisition is performed by means of a backscattering and a transmission detector consisting of four iCDD cameras each. Recent investigations on Ca-Nd-Vanadite and Ba-Ni-Phosphate single crystals will be presented. A further example will illustrate the usage of Laue neutron diffraction to perform 3D grain distribution mapping and indexing of oligocrystalline sampes (Raventos et al., arXiv:1902.03200v1).



FALCON: Backscattering and transmission detector



Transmission Laue image of Ca9Nd(VO4)7

Multichannel scintillation neutron detector for microsample research under high-pressure

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A multichannel scintillation neutron detector was designed and built for an installation for the study of microsamples under the high pressure of the IR-8 reactor of the Kurchatov Institute. The detector consists of 9 modules of 16 detectors. Each detector is a single 50x5 mm linear scintillation detector. Two ZnS: Li^6 scintillator plates with an efficiency of 48% are located on both sides of the optical fiber(fig. 1), light is emitted using SiMP.Thus, it is possible to achieve a neutron registration efficiency (λ = 1.8 Å) of 75%[1], and the use of a coincidence circuit in the amplifier-former completely eliminates the intrinsic noise of the detector.

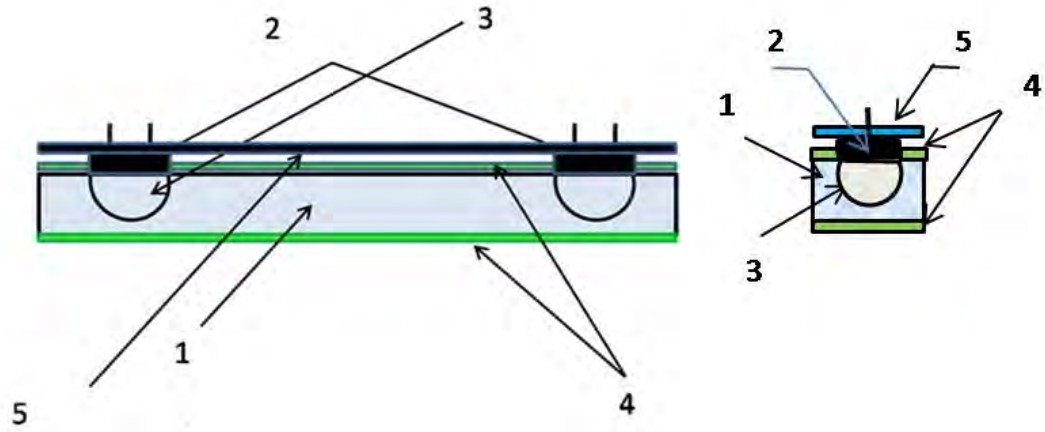

Figure 1. Schematic diagram of a single detector
1. Light guide made of organic glass or polystyrene.
2. Avalanche diodes SiPM.
3. The optical lens implemented in the optical waveguide.
4. The scintillator ZnS (Ag) / LiF
5. Backplane.

Each module is equipped with a 16 channel pulse counter with a CAN interface. The modules are united by a common protection consisting of boropolyethylene. The detector is located on the ring gear rack and is equipped with a stepper motor with an encoder to adjust it to the desired angle.

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Present status of the ANDES, a multi-purpose neutron diffractometer for LAHN

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The Argentinean Atomic Energy Commission (CNEA) is building a multi-purpose research reactor in Centro Atómico Ezeiza, 30 km from Buenos Aires Argentina, with commissioning planned for mid 2020. The RA-10 will be an open-pool facility for radioisotope production, materials and fuel irradiation, silicon doping and neutron techniques applications. Associated to this last goal there is a separate project to build the Argentinean Neutron Beams Laboratory (LAHN), also executed by CNEA and funded by the National Government. The first stage of LAHN project includes two instruments of particular application in (nuclear) materials research and development. One of them is ANDES (Advanced Neutron Diffractometer for Engineering and Science), a multi-purpose neutron diffractometer for materials science and engineering applications, able to perform a variety of analysis, both on intact objects and on small samples. The techniques available include strain scanning, texture measurement, and high intensity powder diffraction on a variety of environments. The development of this instrument is supported in 4 main areas: shielding design, mechanical engineering design, neutron optics and automation and control. In this work we present the advances in the design of the instrument.

Compact neutron supermirror transmission polarizer for SANS

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A new compact neutron supermirror transmission polarizer for SANS is proposed in [1, 2]. This polarizer is considerably more compact then a V-cavity. The polarizer consists of a set of plates transparent to neutrons placed in the magnet gap. There are no air gaps between the plates. A polarizing supermirror coating without absorbing underlayers is deposited on the polished surfaces of the plates. Magnetic and nonmagnetic layers of the supermirror coating as well as the material of the plates have nearly equal neutron-optical potentials for spin-down neutrons. There is a considerable difference, however, between neutron-optical potentials of layers in the supermirror structure for spin-up neutrons. This leads to reflection of spin-up neutrons by the supermirror coating and thus to their removal from the original trajectory or, in other words, from a direct beam. In contrast, spin-down neutrons are not reflected by the coating and, consequently, keep their initial trajectories. As a result, that part of the transmitted beam which propagates along the axis of the incoming beam contains vastly larger number of spin-down neutrons what makes this part of the beam highly polarized.

The compact polarizer on silicon plates with supermirror *CoFe/TiZr* (m = 2) coating has been designed and produced at PNPI.

Experimental results obtained on the polarized neutron reflectometers Super ADAM and D17 (ILL, Grenoble, France) will be presented in details.

The work was supported by the Ministry of Education and Science of the Russian Federation, Agreement No. 14.607.21.0194 of September 26, 2017 (project No. RFMEFI60717X0194).

[1] V.G. Syromyatnikov. Russian patent N 2624633 for an invention. Priority from 21.06.2016.

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Using the LSWT engine SpinW in an experimental workflow.

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[2]

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Measuring spin-wave excitations in magnetic materials has been one of the great successes of neutron scattering. Until recently most researchers had to implement linear spin-wave theory (LSWT) on their specific system themselves, a long, complex and arduous task. SpinW is one of the most successful LSWT simulation libraries. Features include the generalization to arbitrary crystal structures, symmetry, exchange (both symmetric and antisymmetric) interactions and anisotropies to calculate the observed spin-wave spectra in a time efficient manner. The use cases of SpinW will be explored with real life examples, exhibiting the unique features of SpinW and how it can fit in an experimental workflow, integrating with Horace data analysis codes. With limited beamtime available, it is becoming essential to pre-plan and understand your measurement before the experiment. As such, it will also be shown how to optimize measurements, not just for obtaining high quality data, but also for model determination. The future of SpinW will also be explored since it is now being developed as part of the supported ESS software suite. This includes the work on optimizing the code for the high throughput needed at the ESS and the work on moving to free and open source software.

3D printed humidity chamber for neutron scattering experiments

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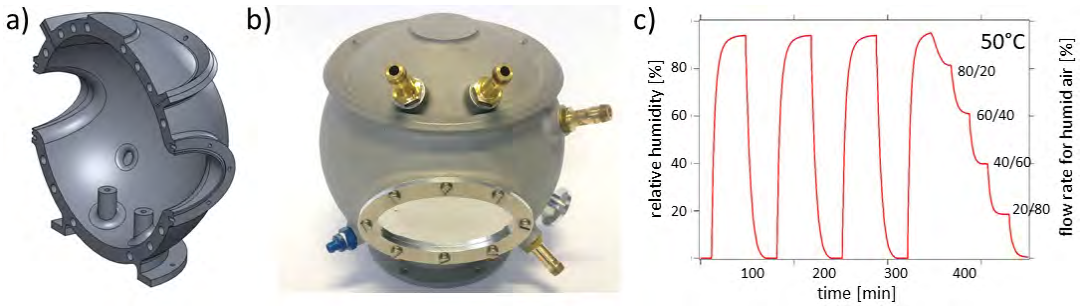
The investigation of organic thin films with neutron scattering techniques such as grazing incidence small angle neutron scattering (GISANS) or neutron reflectometry (NR) allows a non-destructive probe on the inner film morphology. This is especially interesting for films that undergo changes in lateral and vertical structure as well as in film composition due to an external stimulus. As stimuli-responsive materials can be sensitive to a change in temperature, humidity or other environmental conditions, a sample environment is needed that gives precise control over the necessary parameters.

In the framework of the FlexiProb project, which plans a flexible and interchangeable sample environment for various neutron experiments at the European spallation source (ESS), we designed a sample environment for GISANS experiments in varying environmental conditions. Its core is a 3D printed aluminum chamber as shown in figure 1a and 1b, which can be connected to an external gas and fluid flow. The chamber is designed spherical to reduce condensation inside and to provide a uniform heat distribution around the sample. For that purpose, fluidic channels through the chamber walls and lid visible in figure 1a minimize head gradients throughout the chamber. The gas-flow can be composed of up to three different gas streams, each one individually controllable. This can provide pure gas or solvent atmospheres, or allows the mixing of the gas composition to the desired specifications as shown in figure 1c. To demonstrate its options, thin polymer films are humidified and investigated with neutron scattering techniques.



Progress in simulation software, shielding methods and compact Larmor devices: A status report from SINE2020 WP8

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Within the scope of WP8[1] in the EU project SINE2020[2], our collaboration has worked on multiple tasks to pave the way for future European neutron sources:

1. New methods (e.g. MCPL[3]) have been developed for realistic source-to-end simulations of instruments, based on both neutronics (e.g. MCNP[4]) and Monte Carlo ray-tracing (e.g. McStas[5], SIMRES[6] and Vitess[7]).

2. New equipment has been developed to assess background generated by high-energy particles from modern spallation sources and new types of shielding[8,9] have been developed to suppress these backgrounds and improve signal to noise. Short and longer term effects of irradiation have further been assessed.

3. Effective parameters to enable compact, modular Larmor-based devices for the ESS have been derived[10].

On behalf of the international collaboration, the contribution will highlight the main results achieved in SINE2020 WP8.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000

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4. T. Goorley, et al., "Features of MCNP6", 2013, Paris, LA-UR-13-28114 (2013)
5. P. Willendrup et al., Journal of Neutron Research 17 (2014) 35–43 and mcstas.org
6. J. Šaroun, et al. Nucl. Instr. and Meth. A, **634**, Issue 1, Supplement, 1 2011, pp S50-S54
7. See Vitess website
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Time-of-flight spectrometer TOFTOF at FRM2

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TOFTOF is a direct geometry disc-chopper timeof-flight spectrometer located in the Neutron Guide Hall West. It is suitable for both inelastic and quasielastic neutron scattering and the scientific questions addressed range from the dynamics in disordered materials in hard and soft condensed matter systems (such as polymer melts, glasses, molecular liquids, or liquid metal alloys), properties of new hydrogen storage materials to low-energy magnetic excitations in multiferroic compounds, and molecular magnets.

A cascade of seven fast rotating disc choppers which are housed in four chopper vessels is used to prepare a monochromatic pulsed beam which is focussed onto the sample by a converging supermirror section. The scattered neutrons are detected by 1000 3He detector tubes with a time resolution up to 50 ns. The detectors are mounted at a distance of 4 m and cover 12 m^2 (or 0.75 sr). The high rotation speed of the chopper system (up to 22 000 rpm) together with a high neutron flux in the wavelength range of 1.4 -14 Å allows free tuning of the energy resolution between 3 meV and 2 µeV.

The 60 m primary neutron guide has an s-shape which efficiently suppresses fast neutron background. This enables the investigation of weak signals. The prototype of a new focussing neutron guide has been installed recently, as alternative option in the last section of the guide system. The existing linearly tapered neutron guide yields a beam spot size of 23 x 47 mm^2. Using the focussing guide, an intensity gain up to a factor of 3 (wavelength dependent) is observed on a sample area of 10 x 10 mm^2.

TOFTOF represents a versatile instrument combining high energy resolution, high neutron flux (also
at short wavelengths), and an excellent signal-tobackground ratio. It is perfectly suited for both inelastic and quasielastic neutron scattering and scientific topics include e.g.:

• Diffusion in liquid metals and alloys
• Hydrogen dynamics in soft matter systems such as molecular liquids, polymer melts or colloids
• Molecular magnetism, quantum criticality in heavy fermion compounds, low energy excitations in multiferroic materials and novel magnetic phases
• Dynamic properties of energy storage materials, such as solid state hydrogen storage materials, electrolytes for batteries and fuel cells, or gas storage materials
• Energy-resolved quasi-elastic neutron scattering on proteins, vesicles, and biological materials
• Kinetic studies of hydrogen binding, e.g. in concrete
• Aging effects in disordered media and low frequency dynamics in glasses
• Biological activity and functionality of proteins and cells under pressure

Multiple Bragg reflection by mosaic crystals

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We study multiple Bragg reflection from a thick, ideally imperfect crystal by analytical means. The two-ray transport equations of Darwin (1922) and Hamilton (1957), fully solved by Sears (1997), were generalized for out-of-plane trajectories, and measurable corrections to the two-ray approximation were predicted by Wuttke (2014). We now present an efficient numeric solution method, based on a transfer matrix for discretized directional distribution functions.

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Neutron field spectrometry at high energy neutron facilities with extended range Bonner Sphere Spectrometer system

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The shutdown of a SINQ is ongoing to exchange the guides of all cold instruments and improve the shielding of the neutron guide bunker.

Understanding the neutron field at different locations is essential in designing the new high-performance shielding since the source of high-energy neutrons can then be attenuated with effective materials at optimal positions. A Bonner Sphere Spectrometer (BSS) is one of the attractive methods to measure the neutron spectrum over a broad energy range. The energy coverage of a standard BSS system is from $1x10^{-9}$ (thermal) to $2x10^{1}$ MeV (fast) and can be extended above 1 GeV. We are currently developing a in-house mobile Extended Range BSS system (PSI-ERBSS) with collaboration with other departments within PSI.

We have carried out a set of measurements at 6 m and 12 m distances from the SINQ-target in the neutron guide bunker. The unfolded energy spectra were consistent to the ones simulated with MCNP. Therefore, the model of simulation was validated and used for the new shielding design for the SINQ upgrade.

We have extended the PSI-ERBSS to in-beam measurements where the spheres are under illuminated using the dedicated shielding and the fast neutron imaging. While the shutdown for the SINQ upgrade, we are planning to conduct further measurements at other neutron facilities outside of PSI.

The development of new shielding materials will be presented as well in the talk.

Recent Issues from Taiwan's cold triple axis spectrometer SIKA at ANSTO.

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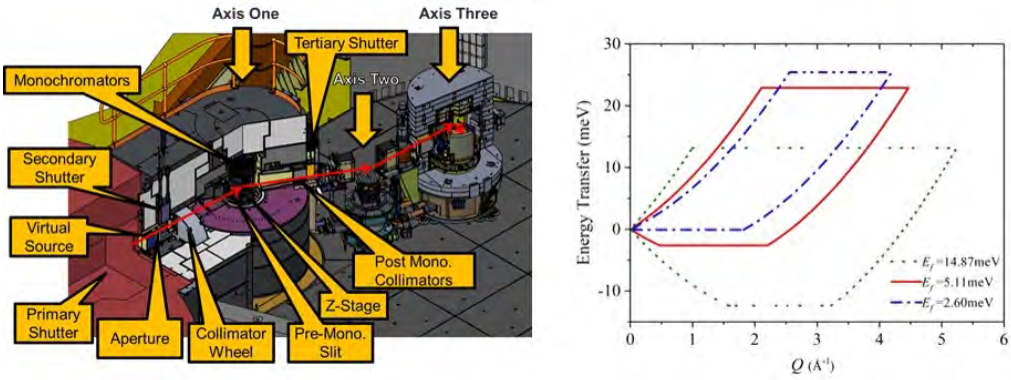
Triple axis spectrometers have been one of most versatile neutron scattering instruments for many areas of condensed matter physics. With using cold neutron, triple axis spectrometer can investigate physical phenomena with high energy and momentum resolution.

In this presentation, I present Taiwanese built cold triple axis spectrometer SIKA at OPAL reactor in Australian Nuclear Science and technology (ANSTO). The SIKA project has been funded by the Ministry of Science and Technology Taiwan to build a cold neutron triple-axis spectrometer at the OPAL reactor in ANSTO since 2005. We are now running user program since 2015 July. The components, capabilities, sample environment, software, and statistics will be presented in this talk.

Then, I present some of our recent scientific outcomes from SIKA. We are working on magnetic scattering from Cu spin chain systems with dilution fridge, new Kagome lattice antiferromagnets under magnetic field, magnon excitations from thin-films and single crystals, phonon dispersion from thermoelectric materials, and so on. We are expecting more to come.

After that, I present current issues on SIKA. We are working on several upgrades. To accommodate 3He Polarization analysis system, we are implementing automation of arms for sample stage and analyzer drum. Also, position sensitive detector (PSD) is under repair. With using PSD, SIKA will have capability of multiplexing analysers. The results from these commissioning will be presented.

Finally, we would like to cultivate users. We are getting healthy number of Taiwanese users while we would like to have more users from European and the other Asian countries. I hope audience in this conference will be interested in SIKA.



Figures (Left) Layout of triple axis spectrometer SIKA (Right) Accessible ranges of the momentum and energy transfer of SIKA at various final energies

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Setup for in situ Neutron Reflectometry on Magnetic Thin Films

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Magnetic thin films and heterostructures thereof are used in many electronic devices. A thorough understanding of the coupling between structural, electronic and magnetic degrees of freedom is essential to improve their functionality and investigate novel aspects like multiferroicity or skyrmion lattices. In order to prepare high quality samples, i.e. avoid incorporation of impurities or surface contamination, these layer structures have to be grown under ultra-high vacuum (UHV) conditions.

For the analysis of the structural and magnetic properties of magnetic thin film samples, the technique of polarised neutron reflectometry (PNR) is excellently suited. Conventionally, the sample growth and analysis are spatially separated: The fully grown samples are typically transported from their growth chamber to the beamline for analysis, which exposes them to ambient conditions. The required protective capping layer or the exposure of the sample can influence or alter the properties of interest.

In this contribution, a compact *in situ* ultra-high vacuum sputter deposition chamber for performing *in situ* PNR experiments is presented [1]. It combines deposition and measurement capabilities into one single device. Its design allows installation at various neutron beam lines, typically REFSANS at MLZ, Germany, and AMOR at PSI, Switzerland. At the latter, we can perform PNR for both non-spin flip channels up to Q_z=0.1Å^{-1} within 30 minutes [2, 3], using the focusing Selene neutron optical concept. The sample environment can provide a variable temperature of 10K - 1000K and a magnetic in plane field of up to 300mT across the sample. This setup opens new opportunities for investigating the magnetic properties of a large variety of novel materials and material combinations as a function of their film thickness and composition, both on one single sample and at different subsequent deposition steps.

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Suite of the Neutron Spectrometers in J-PARC

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The spectroscopy for material science is one of powerful tools to investigate the mechanism of physical properties. For deep understanding of the dynamics in physical degrees of freedom, dynamical structures $S(q, E)$ should be measured in wide area of momentum and energy space. To realize the wide coverage of $q$and Espace, six inelastic spectrometers with different concepts are now part of spectrometer suite in MLF [1]. The spectrometers 4SEASONS, HRC and AMATERAS are direct geometry instruments utilizing Fermi or disk choppers to select the neutron energy. The set of chopper spectrometers covering wide momentum and energy space enables us to realize various researches in diverse field. Another is DNA indirect geometry instrument. A very high energy resolution can be achieved with silicon crystal analyzer and high speed pulse shaping disk choppers. This spectrometer is suitable to investigate dynamical behaviors of proteins, such as human α-synuclein, which form amyloid fibrils. VIN ROSE and POLANO are younger generation of spectrometers in MLF. VIN ROSE is a neutron spin echo instrument with MIEZE- and NRSE-type just opened for user program. Spin echo spectrometer can be achieved the highest energy resolution for investigating slow dynamics in soft matter materials. POLANO is a chopper spectrometer with capability of polarization analysis. The main construction was completed and started unpolarized beam commissioning. Since higher energy polarized neutron experiments up to 100 meV is the target range of the research field in so-called strongly correlated electron systems, final goal of polarization energy is *over* 100 meV in POLANO. Including the POLANO, all 6 spectrometers at MLF are now in operation and open for user program. In this presentation, recent instrumental upgrade and development of devices will be reported as well as remarkable scientific outcomes.

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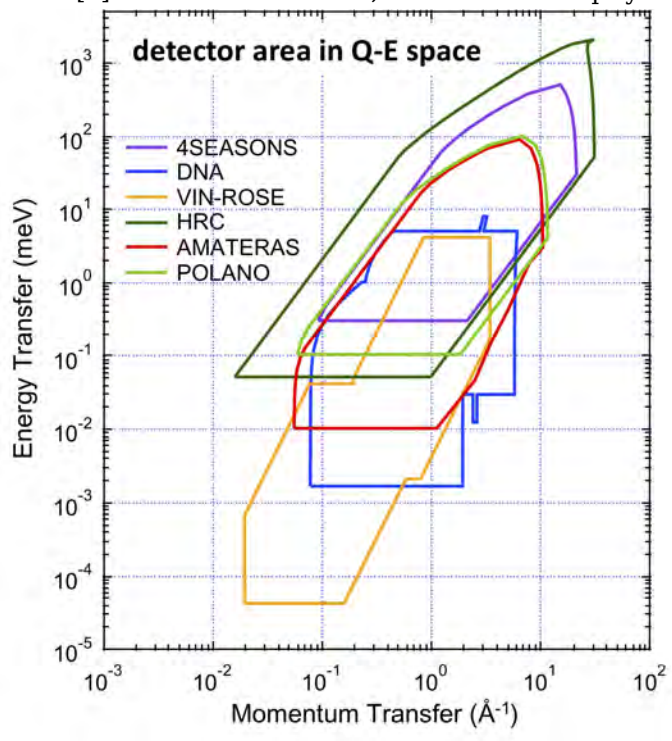

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Since the beginning of 2018, the neutron imaging instrument NECTAR at FRM-II is now ready to switch between different neutron energies for imaging. Apart from the well-established radiography with fission neutrons using the converter facility, NECTAR is now prepared for using thermal neutrons, enabling radiographies with high spatial resolution of at least 100µm.

The NECTAR instrument was originally designed for imaging with fission neutrons. Over the past years, the request for high-resolution thermal neutron imaging was increasing rapidly and a major revision was made to prepare NECTAR to a state-of-the-art facility for this demand. Numerous new equipment such as collimators, flight tube and detector system were designed. The current status of these updates for the NECTAR instrument will be presented.

Free-Film SANS – Container-free in-situ sample environment for neutron scattering

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In-situ small angle neutron scattering (SANS) provides valuable insights into soft matter systems, such as micelles, biological macromolecules or nanoparticle formation. Any scattering experiment is limited by the signal to noise, such – for instance - the detection of ligand shells during nanoparticle formation. For SAXS free-jet setups are established, but the counterpart for SANS was missing, as SANS requires large sample cross sections. [1,2] Here, we introduce a novel free-film setup, where the neutrons only penetrate a flowing liquid film optimized to a sample area of 180 mm^2 with an average film thickness of 0.5 mm as determined from the incoherent scattering of the film. [3] In order to suppress H/D-exchange from the humidity in the air for the operation of the setup with deuterated solvents, we jacketed the setup in a containment filled with Helium. To validate the H/D-ratio over time, three independent methods have been used: IR, gravimetry, incoherent neutron scattering. The main benefit of the free-film is the reduction of the background scattering by 37 % in comparison to measurements in a standard Hellma cell as typically used for SANS. Furthermore, we showcase the setup for the formation of EDTA-capped CdS nanoparticles, in order to investigate the role of the weakly scattering EDTA ligand shell in the nucleation process, having been inaccessible so far.

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Topological Interactions In Polymers Under Shear

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Entangled polymers show unique flow behaviors, since the relaxation processes occur on time scales relevant for our daily lives, ranging from milliseconds to hours or even days. Yet, due to experimental limitations, the nonlinear rheological behavior of complex fluids is only modestly understood. The reptation model, which is currently the best theory to describe polymer dynamics was developed by de Gennes, Doi and Edwards in the early 1970's[1]. It assumes a tube-like confining field restricting the motion of a single chain and originating in topological interactions between polymer chains. The model is exceptionally successful in explaining viscoelastic properties of polymeric fluids and predicting the experimentally observed scaling laws[2]. However, till now it only describes the topological interactions in a macroscopically static case. Polymer dynamics at a molecular level remain yet largely undisclosed for polymeric fluids under deformation.Under flow, the fluids display dramatic changes, like shear thinning which are expected to be associated with changes in the topological interactions at the smallest scales. To explain the macroscopic observable effects, models suggest convective constraint release (CCR) as an additional relaxation mechanism[3][4], total disentanglement, entangled layers slipping past each other, as well as disentangled layers interacting with each other. However, on molecular length scales these theories are difficult to test since the Weissenberg effect makes shear experiments exceedingly difficult. Heretofore, small angle neutron scattering (SANS) studies revealed shear-induced conformational changes at elevated shear rates in polymeric coils in solution as well as in melts[5].

In the past neutron spin echo (NSE) provided indispensable information that allowed to understand the nature of the topological interactions that govern the macroscopic behavior in polymeric fluids through testing the predictions of the reptation model[6]. Establishing rheological measurements in NSE provides the possibility to directly monitor molecular interactions in flowing media and thus a way to explore the physical mechanisms responsible for non-Newtonian flow phenomena, many of which are still not understood.To make the measurements possible, we constructed a fully non-magnetic shear device for NSE. Doppler scattering results in a phase shift of the detected echo, which depends on the macroscopic velocity as well as the wavelength. For a distribution of velocities, a spread of Doppler-induced phase shifts results in a net depolarization of the beam and a damping of the echo. This can result in an apparent faster decay of the intermediate scattering function. In the presentation, we will show SANS and NSE data on entangled polymer solutions and melts (Polystyrene, PDMS) under non-Newtonian flow, as well as the comparison of Doppler effects in simulation and NSE data.

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Microscopic origin of the scattering in aqueous amine mixtures: X-ray and neutron experiments versus simulations

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The structure of aqueous amine mixtures is investigated through X-ray and neutron scattering experiments, and the scattered intensities compared with computer simulation data. The variation of structure factor peak positions and intensities are followed for different compositions. The detailed analysis of the various atom-atom structure factors and snapshots indicates the presence of a significant microstructure, which produces correlation peaks in the atom-atom structure factors, positive for like species atoms correlations and negative for the cross species ones. Distinct differences are seen in the structure of aqueous amines and aqueous alcohol or aqueous DMSO solutions. The peculiar role of water interactions with the amine headgroup and its connection to the microstructure is explained with the help of molecular simulations.

Glucose oxidase from Aspargellius niger studied by small angle neutron scattering

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Conformational stability of biological macromolecules is one of the major problems for biotechnology, pharmaceutical and food industry. Defining a technique suitable for studying the protein conformation is essential for optimizing the properties of proteins. Although considerable research has been devoted to the structure, conformation stability and mechanisms of interactions of glucose oxidase, there is still a continuous interest in studying the properties of this protein to extend its bio-applications.

Glucose oxidase is an enzyme, mainly known as catalyst of the oxidation reaction of β-D-glucose to glucono-β-lactone and H_2O_2, using molecular oxygen. It is a member of the glucose-methanol-choline oxidoreductases family. The glucose oxidase monomer with a molecular weight of 80 kDa consists of a single polypeptide chain of 583 amino acids that are organized mostly in α-helix and β-sheets structures. The monomer chain is folded into two domains and has one non-covalently bound molecule of flavine adenine dinucleotide. The catalytic activity of glucose oxidase and its bio-applications are mainly limited by the conformational stability.

The purpose of the present study is to ascertain the conformational stability of glucose oxidase from *Aspergellius niger* in the optimal environment that presumably preserves its functional properties using small angle neutron scattering (SANS) method. The functional oligomeric state of glucose oxidase is a dimer, although evidence from the X-ray crystallographic structures of the monomeric and tetrameric forms is also available (PDB entry 3qvr, 1gpe and 4moe). Using SANS it was shown that at pH 5.9 in HEPES buffer solution of 100% D_2O and a concentration of 15 mg/mL, glucose oxidase exists in a dimeric state. Also, the low-resolution three-dimensional models of glucose oxidase from *Aspergellius niger* was computed based on SANS results. The results indicate that glucose oxidase neutron scattering structure adopts a slightly more relaxed structure comparing to the compact X-ray high resolution model with a maximum particle dimension, D_{max} of 110 Å and R_g of 34.50±0.02 Å.

Structure organization of silicone-rubber based magnetic and magnetorheological elastomers reveled by means SANS and neutron depolarization methods

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Filling elastomer matrices with ferromagneric nano- and microparticles, specific classes of "smart" composites, magnetic and magnetorheological elastomers (MEs and MREs) are formed. Complex internal structural effects at different length scales that occur under external stimuli control the macroscopic properties of these composites and provide them with a wide range of applications: automotive bushings, engine mounts and adaptively-tuned vibration absorbers and isolators; vibration and seismic shock dampers; sensors and transducers for deformations and mechanical tensions; magnetic field sensors and actuators, coatings, implants and prostheses, etc.

In the present work results on small angle neutron scattering and neutron depolarization techniques applied for the microstructural investigation of such composites, are reviewed and discussed.

The analysis of structural features of silicone rubber and ensemble of embedded Fe_3O_4 particles as resulted from the conditions of preparation of MRs by the variation of particle concentration and the strength of a transversal magnetic field (TF) applied during the polymerization process, have shown a stronger effect on the interparticle correlation distance value is obtained by increasing the particle concentration (for moderate and high particle concentrations), than by imposing during the polymerization process higher values of magnetic field; contrary to this fact, for small particle volume concentrations, have been found that the magnetic field applied during the polymerization process affects the interparticle correlation distance to a considerable extent.

In a series of elastomeric samples composed from silicone rubber and ferrofluid and polymerized in an applied longitudinal magnetic field (LF) and without, a "magnetostrictive effect" was revealed.

Further, silicone rubber-based magnetorheological elastomer with carbonyl iron microparticles samples were analyzed by means of neutron depolarization (ND) method and differences in their magnetic structure depending on the particle concentration and polymerization in and without applied magnetic field revealed.

Acknowledgments

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Small-angle scattering of interpenetrating polymer networks (IPNs) as medical devices with reduced risk of infection

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A common material for urinary catheters is a hydrophobic polymer, silicone elastomer. The properties of silicone make it well-suited for producing medical devices; it has favourable mechanical properties and is chemically inert. However, this hydrophobic surface makes it prone to the adhesion of bacteria and subsequent rapid formation of biofilms. The bacteria that grow in biofilms tend to be resistant to antibiotic treatment, which is a serious problem. Device-associated infections present a real challenge in modern medicine, and therefore, generating materials that resist bacterial attachment and biofilm growth is a worthwhile development for reducing the number of infections.

To reduce the adhesion of bacteria and the risk of infection, at BioModics, we have produced silicone catheters and medical devices that are functionalised by the inclusion of a hydrophilic hydrogel interpenetrating polymer network (IPN). The hydrophilic polymer network is introduced by treating the hydrophobic silicone with supercritical carbon dioxide (at elevated but easily accessible temperature and pressure). This expands the silicone network, and then hydrophilic monomers are introduced to react and form an IPN within the silicone network. This hydrogel not only reduces the risk of infection, but it also has the potential to act as a drug delivery mechanism. The IPN act as a reservoir for hydrophilic small molecules that can be suspended and then controllably released at site from the IPN-impregnated silicone.

The release properties are dependent on the morphology of the IPN. However, it is a challenge to get insights to the micro structure of the IPNs. Therefore, we have performed small-angle scattering measurements (with both X-rays and neutrons) to investigate the distribution of the polymer molecules within the IPN. X-ray measurements are sensitive to differences in electron density, and they primarily revealed the structure of the inorganic filler in the silicone. Neutron measurements are sensitive to isotopes, and by introducing water or heavy water (D_2O) to the IPN, we were able to observe the distribution of water and the hydrophilic domains. Furthermore, we have performed spin-echo small-angle neutron scattering to investigate structural inhomogeneities at longer length scales. We will discuss the insights into the nanoscale structure of these materials obtained with neutron scattering techniques, and how the structural information can be used to understand functional properties and assist in optimisation of the materials for the future.

Elucidating the mechanisms of small molecule cryoprotection using Neutron Membrane Diffraction

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The interaction between membranes and small molecules is a key factor in determining survival of organisms or cells during dehydration and/or freezing. Cryoprotective molecules fall into two categories: those important in desiccation and freezing tolerance in nature (such as sugars), which cannot pass through membranes; and penetrating molecules, such as DMSO, which are used in laboratory cryopreservation. Both types of molecules affect membrane structure, but the interactions, and therefore cryoprotective mechanisms, are different.

To understand these mechanisms we have previously studied the structure of synthetic membranes in the presence of small sugars using SAXS and SANS [eg 1-2]. More recently we have used membrane diffraction, which yields higher order diffraction peaks, allowing Fourier reconstruction of the bilayer structure [3-4]. These experiments are conducted on stacked multilamellar membranes (with and without the relevant molecules) under partially dehydrated conditions (relevant to desiccation and freezing). By deuterating one or more components, and adjusting the neutron contrast of the water by changing the D_2O/H_2O ratio, it is possible to isolate the locations of the molecules in the bilayer region with high precision.

Using the cold triple axis spectrometer MIRA [5] (MLZ, Garching, Germany) we have optimised these measurements to maximise the number of higher order diffraction peaks under conditions of contrast variation. Each subsequent peak, and Fourier term, provides improved spatial resolution and diminishes the effects of truncation artefacts in Fourier series.

We have recently extended these measurements to systems containing DMSO. In this talk we will present these results, and use them to contrast the different modes of action of the two classes of cryoprotective molecules. The implications for our understanding of cryopreservation will be discussed.

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Influence of freezing conditions on the protein stability during freeze-drying and long-term storage of biopharmaceuticals

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Many protein-based pharmaceuticals are stored as frozen solutions or as amorphous solid (lyophilized) phases to minimize chemical and physical degradation during their shelf life using a freeze-drying process. However, aggregation is often observed after freeze-thaw or reconstitution of freeze-dried powder and the stability of the protein are no longer assured. Different pharmaceutical formulations are developed to avoid protein degradation and irreversible aggregation during freeze-drying (lyophilization) and storage, using an appropriate buffer to control the pH or adding polyhydroxy compounds (PHC), including carbohydrates (sugars) and sugar-alcohols, well-known as cryo and lyo-protectors.

The cryo-protective action of PHC is usually related to their ability to interfere with the water-to-ice transition, that is, to keep a portion of water molecules in an amorphous (unfrozen) form during cooling. Depending on the solute concentration, freezing (formation of ice) is inhibited either partially or completely.

Characterization of protein structure and interactions in solutions, freeze-concentrated solutions, and dried systems in presence of PHC become an essential part to both designing stable biopharmaceutical products and understanding the mechanisms of lyo- and cryo-protection of biological systems.

Small-angle neutron scattering (SANS) uses low-energy thermal neutrons to probe information on nm to μm length scales without degrading the sample, making it a well-suited technique to study the mesoscopic structure of proteins in a variety of phases. In particular, SANS can investigate the nature of protein crowding and phase separation in the presence and absence of polyhydroxy components, providing insight into the interactions between the protein and solute molecules during all stages of the freeze-drying process.

In this presentation, small-angle neutron scattering data of a model protein/cryoprotectant system of lysozyme/sorbitol/water, under representative pharmaceutical processing conditions, will be presented. The results demonstrate the utility of SANS methods to monitor protein crowding at different stages of freezing and drying to investigate changes in protein-protein interaction distances. Possible interpretations of interaction peaks in the SANS results will be discussed, as well as the role of PH as a cryoprotectant during the freezing and drying process.

A new methodology to monitor the aggregation of the proteins using a Single-axis Acoustic Levitator (SAL) device available at the Institut Laue Langevin (ILL) in Grenoble will be also presented. This apparatus can be used as a model system for spray drying processes allowing permits the levitation of the sample, suspended in air by means of an ultrasonic field. This method enables contact-free positioning of liquid droplets of 3 to 5 mm in diameter and offers a direct mean to observe the drying of droplets or, using a nitrogen cryo-stream directly on the droplet, to freeze it and to cool it down to low temperatures, up to -20 C. The drying of protein solutions and the formation of new structures via self-assembly or self-organization is followed continuously as the concentration of the sample increases by evaporating the solvent. SANS measurements of protein conformation in solution during drying using this technique will be shown.

Model free description of polymer coated gold nanoparticle dynamics in aqueous solutions obtained by Bayesian analysis of neutron spin echo data

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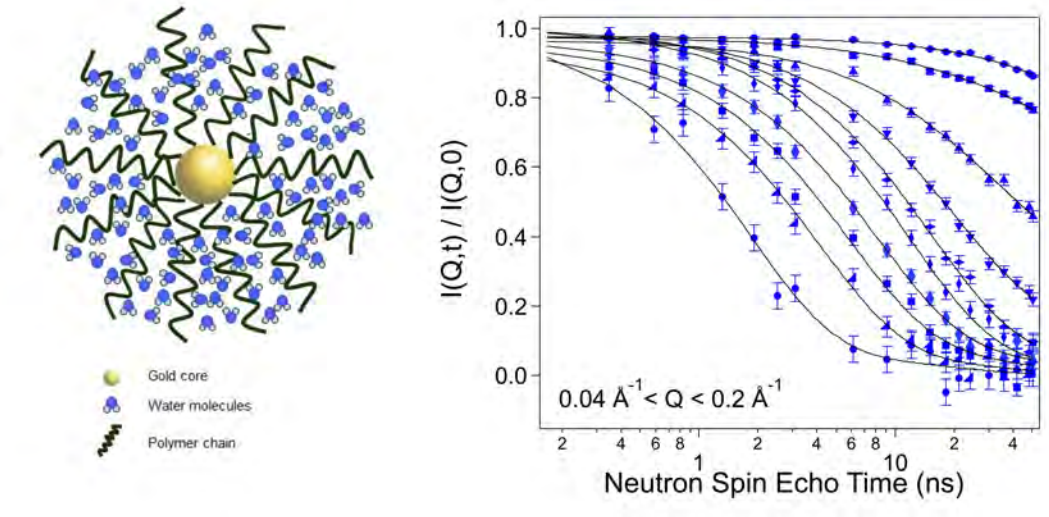
We present a neutron spin echo study of the nanosecond dynamics of polyethylene glycol (PEG) functionalised nanosized gold particles dissolved in D_2O at two temperatures and two different PEG molecular weights (400D and 2000D). The analysis of the neutron spin echo data was performed by applying a Bayesian approach to the description of time correlation function decays in terms of exponential terms, recently proved to be theoretically rigorous. This approach, which addresses in a direct way the fundamental issue of model choice in any dynamical analysis, provides here a guide to the most statistically supported way to follow the decay of the Intermediate Scattering Functions *I(Q,t)* by basing on statistical grounds the choice of the number of terms required for the description of the nanosecond dynamics of the studied systems. Then, the presented analysis avoids from the start resorting to a pre-selected framework and can be considered as model free. By comparing the results of PEG coated nanoparticles with those obtained in PEG2000 solutions, we were able to disentangle the translational diffusion of the nanoparticles from the internal dynamics of the polymer grafted to them, and to show that the polymer corona relaxation follows a pure exponential decay in agreement with the behavior predicted by coarse grained molecular dynamics simulations and theoretical models. In general, the results of our model free Bayesian analysis for the free and tethered polymer chains are in line with the predictions in terms of the Rouse model. This methodology has one further advantage: in the presence of a complex dynamical scenario *I(Q,t)* is often described in terms of the Kohlrausch-Williams-Watts function that can implicitly represent a distribution of relaxation times. By choosing to describe the *I(Q,t)* as a sum of exponential functions and with the support of the Bayesian approach, we can explicitly determine when a finer-structure analysis of the dynamical complexity of the system exists according to the available data without the risk of overparametrisation. The approach presented here is as an effective tool that can be used in general to provide an unbiased interpretation of neutron spin echo data or whenever spectroscopy techniques yield time relaxation data curves.



Structural modification induced by different doping concentration of Ce3+ in silica gels. A SANS study

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Because of their luminescence properties rare earth (RE) ions play key role in many technological applications. In order to obtain functional crystalline or amorphous materials with optical, anticorrosive and catalytic properties, RE ions are widely used as dopants for oxidic materials. Cerium is one of the most frequently used rare earth ion. Because of its great thermal and chemical stability, photophysical and optical inertia, mesoporous silica proved to be an attractive host material for rare earth ions.

The versatility of the sol-gel technique combined with the important features offered by the Cerium ions could lead to interesting Ce^{3+}/SiO_2 composite materials. The structure, size, and composition of the Ce^{3+}/SiO_2 composites can easily be altered in a controllable way to tailor their catalytic and optical properties.

Present work is focused on the synthesis and characterization of the Ce^{3+}/SiO_2 composites, with dopant concentration in the range 1–20 mole% and a step by step calcination at 400 ºC, 600 ºC and 800 ºC.

Small Angle Neutron Scattering (SANS) provided information on the structural features of the composite materials (Figure 1.). Influence of the synthesis parameters, thermal treatment temperature and Cerium concentration have been studied.

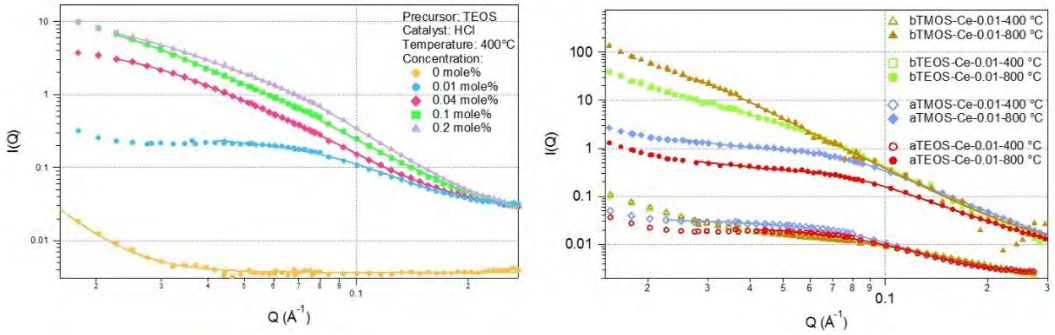

Figure 1. The temperature and Ce^{3+} concentration influence on the SANS curves characteristics

SANS measurements were performed at the Budapest Research Reactor Yellow Submarine pin-hole type SANS instrument. After a proper data normalization, the intensity versus scattering vector curves were produced, and model fitting was made. As a result of the fitting, the gyration radii of the cerium crystallites were determined, and a maximum size at 10 mole% has been found. It was concluded that the maximum crystallite size was only affected by the cerium quantity, and the annealing temperature. The synthesis conditions did not affect the size. At 400°C the formation of the cerium crystallites had started, and the maximum size had been reached at the 800°C annealing temperature. Additionally to the scattering from the cerium crystallites, the silica pore surface scattering was also modelled, and the changes in the fractal behaviour with the synthesis conditions was also studied.

The information provided by SANS were compared and/or completed by electron microscopy (TEM and SEM), nitrogen adsorption. The photoluminescence was used to reveal the optical response caused by the structural modification of the composite materials.

SANS study of organically modified silicas obtained by sol-gel technique

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Combining the advantages offered by the sol-gel technique with the physiological effectiveness of bioactive molecules, new horizons in materials engineering have been opened. Materials with special microstructures obtained in a sol-gel process - where the precursors and the sol–gel processing parameters have been judiciously chosen, proved to be proper carriers for fragile biologically active molecules.

Hybrid silica materials were synthesized via two routes: (1) by using substituted silica precursors and (2) by using natural organic additives.

(1) Methyl, vinyl, isobutyl substituted silica gels were obtained by increasing the substituted precursor molar ratio in the precursor mixture from 5 to 80%. Modification of pH caused important morphological changes on the obtained silica materials.

(2) 3-24 wt.% gelatin aerogels were also synthesized and characterized.

The aim of the study was to establish a relationship between the used synthesis parameters and the obtained physicochemical characteristics of the hybrid silica materials.

Here we describe the structural characterization of the two groups of materials carried out by small-angle neutron scattering (SANS). For both groups of materials other physicochemical characterization techniques (NMR, electron microscopy and contact angle measurement) were used to get a comprehensive picture.

SANS measurements were carried out on the Yellow Submarine pin-hole type SANS instrument of the Budapest Neutron Centre. After proper data processing, the evaluation of the SANS curves has been carried out by model fitting. This offered an understanding of the effects of the various precursors, their concentrations and the used pH values. Figure 1 compares the SANS curves of samples taken from the first group of materials. The graph on the left side presents the effect of pH on the structure. The graph on the right side presents how the various precursors affect the morphology of the obtained materials.

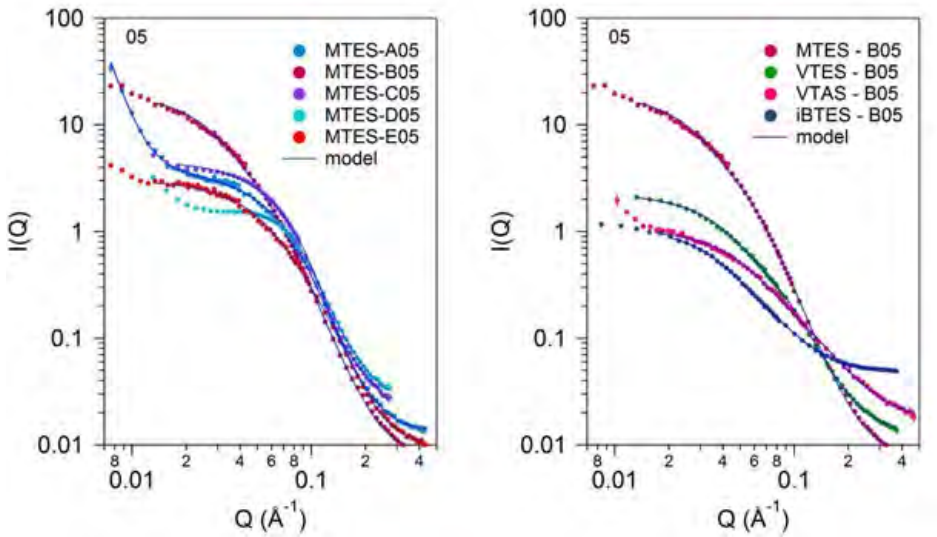

Figure 1. Comparison of the SANS curves of the methyl substituted hybrid silica samples (left) and of the methyl, vinyl and isobutyl substituted silica samples (right)

SANS measurements were made on the gelatin containing aerogels by using a contrast variation technique that allowed the direct study of the morphology changes during hydration.

Influence of divalent cations of essential metals on the structure of lipid membranes: SAND study

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Currently, there is some interest in the studies of the membrane structure and its properties in the presence of salt solutions. Plasma membrane properties such as membrane fluidity, bending and compressibility moduli, electrostatics, and aggregation and fusion are associated with ions that are present inside the membrane and outside the cells. Metals such as calcium, magnesium, iron, manganese, copper, zinc, nickel, and cobalt are usually associated with toxicity; however, at certain concentrations, they are essential for living cells. The divalent metal cations attract a special attention due to their peculiar properties.

Previously neutron studies demonstrate differences in how Ca2+ and Zn2+ affect DPPC bilayer, i.e. changes in lipid bilayer thickness [1]. These results suggested two parameters playing a key role in the mechanism of ion-membrane interaction. First, it is the size and hydration properties of ions themselves. Second, the specific interactions may depend on the density of lipid-ion interactions per lipid, thus correlating with the lipid lateral area.

In this work, a set of essential divalent cations are expanded with Mg2+ which is characteristic of different size. Neutron measurements of samples based on another membrane-forming lipid DOPC with Ca2+and Mg2+ ions of various concentration were also carried out. Neutron diffraction data from well-oriented lipid stacks were collected at D16 instrument at ILL reactor (Grenoble) for three contrast variations (D2O/H2O ratio). Changes in the main structural parameters of the DPPC and DOPC bilayers with increasing ion concentrations are discussed. The evaluated d-spacings for various samples are shown in Fig. 1 and compared to the results published previously [1].

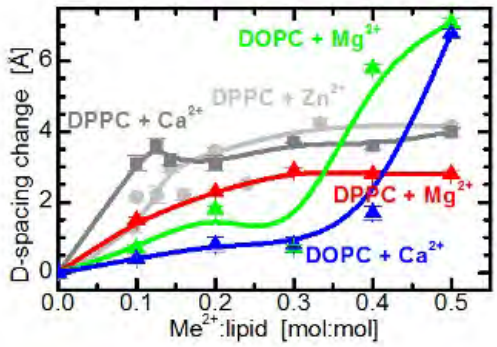

Figure 1. Changes to the transversal lamellar D-spacing in the various multilayered model membranes studied. The changes appear to group by lipids (i.e., DOPC vs. DPPC) rather than by the cations added (i.e., Ca2+, Zn2+, and Mg2+).

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Supramolecular gels based on lithocholic acid and its derivatives: Small-angle neutron scattering vs. atomic force microscopy

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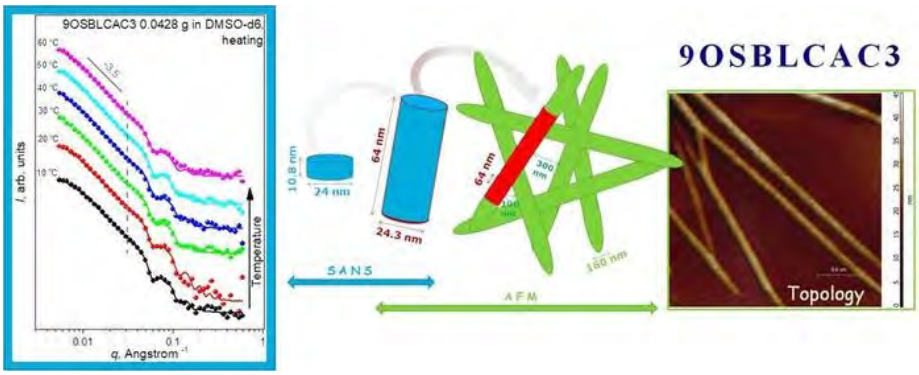
Supramolecular gels, formed by low molecular mass organic gelators (LMOG), have come under intensive study in recent years, since they can be considered as a biomaterial alternative to polymer gels. The potential use of supramolecular gels in medicine: drug delivery, tissue engineering [1], as well as in photoelectronics [2] is related to their responsiveness to the changes of environmental parameters: physical (temperature, light, ultrasound) and chemical (presence of cations and anions in the medium) [3].

The stability, morphology and internal structure of supramolecular gels based on lithocholic acid (LCA, 3α-hydroxy-5β-cholan-24-oic acid, $C_{24}H_{40}O_3$) and its derivatives, synthesized for the first time, are discussed. LCA molecule has a steroid framework with two functional end groups: hydroxyl and carboxyl. Due to such structure, LCA can form self-assembled systems in various solvents by means of hydrogen bonds. A radial spherulite organization of the gel has been observed for LCA in dimethyl sulfoxide (DMSO).

The search for stable supramolecular gels was carried out by modifying the functional end groups of lithocholic acid, and their structure was characterized using small angle neutron scattering (SANS) and atomic force microscopy (AFM). It has been established that a change in the carboxyl group leads to the loss of gelling properties, while a change in the hydroxyl group does the opposite. Moreover, the morphology of organogel at the nano- and micro- level does not change. For example, 7OPhOLCA in DMSO is a stable gel formed by radial spherulites, whose lamellar structure appears to be based upon molecular assembles, mostly dimers, as follows from SANS data [4] and AFM images. Modification of both functional end groups of lithocholic acid, in particular for 9OSBLCAC3 ($C_{50}H_{72}O_6S$), leads to the formation of a very stable transparent supramolecular gel in DMSO and a very stable opaque one in ethanol, consisting of nanofibrils.



The work was carried out in frame of the Poland-JINR scientific program 2015-2019.

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Nanoscale mechanics and energy storage in porous materials: neutron scattering insight

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Sorption of water and hydrogen in porous materials can be used for the development of efficient energy storage devices. For technological applications and the successful design of such materials a detailed understanding of sorption processes and mechanical impact of sorption on the host structure is required. Here we report the results of our in-situ neutron scattering study of water and hydrogen sorption in zeolites and metal organic frameworks with well-defined pores of sub-nanometer size. Though molecular interactions between the adsorber and the adsorbent in all studied materials are expected to be weak, we observe relatively large intake accompanied by pronounced structural deformations of porous hosts. Thus, in CAU-1 metal organic framework with three dimensional pore structure we observe an isotropic adsorption-induced structural contraction [1]. In contrast in CAU-8 and zeolite $AlPO_4$-5 with one dimensional pore channels we observe anisotropic changes such as contractions in the plane perpendicular to the pores and elongation along the pores [2]. Interestingly, the observed structural changes seem to support hydrogen and water intake either by triggering the rearrangement of the adsorbed molecules and the formation of additional occupied positions or by enhancing the guest-guest interactions leading to capillary-like condensation. One can argue that smart tuning of adsorption-induced structural deformation of porous materials could be used for further improvement of storage capacities in metal-organic frameworks and zeolites.

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Dynamics of Rubbery Dead Layers Bound on Carbon Surfaces

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Structure and mechanical properties of polybutadiene (PB) film on bare or surface modified carbon film were examined. There was the interfacial layer of PB in the vicinity of the carbon layer whose density is higher/lower than that of bulk on the hydrophobic/hydrophilic carbon surface. To extract the information about the structure and the properties of PB at the carbon interface, residual layer (RL) adhering on a carbon surface, which is a models of "bound rubber layer", was obtained by rinsing the PB film by toluene. Density and thickness of RL were identical to that of the the interfacial layer of the PB film. In accordance with change of the density, normal stress was also dependent on the surface free energy; the RLs on hydrophobic carbons were not in rubbery state, presumably in glassy state, whereas that on hydrophilic carbon was in rubbery state. Similarly, wear-test evaluated by atomic force microscopic instruments revealed that the RL on the hydrophilic carbon was peeled off by scratch under the condition of certain stress, while the RLs on the hydrophobic carbons were resistant to the scratch. From these results, we conclude that the surface modification of the carbon affect the interaction between the PB molecules and the carbon surface, and the density and mobility of the PB molecules bound to the surface are altered depending on the strength of the interaction.

Small-angle neutron scattering and in situ UV/Vis absorption spectroscopy of photosurfactant worm-like micelles

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The ability to observe chemical processes simultaneously with small-angle scattering is highly desirable for a deeper understanding of biological and soft matter systems. This is particularly crucial for dynamic systems, to ensure sample stability, purity, chemical conditions, and for where it is not possible to perform further measurements or characterisation on intermediate states *ex situ*. However, while such environments are becoming almost mainstream at large scale X-ray sources, they remain rare at neutron facilities.

Consequently, as a part of a larger sample environment development project at the small-angle neutron scattering (SANS) instrument, KWS-2, at the Jülich Centre for Neutron Science, which already includes *in situ* dynamic light scattering and Fourier infrared spectroscopy, we have recently developed a set-up for *in situ* UV/Vis absorption spectroscopy and light irradiation. A proof-of-concept investigation was undertaken to provide mechanistic and kinetic insights into the photoisomerization and self-assembly of a novel photoresponsive azobenzene-containing surfactant (AzoPS). It was shown that the incorporation of spectroscopy with SANS allows the scattering profile, and hence micelle shape, to be correlated with the extent of photoisomerization in real-time.

To the best of our knowledge, this is the first time the degree of AzoPS photoisomerisation has been tracked *in situ* through combined UV-Vis absorption spectroscopy-SANS measurements. This combined UV-Vis/SANS approach could be extended to various other systems to allow monitoring of their self-assembly process, where the only requirement is the presence of a characteristic absorption spectrum.

Reference: E. A. Kelly, J. E. Houston, R. C. Evans, *Soft Matter*, 2018, **15**, 1253.

DYNAMICAL EXCHANGE LIFETIME OF THE BOUND LAYER ON SILICA NANOPARTICLES IN NANOCOMPOSITES

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For decades it has been postulated that a layer of immobilized polymer forms between a polymer matrix and an attractive surface (both flat substrates and dispersed nanoparticles, NPs). This “bound layer” (BL) is thought to bridge the favorable mechanical properties of inorganic fillers with the surrounding polymer in polymer nanocomposites (PNCs) and yield reinforcement well beyond that expected by the Guth-Gold model. Understanding the structure and dynamics of the BL that forms on favorably interacting NPs is critical to revealing the mechanisms responsible for material property enhancements in PNCs. Thus, NPs can increase the PNC modulus by almost an order of magnitude, even at 10 vol % loading. Adsorbed BLs can presented a temperature-dependent exchange kinetics with surfaces, so the question then is whether commonly termed “frozen” BLs on NPs can show such exchange behavior and, if so, under what conditions this occurs. The current understanding of BLs is that the adsorbed polymers assume the form of “trains”, “loops”, and “tails”, making up two regions: the tightly adsorbed, flat region in the immediate vicinity of the NP and the outer swollen tails that mix with the surrounding medium. Attempts to measure the effective thickness of the BL employ different indirect assumptions to infer the effective BL length scale and reported dimensions comparable to the chain radius of gyration.

We used Small angle neutron scattering (SANS) to characterize the BL, and its temperature-dependent exchange behavior in a free polymer matrix with the same chemistry. Here we specifically highlight the BL by using contrast matching methods, so that the NPs (~53 nm diameter silica), the BL (partially deuterated d3-P2VP), and the matrix (h-P2VP, with a glass transition temperature of ~100 °C) are distinguishable. We anneal these samples for different times at two representative temperatures. We find practically no exchange between the BL and the matrix at long times for 150 °C, but substantial chain exchange at 175 °C, even over tens of hours. We therefore suggest that this exchange process has a relatively sharp temperature dependence. We do not perform experiments at much higher annealing temperatures due to concerns with polymer degradation. We postulate that the reduction in BL thickness is due to a combination of two mechanisms that occur simultaneously. Since the BL should have both tightly bound “trains” and the loosely bound “loops and tails,” we suspect that the polymer chains with few surface contacts are able to desorb from the surface relatively quickly at both temperatures. At the lower temperature the more tightly bound chains, with significantly reduced mobility relative to the bulk, have no practical chance of fully desorbing due to the high energy of adsorption from multiple interaction points between it and the NP surface. Meanwhile, at 175 °C the data imply that a large fraction of these strongly bound chains desorb. Our major conclusion is that exchange kinetics of commonly referenced “irreversibly” bound polymers appear at high enough annealing temperatures. We believe that this relatively strong temperature dependence arises from the poly-valency of the binding of a P2VP chain to a NP, i.e., due to the fact that each P2VP chain is adsorbed through multiple monomers. Thus, while the adsorption−desorption process of a single segment is an activated process that occurs over a broad temperature range, the cooperative nature of requiring multiple segments to desorb (to exchange BL chains with the bulk) converts this into a sharp process. In conclusion, we have found that the BL itself is not a frozen object, but rather that it is prone to desorption that bring new insights to the understanding on the structure-properties relationships in PNCs.

Reference: Jimenez et al, ACS Macro Lett. 2019, 8, 166−171

Structure of the monolithic nanostructured aluminium oxohydroxide (NOA): small angle scattering studies

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The present work is focused on the structural study including the structural anisotropy of the monolithic nanostructured aluminium oxohydroxide (NOA), which forms highly porous monoliths upon surface oxidation of an aluminium amalgam in air under controlled temperature and humidity. All the NAO samples (synthesized at 25 °C and annealed at temperatures up to 1150 °C) were comprehensively analyzed using X-ray powder diffraction, thermal analysis, low-temperature nitrogen adsorption, transmission electron microscopy, small-angle and ultra-small-angle neutron scattering, and small-angle X-ray scattering. We showed that the structure of the samples can be described within a three-level model where primary inhomogeneities (characteristic size $r_C \approx 9 – 19$ Å) form fibrils (cross section radius $R \approx 36 – 43$ Å, length $L \approx 3200 – 3300$ Å) or lamellas (thickness $T \approx 110$ Å, width $W \approx 3050$ Å), oriented along the direction of growth of NOA and structured by the type of short-range order with the radius of structural correlations $x \approx 70 – 140$ Å in the direction perpendicular to the axis of growth of NOA. Fibrils and lamellas, in turn, are combined into large-scale aggregates (characteristic size $R_C \approx 1.25 – 1.4$ μm) with slightly rough surface. The high specific surface area (~ 200 m^2/g), intrinsic for the initial NAO, is retained upon its thermal treatment up to 900 °C. Upon annealing at 1150 °C, specific surface area decreases down to ~100 m^2/g due to the sintering of fibrils.

This work was carried out with the financial support of the Russian Foundation for Basic Research (Project 17-53-150007 CNRS_a).

SANS investigations on ligand shells during CdS nanoparticle formation

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Various synthesis strategies employ capping agents to produce stable colloidal nanoparticle (NP) dispersions. The ligands are either injected at the end of the NP growth process or initially mixed with the reactants in the precursor solutions. Yet, little inside is available how ligand molecules interact with precursor clusters and NPs during particle formation. Recent studies showed that ligands alter the internal crystallization of NPs and that ligand shells may vary with NP size [1,2].

CdS nanoparticles without capping agents are synthesized in a precipitation reaction, which involves a two-step process [3]. At first a precursor complex forms, which then congregates to NPs with diameters of roughly 5 nm. For colloidal stabilization, ethylendiaminetetraacetic acid (EDTA) is added frequently, which decelerates the growth process by several orders of magnitude.

Via combined X-ray and neutron small angle experiments (SAXS/SANS) we want to elucidate the influence of the ligand on the evolution of the CdS NPs. To this end, we performed in-situ SANS experiments in a novel free-film setup which provides reduced background scattering due to the lack of any sample container and it is thus more sensitive to the small scattering contribution from the ligands [4]. We expect the EDTA to form a ligand shell around the CdS core of the particles. We employed contrast matching of the solution (different H_2O/D_2O ratios) to selectively match the ligand shell or the CdS core assuming pure components. In addition to SANS and SAXS, the NPs were analysed by transmission electron microscopy (TEM) and dynamic light scattering (DLS). The core sizes as determined by TEM and SAXS match rather well, while DLS points towards larger structures, but is not able to distinguish between hydration or ligand shell. Our SANS free-film experiments reveal structures and dynamics on a bigger length scale, supported by the contrast matching of the core and ligand shell.

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Stabilization of Proteins in Nanopores

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Protein molecules are nature's all-rounders and carry out their specific tasks with great efficiency. For example, some play an important role in converting substances; others are involved in combatting pathogens. As a result, these biological machines are important in technical as well as medical applications. However, proteins tend to clump together irreversibly at high concentrations and thus lose their effectiveness, although this only occurs when they are outside their natural environment of the cell's interior. Spatial restrictions can maintain the activities of concentrated protein solutions. Just why this happens has until now been poorly understood. We demonstrate that despite high concentration levels, proteins do not clump together in nanocavities of porous silicon dioxide, but instead stabilized and behave like a fluid [1]. Crucialreasonsfor such behaviour are on the one hand the interactions between the proteins and the interface, and on the other, the curvature of the nanopores.

Small-angle neutron scattering (SANS) experiment has enabled to directly identify the arrangement of the proteins tested, myoglobin and lysozyme, through the nanostructured materials (SBA-15) [1]. It has been shown that the method enables connections between the characteristics of the pores, the arrangement of the proteins and their activity to be revealed. The knowledge gained can be used for the development of new and better bioinspired applications in biotechnology, medicine and catalytic processes.

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Hydration Interactions in Model Membranes Studied by Neutrons

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Various studies performed utilizing the neutron diffraction reveal intriguing peculiarities in structural properties of model biological membranes. Interestingly, one of the common alterations that is observed at the membrane-water interface underlines the important role of membrane hydration properties. A plausible mechanism of action in the case of many membrane additives seems to be in shifting the water encroachment the way that bilayers absorb more or less water molecules. The difference in water interactions with different lipids and cholesterol has been noted at the interface and up to the bilayer center (Figure A), the ion depending interplay between lipid-water and ion-water hydrations has been shown (Figure B), and the anaesthetic effect also appears to link tightly to hydration (Figure C), to discuss but a few examples. Although a complete understanding of the physicochemical processes taking place in biomembranes is not established fully, the understanding of lipid bilayer structural changes as a result of different properties of environment outside and/or inside the membrane provides a foundation for better insights into the structure-function relationships that most certainly take place in complex biomembrane systems.

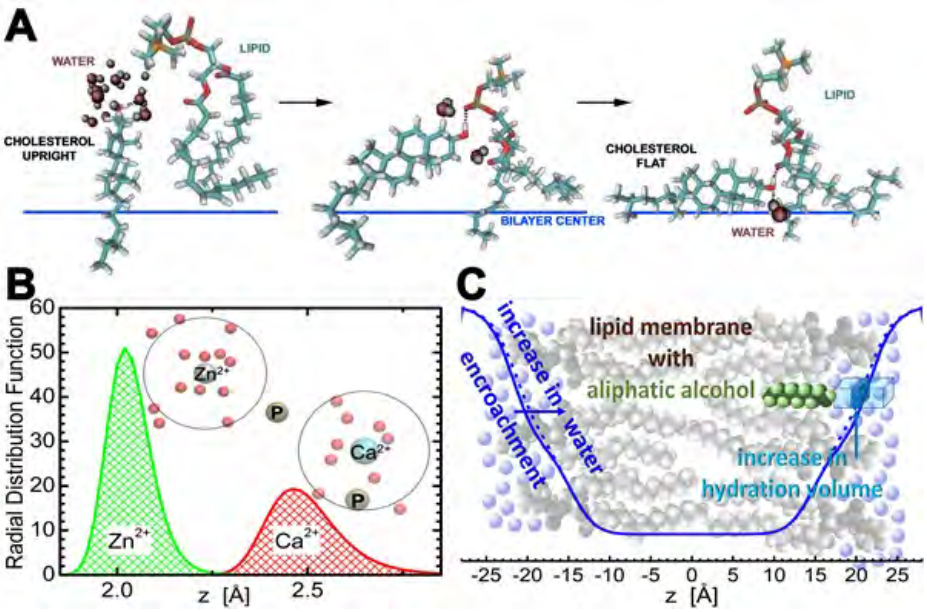

Figure: Schematics of water-altered membrane interactions. (A) Hydrogen bonds between water and cholesterol headgroup facilitate a realocation of cholesterol into the bilayer center. (B) Zinc attracts more water molecules (represented by red balls on top and shaded areas on bottom), while less hydrated calcium can interact closer with the membrane's atoms. (C) Illustration of water encroachment showing increased water penetration and enlarged lateral area when alcohol molecule is present in membrane.

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STRUCTURE STUDIES OF DETONATION NANODIAMONDS COMPLEXES WITH METAL IONS AND POLY(VINYLPYRROLIDONE) BY SMALL-ANGLE NEUTRON SCATTERING

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Nanodiamonds produced by the method of detonation synthesis (detonation nanodiamonds, DND) attract increasing attention as commercially available substances. The chemical inertness and nontoxicity of DND particles core and possibility to functionalize their surface provide wide prospects for their use in biology and medicine. Carboxylated DND are soluble in water and consist of primary diamond nanoparticles with average size of 4-5 nm, arranged in porous chain clusters 30-100 nm in size [1]. Carboxylic functional groups on the surface are responsible for their interaction with water in hydosols and gels with the formation of electrical double layer, preventing the particles aggregation.

Polyvinylpyrrolidone (PVP), being an amphiphilic polymer, provides self-organization with DND particles and conservation of the clusters formed in hydrosol, thus obtaining highly stable DND colloids in isotonic aqueous-saline medium. Wide use of PVP in medicine makes the DND-PVP complex to be a promising carrier in drug delivery systems [2].

DND particles can also serve as carriers for rare-earth and other metal ions, allowing them to be used in medical and other applications as luminescent materials (Eu) or agents for MRI (Gd). Using 2- and 3-valent metals (Cu, Eu, Gd) allows to conjugate the neighbouring DND particles, thus saving the cluster structure in general, making the clusters more organized.

The fine structure of DND-PVP complexes in aqueous solutions and DND-Me, including the presence of PVP, was determined by small-angle neutron scattering using the contrast variation technique.

The work is supported by the Russian Foundation for Basic Research (project 18-29-19008).

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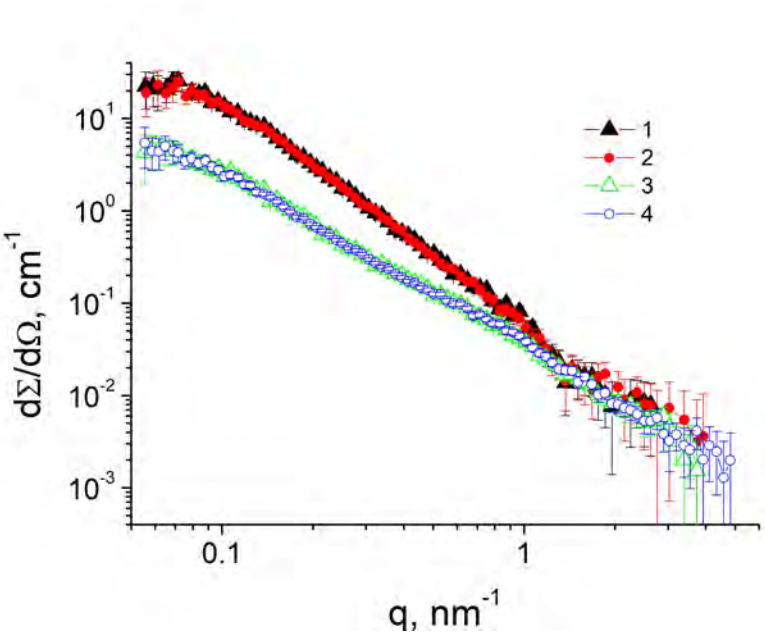

SANS of DND-Gd-PVP complexes in H_2O (1, 2) and 75% D_2O (3, 4). Pure water (1, 3) and isotonic medium (2, 4) were used. Incoherent background is subtracted.

SANS measurements on new Rh(III) chromonic-like coordination complexes

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Chromonic liquid crystals (CLCs) are considered as a sub-class of lyotropic liquid crystals, although they have different molecular structures (planar organic molecules with solubilising groups at the periphery) and well-defined new liquid crystalline structures and properties. Chromonic molecules in polar solvents aggregate into stacks by isodesmic aggregation, instead of exhibiting a critical micellar concentration (cmc), like conventional lyotropic amphiphiles. If the concentration is high enough, the stacks of molecules interact and thus chromonic liquid crystalline mesophases are formed.

Lately chromonic or chromonic-like mesophase were reported for non-conventional molecular structure high coordination number coordination complexes, like tetrahedral Ag(I) and octahedral Ir(III) [Y. J. Yadav et al. 2013; D. Pucci et al. 2014, C. Oliviero et al. 2017]. Several rhodium complexes structurally analogues with the Ir(III) complexes previously reported [Y. J. Yadav et al. 2013; C. Oliviero et al. 2017], have been recently synthesized and structurally characterized. Such as their Ir(III) analogues, the Rh complex molecules self-assembly in water into supramolecular ordered gel phases with chromonic-like structures as showed by Polarized Optical Microscopy investigations.

The complexes were obtained as yellowish powders and were structurally characterized by elemental analysis, NMR and IR spectroscopy. The two complexes, Rh_1 and Rh_2, dissolved in D_2O - with 5.5w/w% and 8.0w/w% concentrations (where they are assembled into chromonic mesophases), respectively - were investigated by Small Angle Neutron Scattering (SANS) in order to reveal the supramolecular organization of the gel phase.

SANS measurements have been performed at the Yellow Submarine pin-hole SANS instrument at the Budapest Neutron Centre. The normalized SANS curves are shown on Figure 1. The present work discusses the form factor changes, presence and absence of the structure factor peaks with temperature, the contribution of interaction between objects to the SANS scattering, formation of columnar primary and hexagonal secondary structures.

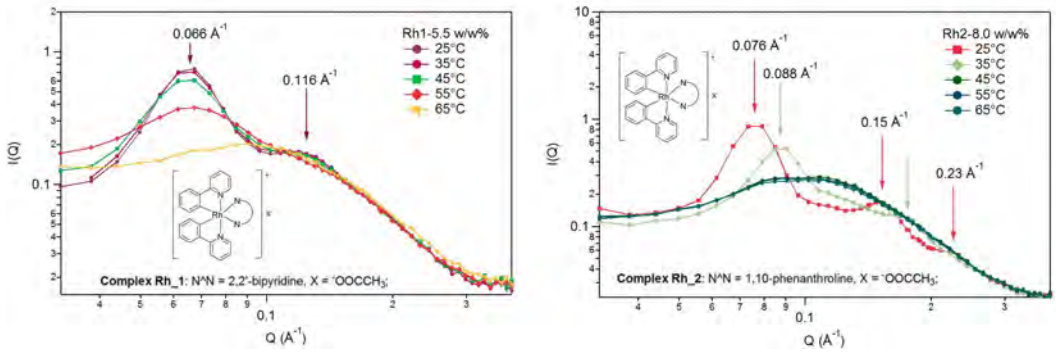

Figure 1. SANS curves of Rh_1 (left) and Rh_2 (right) complexes

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Formation and characterisation of supported lipid bilayers composed of POPE and POPG by vesicle fusion - a simple but relevant model for bacterial membranes

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Supported lipid bilayers (SLBs) are often used as models of biological membranes to either characterise the structural and dynamic properties of the membrane itself or to study biomolecular interactions at the interface, e.g. with antimicrobial drugs.[1] The great majority of the studies include SLBs formed either from saturated or unsaturated phosphatidylcholine (PC) species, which are reasonable models of mammalian cell membranes. PC is sometimes mixed with either sterols or charged lipids such as phosphatidylserine (PS), phosphatidylglycerol (PG) and most recently phosphatidylinositol (PI).[2, 3] For bacterial membranes, on the other hand, mixtures of PC with PE and/or PG have been used largely due to the difficulties forming SLBs *via* the vesicle fusion method using PE and PG lipids.[4] The lack of success in forming SLBs with PE and PG has been explained in part to the negatively charged PG head groups and in part to the molecular shape of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine (POPE). It has been argued that lipids with cylindrical shapes and a packing parameter close to 1 such as PC lipids are required in order to form SLBs.

Here we present the optimization of the formation of SLBs composed of negatively charged 1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (POPG) and zwitterionic POPE on silica *via* the vesicle fusion method. We define specific properties of the experimental setup and physical parameters such as temperature, flow rate, and divalent cation concentration that are crucial for a successful bilayer formation. The optimization was performed using both neutron reflection and quartz crystal microbalance, and the structure of the SLB is reported for the first time. We varied the PG content in order to create mimics of the outer and cytosolic membranes of Gram-negative bacteria and tested the deposition with lipid mixtures containing between 10-25 mol% PG. We also show that the PG content has a pronounced effect on the kinetics of bilayer formation.

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Interfacial behaviour of stimuli responsive nanogels at interfaces by neutron reflectivity

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The interfacial behaviour of stimuli responsive acrylamide-based nanogels differs from solid nanoparticles because of their soft structural character. These nanogels are surface active and have a variable degree of rigidity (softness) controlled by the percentage of cross-linkers, leading to a close packing structure at the interface. Understanding the adsorption dynamics of those particles and the mechanisms that allow them to adsorb the interface are the critical issues that need addressing to achieve tailored particles.

In this work a series of acrylamide based nanogels with different amount of cross-linker have been prepared and characterized in terms of size, phase transition temperature and the surface tension. Neutron reflectivity (NR) technique has been used to probe the interfacial conformation of these nanogels at the air/liquid and solid/liquid interfaces as a function of pH, concentration and temperature. The NR data for a series of different % of cross-linker, concentrations, temperatures and contrasts will be presented. The data of D_2O and NRW contrasts have been fitted simultaneously to a single model. The structure, adsorbed amount and volume fractions of these nanogels at interfaces have been determined. The obtained data indicate that the structural rigidity and the hydrophobic interactions are major driving forces for their surface behaviour and conformation. The results obtained aid the understanding of the adsorption of these stimuli responsive nanogels at interfaces. This will contribute to the applications of these smart materials

A portable SAXS system for simultaneous SANS/SAXS measurements at ILL

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In the last few decades, small angle X-ray and neutron scattering (SAXS/SANS) methods have been used extensively for investigating nanoscale structured materials. Combining both SAXS and SANS techniques in a single experiment will open a new route for a novel nano-analytical method. Simultaneous SAXS and SANS measurements will provide structural information from the same sample volume allowing unique different contrast conditions. Moreover, exploiting X-ray and neutron radiation for time-resolved studies will simultaneously provide nanoscale structural information at two different contrast situations, ensuring the exactness of the probed samples compared with independent experimental approach. Here, we introduce an advanced portable SAXS system that is dimensionally suitable to be installed on D22 instrument at ILL. The new portable SAXS system is based on Copper/Molybdenum switchable microfocus rotating anode X-ray generator and a Dectris detector with a changeable sample-to-detector distance of up to 1.5 m in a vacuum tube. The unprecedented combined experimental approach using simultaneous SAXS/SANS methods will open the way for investigating a truly wide range of innovative materials such as smart self-assembling nanomaterials, multifunctional materials, and organic/inorganic hybrid nanomaterials.

Collapse-kinetics of block copolymer PS-PNIPAM and PnBA-PNIPAM micelles

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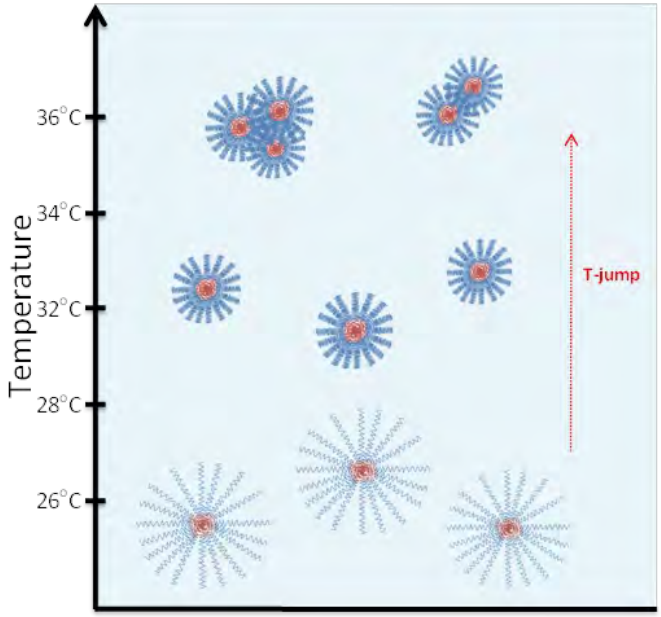
Polymers containing thermally responsive poly(N-isopropyl acrylamide) or PNIPAM are in the focal point of the interest biomedical field and colloid science due to the volume phase transition of PNIPAM in water at physiologically relevant temperature. The polymer shows an entropically driven lower critical solution temperature (LCST) around 32°C, above this temperature polymer chains become hydrophobic and collapse. For many applications, the kinetics of the phase transition plays an important role because it determines the response-rate of devices. However, details of the kinetics are still unknown.

We expect that the phase transition kinetics critically depends on the local mobility of the hydrophobic polymer blocks in aqueous solution. For our investigation we have chosen two block copolymers, PS-PNIPAM and PnBA-PNIPAM with different hydrophobic components and compare them with linear PNIPAM. The polymers were synthesized by reversible addition-fragmentation chain transfer polymerization. Scattering techniques were used to investigate the collapse of the micelles at the LCST and behavior above this temperature. The temperature-jump experiment was performed at Heinz Maier-Leibnitz Zentrum in Garching using the stopped-flow device with time-resolved small-angle neutron scattering (SANS). From the light scattering by comparison the changes of the hydrodynamic radius of the micelles we observed different behavior at and above LCST. Above the transition temperature, PS-PNIPAM creates clusters whereas the micelles in the solution of PnBA-PNIPAM were colloidally stable. If we compare temperature response for both copolymers we observe fundamental differences with the time of response and shifting of the LCST.



Equilibrium structure, hydrogen bonding and proton conductivity in half-neutralised diamine ionic liquids

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Room temperature ionic liquids (RTIL) are liquid around 300K and used already in advanced chemical processes, nanotechnology, catalysis, biomedicine, lubrication among others. Thanks to their ionic character, RTIL are electrolytes suitable for electrochemical applications. Tunable ionic charge density, high thermal and electrochemical stability are just some of the attractive properties of such liquids. Protic ionic liquids (PILs) are suited to be studied by quasi-elastic neutron scattering (QENS), thanks to the high hydrogen content of the cation and the possibility of having H-free anions. The electrical conductivity in PILs occurs via a bi-stable proton between two (or more) complementary and competing sites. Proton transport can then be followed in QENS using partial deuteration of non-acidic hydrogens. Furthermore, molecular dynamics simulations are a proven tool to complement neutron experiments. With their help, it is possible to reproduce QENS spectra in the same time-window, calculate the coherent and incoherent share and then disclose possible dynamical processes happening in the scattering system, such as ion rotation or estimation of diffusion constants [3].

In this work, we show how by using ab-initio methods and classical MD it is possible to identify the structural paths needed for charge transport via non-vehicular mechanisms. The selected system was the diamine based PIL: 2-Aminoethanaminium Triflate (DAEt-TF) which experimentally showed the onset of Grotthuss like proton transport process [1]. The structure and energetics optimization was achieved via DFT computations, and then the classical force field was optimized. Its functional form, is the one of the potential used for liquids simulations (OPLS) and is supported by most of the molecular dynamics software packages, moreover it was integrated to GROMACS software package.

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Amphiphilic properties of drug molecules and their self-assembly in presence of phospholipids

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Introduction

Many pharmacologically active compounds consist of amphiphilic molecules and possess many similar properties to ordinary surface active agents. The amphiphilic nature of these molecules is believed to play a crucial role in their pharmacological activity as well as important properties related to toxicity and hemolysis.

On the other hand, the self-assembly behavior of amphiphilic drugs are expected to largely depend on the presence of an additional surfactant or phospholipid components. While hydrophobic components are expected to be solubilized into the hydrophobic cores of micelles and bilayers, amphiphilic molecules may mix with surfactants and phospholipids and so largely influence the structural behavior of self-assembled aggregates.

Aim

Investigating the self-assembly properties of amphiphilic drugs in the presence of surfactant, phospholipids and the effect of an environmental variable on the process. Determining the influence of the presence of amphiphilic molecules on the structural deformation of the bilayer membrane.

Method

Small angle scattering techniques (SLS, DLS, SANS, and SAXS) are mainly utilized to investigate the self-associated aggregates and their correlations. By means of analyzing data with various geometrical models for the self-associated aggregates, makes it is possible to generate detailed structural information, such as aggregation number, geometrical shape, flexibility and polydispersity of aggregates and complexes that are formed.

On the interaction of softwood hemicellulose with cellulose surfaces in relation to molecular structure and physicochemical properties of hemicellulose.

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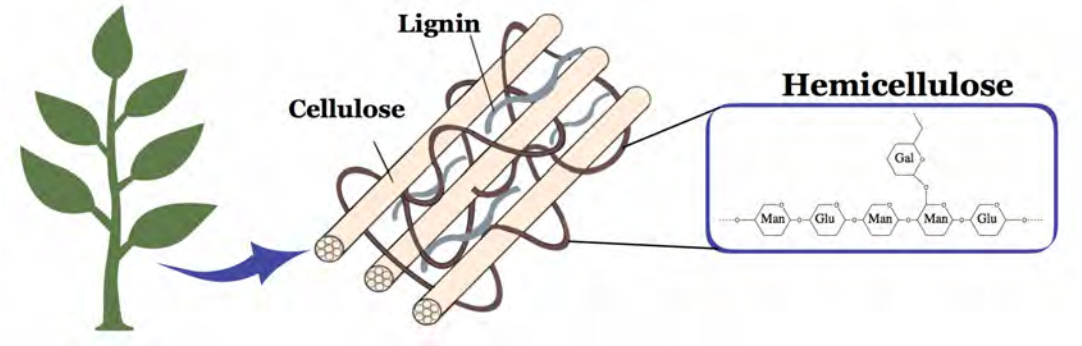
The water-soluble hemicellulose fraction obtained during wood processing has so far been discarded. Softwood contains up to 20% of hemicelluse which makes it an abundant and underutilized resource. The aim with this work is therefore to explore the interfacial properties of hemicellulose for new applications. Previously it has been demonstrated that hemicellulose has high affinity towards cellulose and alter the properties of cellulose based products like paper and wood resin in emulsions. Here we focus on the interactions between softwood hemicellulose (galactoglucomannan, GGM) and cellulose at the surface on a molecular scale. We have revealed how two structurally different GGM samples as well as two galactomannans adsorb to silica, hydrophobized silica and cellulose surface by using a combination of ellipsometry, QCM-D and neutron reflectometry. The solution structure of the GGM samples had been characterized with SAXS, SANS and light scattering to establish how branching and molecular weight affect the conformation of these polymers in bulk. More of the polysaccharides was found to adsorb on cellulose than on hydrophobic surfaces. This indicates that the driving force for the adsorption of polysaccharides is not only hydrophobic interactions. A clear correlation between the molecular weight of polysaccharides and the adsorbed amount on cellulose was found, while the adsorption to the hydrophobic surface was fairly constant. The obtained layer thickness was compared with the hydrodynamic radius, R_H, and radius of gyration, R_G, from bulk scattering data. The results indicated a flat conformation on the surface. The R_G/R_H ratio suggests an elongated rod-like structure of the polysaccharides.



Neutron reflectivity studies on crystal growth of cocoa butter at the solid substrate

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Ingredients of chocolate are mainly cocoa butter (CB), sugar, milk and cacao mass. Since the texture of chocolate is dominated by crystal structure/phase of CB, controlling polymorph of CB is the major process for manufacturing chocolate. CB, the mixture of three kinds of triacylglycerol molecules with y-shape geometry, forms hexagonal, tetragonal and triclinic crystals having layer structure due to their longitudinal anisotropy. Among these structures, a metastable phase having triclinic structure called form V crystal (form V) shows melting temperature 33ºC slightly lower than human body temperature and it is suitable for foods because it melts only in body but not on hands. The conventional process of manufacturing form V so-called tempering is as follows; cooling from above isotropic melting point of CB to 28 ºC which is melting temperature of tetragonal structure called form IV crystal (form IV), forming seed crystal, and heating to 30 ºC to grow form V with mixing on solid board. X-ray diffraction studies show that form V grows as the layer normal of form V is perpendicular to the mixing shear flow. However, the role of surface and the crystal growth under shear at the surface are unclear, though they should be dominant for epitaxial growth of CB crystals. In this study, we performed time-slicing neutron reflectivity measurement (TSNR) to investigate effect of pulse shear flow on the crystal growth of CB at the solid substrate.

We employed CB as a sample. Isotropic melt of CB at 40 ºC was dropped on silicon substrate kept at 22 ºC and pulse shear flow was applied using spin-coater. Steady rotation speed, acceleration time and rotation time were changed to varying strength of shear. BL16 SOFIA at J-PARC MLF was used for TSNR and incident/reflected angle was fixed to 1.6º. White pulse neutron enables obtaining reflectivity data of wide Q-range.

Fig. 1 shows NR data for samples of (a) slow acceleration/rotation and (b) fast acceleration/rotation. For the fast sample form V at $Q = 0.9$ nm^{-1} and form IV around $Q = 1.4$ nm^{-1} were observed, while the slow sample only shows form IV. These results indicate that the layer grows parallel to substrate and both the acceleration (radial and tangent force) and the rotation (radial force) affects the growth of form V. The time dependence of these peak profiles will be discussed in the presentation.

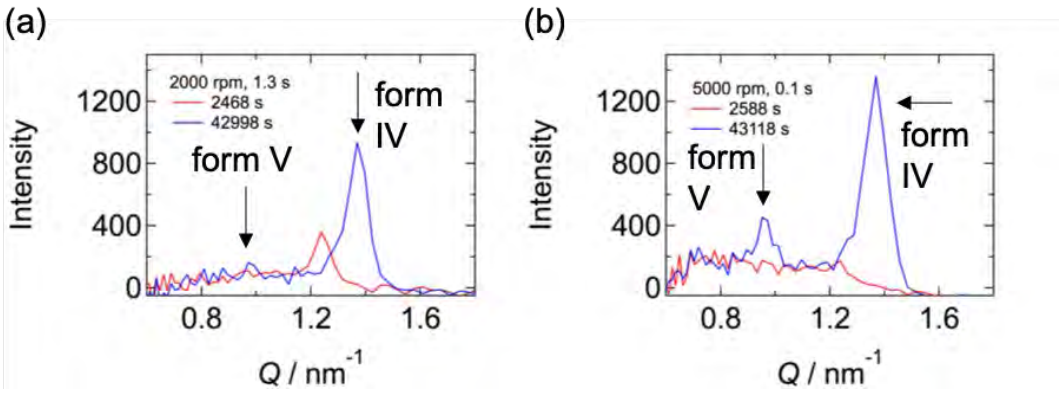

Fig. 1 NR patterns for samples of (a) slow acceleration/rotation and (b) fast acceleration/rotation

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Investigations on surface active ionic liquid micelles modulated by bile salts: A SANS study

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Due to the potential use and widespread applications of mixed micelles, interaction between surface active ionic liquids and biologically important bio-surfactants known as bile salts have been examined. Mixed micelles of sodium deoxycholate (NaDC) and sodium cholate (NaC) with 1-decyl-3-methylimidazolium chloride (C_{10} mim Cl) have been assessed by spectral and scattering techniques. These bile salts display electrostatic and hydrophobic interactions with the IL. The incorporation of bile salts in IL micelles leads to an increase in solution viscosity suggesting micellar growth and transitions. These observations are confirmed by dynamic light scattering (DLS) and further supported by small angle neutron scattering (SANS). The unusual viscosity behavior is observed by altering the solution pH. ^{1}H NMR provided information on deeper penetration of NaDC molecules in IL micelles. Such a bile salt induced sphere-to rod micellar transition further modulated by pH is of its first kind in an IL–bile salt mixed system.

Structural ordering of Magnetic Nanoparticles in a Ferrofluid on Silicon Surfaces

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Neutron reflectometry was used to study the assembly of magnetite nanoparticles in a water-based ferrofluid close to a silicon surface. Under the conditions of with and without a magnetic field, the depth profile is extracted. The study involves the analysis of structure evolution with time for three different magnetite particle sizes 5 (below superparamagnetic limit), 15 (above superparamagnetic limit) and 25 nm; for three different chemical terminations viz., hydrophobic, hydrophilic and (3-aminopropyl)triethoxysilane (APTES) functionalized surfaces. The particles have a volume density of 5% in a D2O–H2O mixture and are surrounded by *N*-succinimidyl ester for steric repulsion. The reflectivity data were fitted to a model using a least square routine based on the Parratt formalism. From the scattering length density depth profiles, the following behavior is concluded: the fits indicate that excess surfactant covers the silicon surface and almost eliminates the water in the densely packed wetting layer that forms close to the silicon surface. Under magnetic field, the nanoparticles assemble into close-packed layers on the surface followed by more loosely packed ones. The layering evolves with time and is best observed in 15 nm particles. The ordering in 5 nm particles is perturbed due to strong thermal vibrations whereas, in 25 nm particles it evolves with time at first but after 20 hrs the layers are found to be with increased water content showing influence of gravity or sedimentation on the heavier particles in the vertical orientation geometry. The particles self-assemble best onto APTES coated surface due to the formation of amide linkages with the interface followed by hydrophilic surface and least onto hydrophobic surface. Detailed analysis of neutron reflectometry data together with model calculations of the arrangement of the nanoparticles within the layers and input from small-angle scattering measurements provide full characterization of the core/ shell nanoparticle dimensions, degree of chaining, arrangement of the nanoparticles within the different layers, and depth profile.

Macroscopic Alignment of Micellar Crystals with Magnetic Micro-Shearing

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The effect of small quantities of magnetic polymer nanocomposite (formed by surfactant Pluronic F127 @ Fe_3O_4 nanoparticles of 10 and 30 nm diameters) on the crystallization behavior of Pluronic F127 micelles solvated by 20 % in water was investigated in the vicinity of hydrophilic and hydrophobic interfaces. Introducing magnetic nanoparticle at the core imparts magnetic properties to the polymeric micelle and increases its hydrodynamic diameter. These magnetic polymer nanocomposites act as defects in the Pluronic crystal and hinder crystallization in comparison to pure Pluronic F127 micelles behavior. Magnetic field results in a motion of the magnetic micelles and a micro-shear effect. This micro-shearing assists self-organization of the crystal. Addition of magnetic micelles formed using 30 nm magnetite particles show similar crystallization behavior, however, with an overall reduced crystallinity due to their significantly larger size compared to the lattice parameter and the dimension of the interstitial cavity for a fcc structure.

Vibrational density of states and molecular mobility in a polymer with intrinsic microporosity PIM-1 as revealed by inelastic neutron scattering

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Polymers with intrinsic microporosity are promising candidates for the active separation layer in gas separation membranes. Here, by means of inelastic neutron scattering, the vibrational density of states (VDOS) and the molecular mobility were investigated for PIM-1, the prototypical polymer with intrinsic microporosity. The results are compared to data measured for a more conventional high-performance polyimide used in gas separation membranes (Matrimid).

The measured data show the characteristic low frequency excess contribution to the VDOS above the Debye sound wave level, generally known as the Boson peak in glass-forming materials. In comparison to the Boson peak of Matrimid, that of PIM-1 is shifted to lower frequencies. This shift is discussed considering the microporous, sponge-like structure of PIM-1 as providing a higher compressibility at the molecular scale than for conventional polymers [1].

Elastic fixed window scans were measured on a neutron backscattering spectrometer to have an overview about the molecular dynamics at a time scale of ca. 1 ns. The temperature dependence of the estimated mean squared displacement shows a step-like increase in the temperature range from 100 K to 250 K indicating the onset of some molecular mobility. The nature of this motional process was analyzed in detail by quasielastic neutron scattering combining Time-of-Flight and backscattering where the data are discussed with regard to both the q- and the temperature dependence.

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ELUCIDATING THE SELF-ASSEMBLY OF DENDRIMERS AND OPPOSITELY CHARGED DYES USING SMALL-ANGLE NEUTRON SCATTERING AND ITSOTHERMAL TITRATION CALORIMETRY

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Self-Assembly is a widely occurring phenomenon in nature. Understanding the shape-determining factors is key for tailoring nanoparticles with desired structural properties. Furthermore, switchability between disassembled and the assembled state through external triggers would increase the application potential.

We will discuss nanoparticles consisting of positively charged polyelectrolytes (Polyamidoamine (PAMAM) dendrimers) and oppositely charged multivalent organic dye molecules. [1, 2, 3]. Depending on the dendrimer generation and the valency of the employed dye molecule a vast variety of either elongated shapes or spherical shapes can be generated. pH triggers the assembly process as at high pH the PAMAM is neutral and thus not forming complexes with the dye molecules. The nanoparticles were characterized using static and dynamic light scattering (SLS & DLS) as well as small-angle neutron scattering (SANS). The results were complemented by UV-Vis spectroscopy and isothermal titration calorimetry (ITC). Gathering all the information from structural characterization and thermodynamics allows to elucidate the self-assembly process and consequently to predict the shape of nanoparticles formed. A general combination of interactions like electrostatics, counterion release and geometric constraints governs the self-assembly process rather than one specific binding motif.

UV light may also serve as a trigger to change the size and shape of self-assembled nanoparticles, as illustrated by an example using a linear cationic polyelectrolyte together with an isomerizable dye molecule.

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Changes in the structural parameters of model membranes of DMPC phospholipid under high pressure by the SANS method

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Changes in the structural parameters of 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) model lipid membranes occurring under the influence of increasing external hydrostatic pressure were studied. The dependences of the thickness of the lipid bilayer, the aqueous layer and the size of the multilayer vesicles on the external pressure were obtained.

Dispersion of multilayer DMPC vesicles in heavy water with a lipid concentration of 17.5% wt/wt was studied by small-angle neutron scattering method (SANS) at YuMO spectrometer (IBR-2, JINR, FLNP, Dubna, Russia) [1] in the pressure range from 1750 to 2400 bar. During the experiment, the sample was maintained at a temperature of 60 °C by a Lauda thermostat with an accuracy of 0.03 °C. Thus, the DMPC membrane initially was in the liquid phase, and the process of pressure change was considered to be isothermal.

The primary TOF small-angle spectra were treated by specialized SAS program [2]. The obtained neutron scattering curves were processed using ATSAS and SasView small-angle scattering data treatment software. The positions of the diffraction peaks observed on the scattering curves reveal the changes in the repeat distance of the multilayer lipid membrane with increasing pressure. It is shown that with an increase in pressure from 1750 to 2400 bar, the repeat distance changes nonlinearly. A minimum of repeat distance is observed near the pressure point of 2200 bar, that allows to make an assumption about the possibility of a phase transition of the lipid membrane under the indicated external conditions. Using the Kratky-Porod approximation [3], the thickness of the lipid bilayer and the aqueous layer between the bilayers are determined. The obtained parameters are refined in the SasView program by the method of approximation of experimental curves with model functions.

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Size and structure of fibres in meat analogues studied by neutron scattering

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Fibre-like structures can be used to produce meat analogues; the structural hierarchy is crucial[1] as it determines the extent to which it mimics the texture of real meat. Few techniques are available to quantify the structure of meat analogues from the nano- to micro-meter length scale. Calcium caseinate dispersion can be transformed into a fibrous gel upon shear deformation, which makes it a promising meat analogue candidate (figure 1A). We present Small Angle Neutron Scattering (SANS) data studying the size, orientation and degree of anisotropy of the fibres formed in the calcium caseinate gels produced at different shear rates. By fitting the annular intensity of the 2D scattering patterns (figure 1B) with a Legendre polynomial[3] (figure 1C), we find the degree of anisotropy first increases with shear rate and then decreases. The parallel and perpendicular (to the shear flow) 1D sector cut data are fitted simultaneously using a Guinier-Porod model[4] (figure 1D). The fibres' lengths show a similar trend as the degree of anisotropy while the radii remain the same with increasing shear rate. SANS combined with a model-free fitting approach identifies the optimal conditions to produce the fibres and it can help further with a rational design of food structures and processing methods.

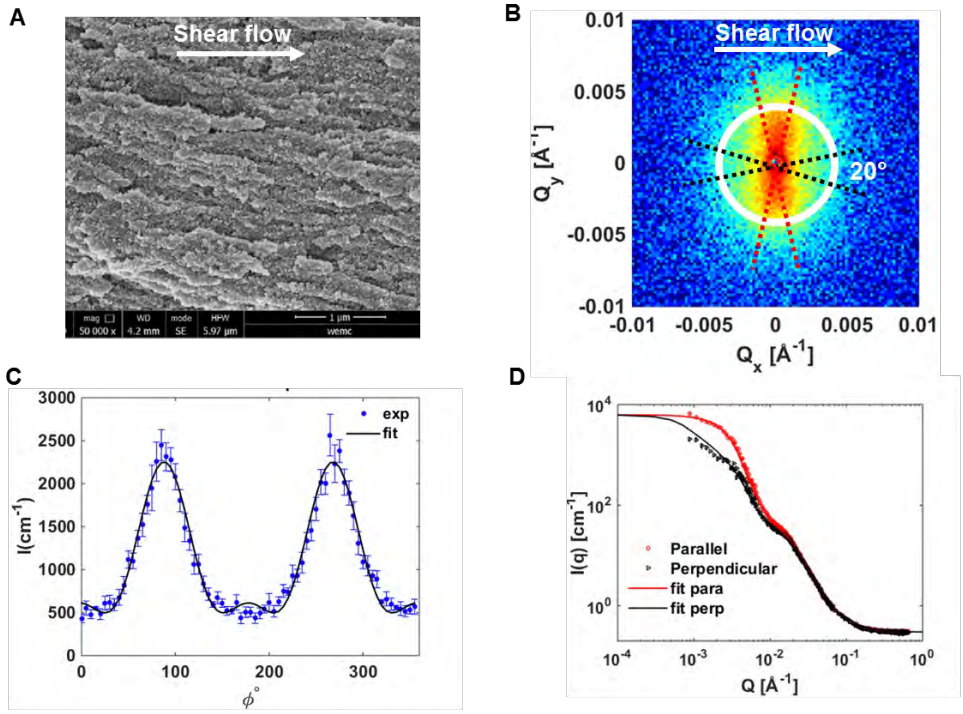

Figure 1 A: SEM picture of the calcium caseinate fibrous gel, the scale bar is 1μm. B: 2D SANS pattern of one sample. C: Annular intensity plotted at Q=0.003±0.0006Å^{-1} (dots) and fitted using a Legendre polynomial (line). D: 1D sector cut along and perpendicular to the shear flow, fitted using a Guinier-Porod model.

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Towards understanding of glass-forming by some isomers of globular alcohols. A QENS approach.

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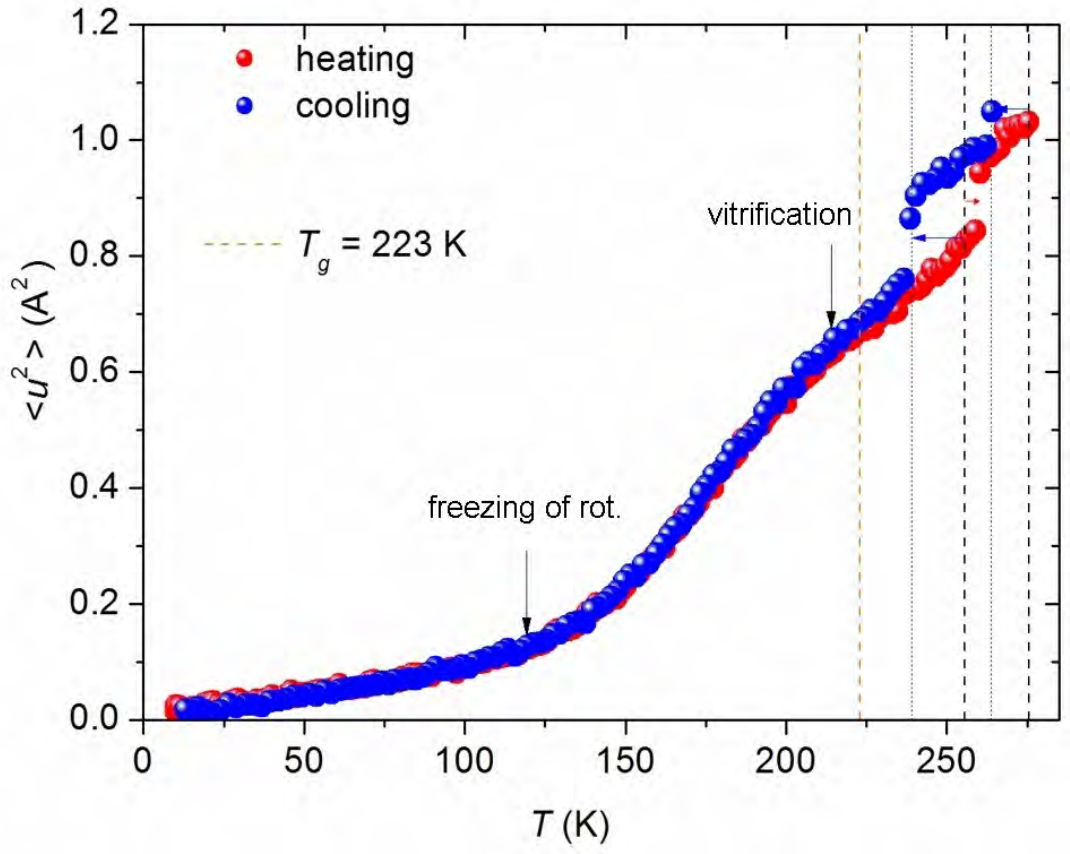
Despite much research work aimed at formation, nature and properties of glassy state, there are still many unknowns concerning, in particular, various glassy states of molecular matter. Such states arise as a result of freezing-in translational, rotational (both molecular and intramolecular) degrees of freedom, or conformational disorder. Hexanol, a relatively simple chemical compound ($C_6H_{13}OH$) has seventeen isomeric forms. Some of them form crystal structures and never assume any glassy state, e.g. 2,3-dimethylbutan-2-ol (23DM2B), the others, such as 3,3-dimethylbutan-2-ol (33DM2B), easily undergo glass transitions.

Both named isomers were subjected to quasielastic neutron scattering experiment with the aim to gain more understanding of the factors influencing the glass formation. Unlike many thermodynamic phase transitions, especially in liquid crystals, which sometimes do not influence intramolecular stochastic motions, a glass transition, being of kinematic nature, often consists in freezing-in such motions. And thus, the softening of the glass-of-rotational state in 33DM2B could only be detected by the QENS experiment, as shown in the figure below on the derived mean-square atomic displacement vs. reciprocal temperature (softening is the discontinuity in the red trace).



The structure, and the development of a glassy state in hexanol, depends upon the hydrogen bonds created in the system. If this happens, the activation energy for stochastic motions of hydrogen atoms involved, are of course affected. This is seen in the QENS experiment.

Controllable electrophysical and optical properties of granulated thin films: the 4D-laser-induced topological nanoclusters

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1. Laser-induced nanostructures and thin films with controllable topology are depended on the laser pulses duration, and may be associated with the 4D-laser technology fabrication of new structures and materials. In fact, the interaction effects of solid targets with laser pulses of different durations for obtaining of various nanocluster structures can be viewed as the possibility of synthesizing the 4D-objects. The result depends not only on the stationary topological/geometric parameters of the system, but also on the dynamic interactions in the system leading to different final stable structures. This is due to the fact that for different durations of laser pulses the specific mechanisms of nanostructuring are activated. Therefore, time plays the role of a control parameter responsible for phase transitions, as well as the spatial parameters do when nanostructures of various dimensions arise – from quantum dots (0D) to 3D nanostructures.

2. Several topological structures for nanoobjects, obtained by computer simulation in arbitrary units, was modeled by us by different numbers of key parameters. The topology peculiarities of the granulated metallic film deposited on dielectric substrates are discussed in clustered metallic structures for both Volt-Ampere characteristics and the optical transmission spectra of deposited bimetallic films.

3. The problem of high temperature superconductivity, due to topological surface structures with correlated states, is under our consideration in frame of nonlinear dynamic modeling resulting in the electronic Cooper pairs appearance. Random temporal and spatial variations in selection topological parameters may result in large variations of such coupling.

Exchange interactions at the manganite/manganite interface of FM/AFM type

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Understanding interface phenomena is one of the greatest challenges in both fundamental and applied physics. In particular, interfaces made of strongly correlated oxides have shown unexpected physical properties, such as the exchange bias, proximity effects, charge transfer, exchange springs and orbital reconstruction [1-3].

Given the complexity of its structural and magnetic phase diagram, LSMO offers a wide range of tunable properties that we can stack into heterostructures. With the atomic precision of the oxide MBE we were able to tune the Sr-concentration x layer by layer (at 0.4 obtaining a ferromagnetic half-metal and at 0.8 an antiferromagnetic insulator), and synthesize superlattices with a large gradient in hole-doping, as a promising platform to study the competition between diverse exchange interactions, such as exchange bias and charge transfer.

In this work we will discuss the results obtained by polarized neutron reflectometry and SQUID magnetometry of these heterostructures, while trying to shed light on the macroscopic and local magnetic properties and their connection to the Sr-doping depth profile.

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Thin silica films containing bimetallic Pt/Pd nanoparticles

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One of the promising areas of research is the synthesis of catalysts of metal nanoparticles of mixed composition, which include various noble metals. The catalytic properties of bimetallic nanoparticles are determined by their size and structure, and may differ markedly from the properties of their constituent metals. Using sol-gel synthesis, bimetallic nanoparticles of various structures can be obtained, for example, particles with a common crystal lattice.

The work is devoted to the study of the composition and structure of thin "spin-on glass" films prepared from silica sols containing platinum and palladium compounds. Tetraethoxysilane $Si(OC_2H_5)_4$ was used as a precursor forming a silica net. Alloying components were prepared from salts, hexachloroplatinic acid $H_2PtCl_6 \bullet nH_2O$ and palladium chloride $PdCl_2$. The thickness of films and concentration distribution of Pt/Pd nanoparticles in silica films depending on concentration of precursors of platinum and palladium is silica sols were determined using the method of X-ray reflectometry. The composition and size of Pt/Pd nanoparticles formed in thin films were determined in the nanometer and submicron ranges by means of atomic force and transmission electron microscopy of high resolution as well as by means of X-ray diffraction analysis

It was determined that thickness values of the films lie in the range of 20÷50 nm depending on the concentration of dopants. The size of crystallites formed in films is ~5-6 nm and their aggregates to 50 nm. Bimetallic Pt/Pd nanoparticles in thin silica films possess a common crystal lattice forming clusters with the structure of a mixed alloy type.

Investigating the Effect of Processing Conditions on the Vertical Profile of Non-Fullerene Organic Bulk Heterojuntion Thin Films

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Thin film photovoltaic (PV) technologies such as organic solar cells (OSCs), have recently attracted significant interest as they offer scalable, inexpensive, non-toxic fabrication routes and power conversion efficiencies (PCEs) as high as 15% are now achievable[1], rivalling current commercial single-junction devices. The highest efficiency OSCs are typically achieved through the fabrication of a nanostructured bulk heterojunction (BHJ) blend, consisting of a phase separated network of conjugated polymer and electron acceptor domains. Improved performance of OSCs is largely the result of a new generation of small molecule, non-fullerene electron acceptors (NFAs). Compared to fullerene-based acceptors, NFAs possess a number of more favourable attributes such as easier energy level modification, better absorption matching with the solar spectrum and improved material stability[2]. One of the most promising new NFAs is ITIC[3], which when combined with a recently developed conjugated polymer PBDB-T, can reach PCEs as high as 11%[4]. Although initial polymer:NFA device performance shows promising potential there is a lack of fundamental understanding of the relationships between the nanostructure of the BHJ blend, the processing parameters during fabrication and the resulting device performance. In particular, as a consequence of device architecture, the vertical composition and interfacial layers of the BHJ blend film play a significant role in the resulting PV performance of devices.

In this study, the effect of casting solvent, solvent additives and thermal annealing temperature on the vertical profile of PBDB-T : deuterated ITIC thin film blends was investigated with neutron reflectivity (NR) using the SURF reflectometer at the ISIS pulsed neutron source. It is found that the blend film is inhomogeneous in the vertical plane with a PBDB-T enriched layer present at the surface and a dITIC enriched layer at the blend/ electrode interface. The characteristics of these interfaces are strongly dependent on the solution environment and post annealing treatments of the blend as they impact the drying process during film formation. Understanding and controlling this drying process is key to achieving a favourable morphology and vertical material composition. The NR measurements performed in this study provide insight into the inner morphology of BHJ polymer:NFA blends, which correlate to the processing conditions used and the resulting device performance.

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Skyrmions in multilayers Fe/Gd: Investigation of the morphology

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Magnetic skyrmions are a kind of magnetic vortices that are currently of great interest. They can be observed in thin magnetic films with competing interactions [1]. Recently, the attention has shifted to ultrathin ferromagnetic/heavy metal films deposited by sputtering, allowing to explore how the balance of ferromagnetic exchange, anisotropy, and dipolar energy might result in cylindrical domains. Fe/Gd multilayers of the composition $[\mathrm{Fe}(0.34\mathrm{nm})/\mathrm{Gd}(d)]_{\times 80}$, in which Fe and Gd are antiferromagnetically coupled reveal a skyrmion lattice at room temperature [2]. In this contribution, we present our result on the systematic investigation of the structural properties of multilayers $[\mathrm{Fe}(d)/\mathrm{Gd}(d)]_{\times \mathrm{N}}$ for thicknesses in the range 0.3 nm < d < 4 nm and the repetition of N=10,40, and 80 using X-ray diffraction and reflection. In addition, we show the magnetic structure as determined by polarized neutron reflectometry experiment. The results are compared with MFM and bulk measurement techniques.

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Combination of neutron and X-ray reflectometry for the investigation of thin metal films and multilayers

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Neutron reflectometry and X-ray reflectometry are non-destructive methods that provide information about the thickness and roughness of thin films and multilayers. Both methods are based reflection of waves from the interfaces of different materials. Reflectivities are determined by the density and composition of the materials and the type of radiation interacting with it. The high intensity of X-ray sources allows one to study thin films with high resolution. Compared with the X-ray, neutrons can penetrate deeper into the inner regions of materials.

The results of the study of thin Ti, Ni films and Ni/Ti multilayers produced by magnetron sputtering are presented. The samples are studied by both X-ray and neutron reflectometry. We show that the X-ray reflectometry is complementary to neutron reflectometry due to differences in contrast between the materials.

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Grain boundary self-diffusion in 56Fe/57Fe multilayers by in situ neutron reflectometry

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For the stability of nanostructured materials, grain boundaries (GBs) can be controlled by the grain size. When the diffusion length $L_d=(2Dt)^{1/2}$ is small compared to d (~0.5 nm), the GB width, the volume diffusion at low temperature is slow compared to the GB diffusion (type-C regime), D being the volume diffusivity and t the isothermal annealing time. We studied self-diffusion active at the GBs at temperatures 150^o, 175^o, 200^o and 225^o C (consequtively for 600 min each) from the change of the ^{57}Fe isotopic fraction monitored *in situ* by neutron reflectometry on the sub-nanometer length scale on Pt(4 nm)[^{56}Fe(x nm)/ ^{57}Fe(x nm)]$_4$/Si with (x=4 and 8), in a dedicated furnace at REFSANS of HZG at FRM II in TOF mode. The samples of different thicknesses represent different average grain sizes without their evolution within a sample [1]. *In situ* experiments is expected to follow the dynamics more efficiently and therefore the mixed interface width has been mapped with time at short intervals. Specular profiles, extracted from the 2D detector maps, were analyzed by the Fitsuite code (www.fs.kfki.hu) simultaneously at each temperature as a function of momentum transfer vector Q and annealing time t to extract the GB diffusion coefficient. The regular diffusion (decaying Bragg peak) regime starts above 200^o C. We find an increase in the intensity of the first Bragg peak at lower temperatures which is probably related to initial smoothening of the interfaces of the as-prepared state of the multilayer. We plan to analyze this aspect further from the corresponding off-specular scattering in the near future.

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The Neutron Depth Profiling Instrument N4DP at the Heinz Maier-Leibnitz Zentrum in Garching, Germany

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Neutron Depth Profiling (NDP) is a non-destructive, isotope-specific, high-resolution nuclear analytical technique and it is often used to probe lithium or boron depth profiles in different host materials. The presented N4DP experiment is carried out at the PGAA facility of Heinz Maier-Leibnitz Zentrum, which provides a cold neutron flux up to 5E10 s-1cm-2 [1]. Upon neutron capture the investigated ^{6}Li nuclei decay via emitting charged particles with well-defined energies. The energy loss of the charged particles traveling through the host material is then related to the depth of origin at a resolution level up to a few ten nanometers [2]. We investigated NDP on several applications such as heat-treated superalloys with boron additives and OLED prototypes with lithium. In this contribution lithium concentration profile measurements in different lithium-ion battery components are presented. Here NDP reveals new insights into the evolution of immobilized lithium in battery electrodes [3], which is one of the main causes of battery lifetime limitation.

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Depth Profile of Replicated Interface Roughness Correlation in NiTi Supermirrors by GISANS

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Neutron supermirrors (SMs), the major components of neutron optical devices, are depth-graded *d*-spacing multilayers of several hundreds to several thousands of bilayers. The interface roughness is a major factor in the reflectivity of multilayers of large bilayer number. Beside the technical interest, scaling and kinetic roughening of growing surfaces of thousands of layers is a challenging scientific subject. The interface roughness and its correlations were studied in DC-sputtered Ni-Ti normal (increasing bilayer thickness from the substrate) and reverse (decreasing bilayer thickness) SMs by off-specular neutron scattering and GISANS. In the detector scans the in-plane and out-of-plane roughness correlations are manifested in diffuse scatter plateaus and peaks which are interpreted in terms of Resonant Diffuse Scattering. Distorted Wave Born Approximation simulations quantitatively reproduce the characteristic features of the measured detector scans with reasonable roughness correlation parameters. The different character of resonant diffuse scatters from normal and reverse-layer-sequence SMs is qualitatively explained and systematized using quasi-kinematical considerations in terms of material and SM parameters. [1]

Off-specular neutron reflectometry study is complemented by GISANS experiments which lift the inherent uncertainties of reflectometry caused by the slit-direction averaging. The depth-graded *d*-spacing in SMs allows us to study in-plane roughness correlation and out-of-plane roughness replication as a function of depth/bilayer thickness. In normal sequence SMs the in-plane correlation length increases with bilayer thickness. Due to various asymmetries the reverse sequence case is controversial. Roughness correlation is 2-scaled in the direction parallel with the substrate movement during sputtering: the diffuse scatter comprises a wider Gaussian and a narrower Lorentzian. The 2-scaledness is more pronounced in reverse sequence SMs. The roughness correlation function is anisotropic, differs in parallel and in perpendicular direction with respect to substrate movement during sputter deposition. Reverse sequence SMs exhibit an up-down asymmetry, too (with respect to horizontal substrate movement during sputter deposition) which can be explained by a ~2° inclination of the roughness replication direction with respect to the substrate normal.

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Relaxation of magnetization in the ferromagnetic-superconducting structure V/Fe70%V30%/V/Fe70%V30%/Nb, measured by real-time neutron reflectometry

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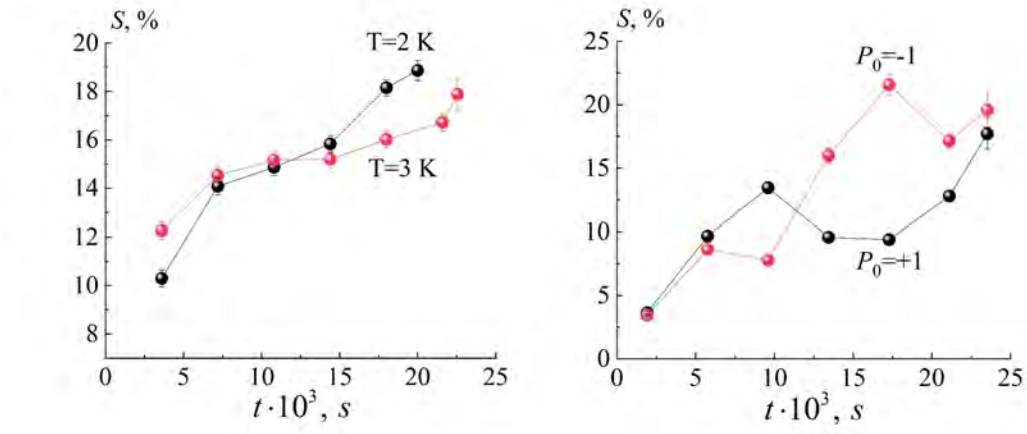
Investigation of the coexistence of ferromagnetism and superconductivity is relevant because of the rapid development of superconducting nanospintronics. Many effects are known for low-dimensional ferromagnetic/superconducting heterostructures: proximity effect, LOFF phase, spin-triplet Cooper pairs, cryptoferromagnetic domain phase [1], etc. Direct detection of the last is possible by neutron scattering measurements. Time dependence investigation of the neutron scattering allowed us to establish the nature of the inhomogeneities in the structure. In this work [2], magnetic state's relaxation of the inhomogeneous superconducting-ferromagnetic structure V (150nm) /$Fe_{0.7}V_{0.3}$ (1nm) / V (1.2nm) /$Fe_{0.7}V_{0.3}$ (1nm) / Nb (150nm) was investigated. Increasing of the domain's walls density was established in a magnetic field with time. At $T < T_c$ (Nb), the time dependence had two-step character (Fig. 1a). This may indicate the formation of a smaller domain structure in the ferromagnetic domains, in particular, the cryptoferromagnetic phase. Simultaneously with the formation of a structure with small domains, the amplitude of oscillations of the clusters magnetic moments increased from the direction along the magnetic field to the direction opposite (Fig. 1b), in the magnetic field of an average value of 1 kOe. The oscillation frequency was ~ 0.1 mHz. This phenomenon can be associated with a weakening of the magnetic interaction of clusters with domains, and, consequently, the appearance of an unstable state, leading to transitions of clusters magnetic moments between two energy minima in the magnetic field. In a larger magnetic field of 5-6 kOe, depinning of superconducting vortices was observed. Thus, real-time neutron reflectometry is an effective method for ferromagnetic-superconducting structures investigation. At present, at the REMUR spectrometer of the IBR-2 pulsed reactor, the maximum frequency of magnetization oscillations available for measurements is f_{max} = 3.3 mHz. It's shown that in the future it will be possible to achieve f_{max} = 0.1 Hz.



(a) (b)

Fig.1. (a) Dependence of the neutron scattering from the coherent channel S (t) in the magnetic field 17 Oe, in the case of a pre-magnetized sample in the 2 kOe magnetic field, at temperatures T = 2, 3 K for λ = 1.8 Å at sliding angle 5.4 mrad; (b) The dependence of S (t) in the magnetic field 1 kOe at T = 2 K for λ = 1.8 Å for two different input spin states of neutrons.

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Development of reference layer method in resonant neutron reflectometry

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Appearance of the new scientific and technological areas demands development of novel diagnostics methods, which allow us to determine the atomic and magnetic structures of nanoobjects. The slow neutrons scattering and, in particular, neutron reflectometry, is one of the most powerful methods for investigation of planar nanostructures, surfaces, and interlayer boundaries. The method is based on the analysis of the specular reflection of slow neutrons with small incident angle to the sample surface. It provides information about the neutron-optical potential dependence on the depth from the sample surface. When working with polarized neutrons, it is also possible to determine the magnetic moments distribution versus depth.

The model-independent approach of reflectivity analysis has been proposed [1], which allows to determine the modulus and phase of the reflection coefficient. This approach is based on the resonant interaction of the neutrons with gadolinium isotopes.

Additionally, it was proved that phase problem can be solved using a reference layer of gadolinium, since the two isotopes of gadolinium Gd^{155} and Gd^{157} have the resonant absorption of neutrons [2].

Various layered systems with reference layer Gd(50 Å)/V(20 Å) were synthesized to determine the modulus and phase of the complex reflection coefficient. The single-layer film Si//Ti (550 Å)/Gd(50 Å)/V(50 Å) and the three-layer film Si//Cr(300 Å)/Fe(300 Å)/Cr(200 Å)/Gd (50 Å)/V(50 Å) have been investigated. The V layer protects the film from oxidation. Layer thicknesses were determined on the x-ray laboratory diffractometer.

The neutron reflection has been measured in an unpolarized beam using a time-of-flight reflectometer REFLEX-P located at pulsed reactor IBR-2 (JINR, Dubna). The sample containing the Fe layer has been demagnetized before the measurements, therefore the total magnetic moment in the layer is absent. Neutron reflection data for samples was obtained at three different incident angles in the Q-range from 0.015 to 0.045 $Å^{-1}$.

The modulus and phase of the complex reflection coefficient for the studied part of the Si // Ti (550Å) and Si // Cr (300Å) / Fe (300Å) / Cr (200Å) samples have been calculated. Comparison of these results with theoretical curves, based on X-ray reflectometry data, has been spent. The qualitative agreement has been obtained.

At present, research work is continuing in order to improve the proposed method and to determine the limits of its application.

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Micelle growth in cationic and anionic surfactant solutions

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Small-angle neutron scattering measurements of micellar solutions of cationic and anionic surfactants reveal a different mechanism of micelle growth in the region of intermediate surfactant concentrations.

THE MODEL OF CRYSTALLIZATION IN A FRACTAL STRUCTURE UNDER CONDITIONS OF A SUBSTANCE SHORTAGE: EXPERIMENTAL STUDY IN CASE OF ZIRCONIUM DIOXIDE

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The fractal concept has been increasingly used for the structures of soft matter description. However, the mechanisms to control the fractal dimension of the objects are currently poorly understood. A convenient object for such studies is zirconia xerogel (ZrO2).The variation of the annealing temperature and pH during the synthesis is able to produce structures with different parameters, such as specific surface, particle size, and fractal dimension [1,2].

The parameters of the mesostructure of zirconium dioxide xerogels synthesized by the sol-gel method were determined at different stages of the heat treatment (60 ÷ 500 ℃) by small-angle and ultra-small-angle neutron and X-ray scattering (SANS, USANS and SAXS). It is well known that if the small-angle intensity curve I(Q) is described by a power law $(I(Q) \sim Q^{-D})$, then the parameter D characterizes the fractal properties of the sample: for the surface fractal $3 < D < 4$, for the mass fractal $2 < D < 3$, and for the logarithmic fractal $D = 3$ [3]. It was shown that particles of the initially amorphous zirconium dioxide form the structure of the surface fractal. Depending on the synthesis conditions, such as the annealing temperature, degree D can either increase to $D = 4$ (solid homogeneous particle) or decrease to $D = 3$ (logarithmic fractal [3]). Based on the data obtained, we propose a model of crystallization in a fractal structure under conditions of a substance shortage. This model assumes crystal growth from the initial fractal structure and takes into account the effect of constitution water on crystal formation.

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EFFECT OF DEUTERIUM ON PHASE TRANSFORMATIONS IN AMORPHOUS PHASES OF FULLERENES AT HIGH TEMPERATURES (HT) AND HIGH PRESSURES (HP)

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Fullerenes are metastable carbon modifications, which under HT and HP undergo a series of phase transformations that have been well studied in the crystalline modifications of fullerenes C_{60} and C_{70}. In this work, phase transformations in amorphous phases of fullerene C_{70} and a mixture of fullerenes C_{60}/C_{70} (50/50) at pressures of 2-8 GPa and temperatures of 300-1100°C and the effect on these transformations of low D concentrations were studied by the methods of neutron diffraction, Raman spectroscopy and HRTEM. Amorphization of fullerenes was carried out by grinding powders in a ball mill and saturation with deuterium (~2 at.%) was carried out from a gaseous medium at 300°C. After that, the powders were sintered in a toroidal-type chamber under quasi-hydrostatic pressure.

It was shown that at temperatures of 300–500 °C, in contrast to crystalline fullerenes, in amorphous fullerenes, polymerization is not observed and the structure of the amorphous fullerene phase remains. At 800-1100 °C, disordered (amorphous) graphite is formed and its transition to crystalline graphite begins. According to neutron diffraction data, anisotropy of disordered graphite was detected (the dependence of the diffraction spectra on the position of the sample relative to the neutron beam). No similar anisotropy is observed in the initial amorphous fullerenes.

The introduction of small amounts of D into the initial amorphous phases of fullerene C_{70} or into a mixture of amorphous of fullerenes affects their transformations to disordered graphite, to the nanostructure of this disordered graphite, its anisotropy in various ways, but equally reduces the stability of amorphous graphite to become crystalline graphite. In particular, in the disordered graphite obtained from amorphous phases of fullerene C_{70} , it leads to the release of graphite nanoclusters, whereas in the case of the transformation of the initial amorphous mixture, it promotes the dissolution of nanoclusters. In general, it was shown that even small concentrations of deuterium can significantly affects the structure and properties of the phases formed from amorphous fullerenes at HT and HP.

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Dynamics in water-methanol mixtures

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The interaction of water with small or large molecules in aqueous solutions is a fundamental topic in a number of disciplines, ranging from physics to chemistry, from material science to biology till astronomical problems. Small amphiphilic molecules, such as in lower alcohols, can be used as model probe to understand the interaction between amphiphilic groups from much larger molecules and water.

To investigate the structural and dynamical nature of these interactions, we combine neutron spectroscopy with molecular simulations on water-methanol mixtures in a wide range of concentration and temperature. We will present here the results of our investigation, and how they do relate with data and models in literature.

In particular, we used quasielastic neutron scattering to probe the single particle dynamics. Our findings agree with the clustering model [1]. Following a data analysis protocol recently introduced for pure liquid water [2], and with the support of molecular dynamics simulations, we could determine the diffusion coefficient of water and methanol molecular species and discuss the general dynamical properties of water-methanol mixtures in terms of jump diffusion between dynamical basins as a function of the concentration. We will then discuss the main outputs of the vibrational dynamics investigation of the mixtures in the solid phase, and which information can be derived on the mixtures properties.

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High-pressure study on an ionic liquid with simultaneous dielectric and neutron spectroscopy

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By combining dielectric spectroscopy (DS) and neutron scattering (NS) in our newly developed high-pressure DS-NS cell [1], we study conductivity and dynamics simultaneously in the ionic liquid Pyrr14-TFSI. We show that conductivity and the fast dynamics measured with backscattering and time-of-flight from IN16B and IN5 at Institut Laue-Langevin are controlled by the same parameter.

The dynamics in real glass-forming systems is rich and includes a large range of dynamical processes taking place on different timescales. The main dynamical feature in glass-forming liquids is the α-relaxation. There is no common understanding yet of what governs the timescale and the spectral shape of the relaxation. It has several times been suggested that there is a close connection between fast and slow dynamics, even though they can differ in timescales by more than ten orders of magnitude. A recent theoretical development in the physics of liquids, the isomorph theory, rationalises this [2]. The fundamental prediction of isomorph theory is the existence of isomorphs, i.e. curves in the phase diagram along which all dynamical phenomena and structure are invariant, i.e. for isomorphic state points, all dynamic processes are expected to be invariant on all timescales.

We have previously shown that both the fast and slow dynamics in a glass-forming liquid along isochrones, i.e. constant relaxation time $\tau_\alpha(T,P)$, is invariant, as predicted by isomorph theory using DS and QENS. We showed the difference in behaviour between two simple van der Waals liquids and a complex hydrogen bonding liquid in agreement with predictions from isomorph theory along the glass transition isochrone, i.e. τ_α = 100 s [3], and along isochrones found from IN16B, i.e. τ_α ~ nanoseconds [4]. We have now tested the predictions on an ionic liquid with Coulumb interaction [5].

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Investigation of tectonically disturbed zones of coal seams of the Kuznetsk coal basin using SANS

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Three methods used for a comparative analysis of the structural characteristics of the coals of the two seams, Boldyrevsky and Polenovsky of the Kuznetsk coal basin: small-angle neutron scattering (SANS), low-temperature nitrogen adsorption (BET) and Raman spectroscopy. Each of them has its own quality. The advantage of SANS is the ability to study the structure of a porous substance in the volume, not limited to the surface layer of the samples.

SANS measurements were carried out on the small-angle spectrometer YuMO of Joint Institute for Nuclear Research (JINR) in Dubna. In our study we tried to reveal the sensitivity of these methods to changes in the physical characteristics of coal at the tectonic disturbances unlike traditional studies of coal, where results are obtained showing changes in the structural and sorption properties of coal depending on the metamorphism stage. Measurements made for samples from the disturbances and from quiet zones of the coal seam to establish regularity.

The BET and SANS methods are necessary to understand the variation of the Raman spectra of coal from disturbances. Thus, an increase in specific surface area and fractal surface dimensions indicates the potential danger of emissions in the area of the tectonic disturbances.

Measurements carried out for coal seams Boldyrevsky and Polenovsky, showed that their structure characterized by surface fractal dimension are close to three. The calculated specific surface areas of the pore space make it possible to distinguish zones of disturbances from calm areas of the same coal seams. It was possible to identify the contribution of microscopic porosity to neutron scattering in the zones of geological disturbances, which correlates with the results of the BET method.

The conclusions were made according to the data of small-angle neutron scattering for fossil coals:

1. Measurement results for all samples from the mine after S.M. Kirov correspond to the surface fractals. The coal in the Polenovsky and Boldyrevsky seams has highest surface fractal dimensions from the point of view of the hierarchical organization of the structure. According to this parameter, the seams can be characterized by prone to sudden outburst of coal, rock and gas.

2. The surface fractal dimensions derived from scattering curves are close to the value 2.9. However, the specific surfaces of pores calculated taking into account the fractality are significantly different for zones of tectonic disturbances and other areas of the seams, which allows to conclude about importance of micropores in an increased rate of gas release in disturbed areas of coal seams.

LOCAL STRUCTURE AND DYNAMICS IN IONIC LIQUIDS

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Ionic liquids are salts with a melting temperature below 100 °C. They typically consist of a large organic cation with an asymmetry introduced by adding alkyl side chains of varying lengths, and an inorganic anion. The flexibility in the design of the anions and cations makes it possible to tune the properties of the ionic liquid to suit particular applications, such as batteries, fuel cells and carbon capture [1]. However, ionic liquids are also interesting from a more fundamental point of view. Unlike most other liquids they show structural heterogeneities on the mesoscopic length scale. The heterogeneities are suggested to originate from the segregation of the alkyl side chains in a charge matrix. The length scale and interactions of these heterogeneities can be tuned by the architecture of the constituent ions of the ionic liquid, providing a systematic way to investigate their influence on the dynamics.

In this contribution we discuss the dynamics and structure of ionic liquids directly on the mesoscopic length scale of the heterogeneities. Our aim is to understand the correlation between the local dynamics, the structural heterogeneities, and the ionic conductivity. With the back-scattering spectrometer IN16B and ToF spectrometer IN5 at ILL we can access the local dynamics at the relevant time and length scales. A key feature of our experiment is that we have used a sample cell where neutron scattering and dielectric spectroscopy are performed simultaneously [2]. In addition, this cell also allows to change both the temperature and the pressure on the sample. In this way we can monitor the conductivity directly at a given pressure and temperature as we are doing the neutron scattering experiment. Structural measurements were done on the Small Angle X-ray Scattering beamline I22 at Diamond Light Source. By using the pressure jump cell of I22 [3] the structure of the heterogeneities could be investigated as a function of pressure and temperature. With these experiments we have been able to explore the effects of both pressure and temperature on the dynamics and structure at different state points (P,T) where the conductivity is invariant. A key question is, if the local dynamics and structure are the same in these points, which gives us insight in the mechanism of ion transport.

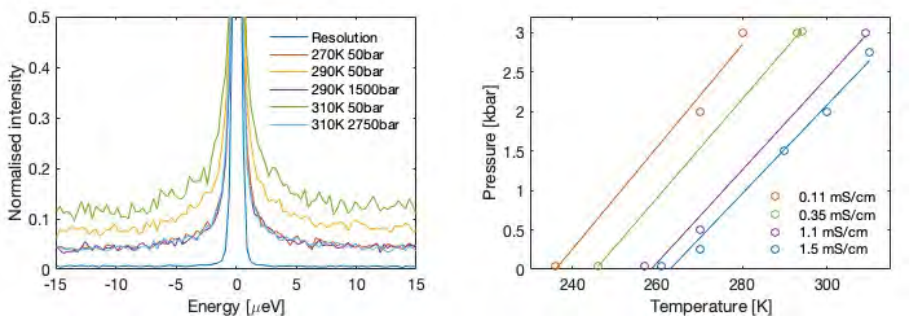

Figure: To the left; QENS spectrum for different state points (P,T). To the right; lines of constant conductivity.

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Classification of the fractal and non-fractal objects in two – dimensional space

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The classification of fractal objects on a nanometer scale in the three-dimensional space is well developed using small-angle neutron and X-ray scattering. It implies that using the power law of the scattering intensity vs momentum transfer ($I \sim q^{-\Delta}$) one can distinguish between the surface fractals ($3 < \Delta < 4$) and mass fractals ($2 < \Delta < 3$) as well as the logarithmic fractals ($\Delta = 3$) [1, 2]. To study the fractal properties of two-dimensional space, we use often the method of numerical Fourier analysis [3]. This method simulates the small-angle light scattering experiment. For homogeneously filled objects with a sharp boundary in 2d space, the scattering intensity decreases with q obeying the power law ($I \sim q^{-\Delta}$) with an exponent $\Delta = 3$. This exponent is a unit less than for similar objects in the 3d space. Fractal objects in the 2d space can be classified and separated in analogy with those in the 3d space onto two classes of the "planar" fractals ($1 < \Delta < 2$) and "boundary" fractals ($2 < \Delta < 3$). Here $\Delta = D$ for the planar fractal and $\Delta = 2d\text{-}D = 4\text{-}D$ for the boundary fractals respectively, and D is a fractal dimension. As to the logarithmic fractals [4], the scattering intensity depends on momentum transfer q as ($I \sim q^{-\Delta}$) with $\Delta = 1$ and $\Delta = 2$ for fractals with the topological dimension equal 1 or 2, respectively. Thus, we suggested and proven with numerical experiments the classification of the fractal and non-fractal objects in the two-dimensional space.

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The use of fractal analysis to assess the characteristics of the spread of radioactive substances in geological environments

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In order to analyze and predict the processes of radioactive substances distribution in geological formations (soils), a mathematical model using the methods of modern dynamics or fractal geometry is presented. For a reliable determination of the required values of the fractal parameters requires a large array of source data values of activities of radionuclides. Therefore, new parameters were introduced: the dimension of the minimum cover and the fractality index in order to reduce the required values. A spline method was also used to smooth the function graph describing the migration of radionuclides in the soil. Studies of non-classical radionuclide transport processes in highly heterogeneous geological media (soils) reflect the most significant features of these processes.

According to the results of the study, it was concluded that the decrease in the concentration of the impurity of radioactive substances does not correspond to the classical laws and occurs according to the power law. This decrease in the superdiffusion mode is faster, and in the subdiffusion mode it is slower than in the classical (Gaussian) law. It is shown that the concentration of radionuclides in the" tails "of the distribution decreases according to the power law, which is characteristic of formal mathematical models of fractional diffusion-the presence of" heavy " tails of the distribution. This pattern of radionuclide proliferation can pose a significant risk because of the possibility of their migration over distances greater than previously thought. The results obtained have applied and theoretical values, can be used in the development of techniques for the management of spent nuclear fuel and radioactive waste, in justifying the safety of final isolation of high-and medium-level waste, as well as in the framework of environmental analytical monitoring.

An In Situ Neutron Scattering Study upon Cooling Confined CO2 on a Carbon Material below the Bulk Triple Point

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Ordered mesoporous carbon materials have attracted great attention in many areas of modern science and technology, with a wide variety of applications, such as catalyst supports, electrodes, materials for gas storage systems, adsorbents for gas and liquid purification, electrochemical sensors and drug delivery systems. Their popularity is mainly attributed to their unique pore structure and surface properties [1].

One of the most widely-studied ordered mesoporous carbons is designated as CMK-3. A typical synthesis of the CMK-3 involves nanocasting of SBA-15 ordered mesoporous silica (template) by sucrose (carbon precursor), followed by carbonization and silica etching [2]. By following this route CMK-3 is an inverse replica of SBA-15 that retains the structural symmetry of the template. To this end, CMK-3 type materials comprise hexagonally ordered carbon rods (p6mm space group) with a noticeable volume of micropores and highly interconnected uniform mesopores between them [3].

In the present work CO_2 was confined in the pores of a CMK-3 type sample and its phase behavior was studied by in situ total neutron scattering, during freezing below the bulk triple point (T_3=216.6 K, P_3=5.19 bar) down to 160 K. The experiment was carried out at NIMROD instrument, ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, UK. NIMROD bridges the gap between conventional small- and wide-angle neutron scattering and is thus ideal for the structural properties of fluids confined in porous materials [4].

In a previous NIMROD experiment, the phase behavior of CO_2 sorbed on an ordered mesoporous silica sample (SBA-15) was investigated during cooling below T_3. Surprisingly, the pore-confined CO_2 molecules neither freeze nor remain liquid as expected, but escape from the pores at some characteristic temperature [5]. The process is reversible and, upon heating, the pores are refilled nevertheless with a temperature hysteresis. In the present study, upon cooling below T_3, partial CO_2 depletion from the pores of the CMK-3 type sample was also observed but in a different way compared to its inverse replica SBA-15. In addition, close to T_3, the pore-confined CO_2 was found to be in a strongly densified state.

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Momentum distribution of nickel and niobium in the Ni44Nb56 metallic glass by neutron Compton scattering: isotopic substitution in action.

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Drawing from our proven track record of Neutron Compton scattering (NCS) work performed on VESUVIO spectrometer at ISIS, we carried out experiments for the two samples with same chemical composition ($Ni_{44}Nb_{56}$) but with different Ni isotopes [^{58}Ni (cross section =26.1 barn) and ^{60}Ni (cross section = 0.99 barn)].By measuring the nuclear momentum distributions of Ni and Nb nuclei we traced the changes to $g_M(\omega)$ (M=Ni, Nb) . To aid the data analysis the widely used technique of stoichiometric fixing was applied. Namely, the ratio of peak intensities, A_{Ni} /A_{Nb}, where A_{Ni} and A_{Nb} are the fitted scattering intensities from the Ni and Nb atoms, were fixed to $N_{Ni}b^2_{Ni}$/ $N_{Nb}b^2_{Nb}$, where N_{Ni} and N_{Nb} are the corresponding numbers of atoms in the beam. The total scattering cross-section for nickel is $\sigma_{Ni} = 4\pi b^2_{Ni}$, where bNi is the neutron–proton scattering length, with a similar expression for σ_{Nb}. Since neutron–nucleus cross-sections for both nickel isotopes have different values the fitted values of the constants A_M were different , what permitted us to calculate partial kinetic energies of Ni and Nb atoms. In order to obtain $g_M(\omega)$ in $Ni_{44}Nb_{56}$ system the Schommers algorithm was used . Obtained results were compared with existing inelastic neutron scattering data and computer simulation. As the result we obtained much deeper insight into the interatomic bonding interaction and atomic dynamics in the metallic disordered systems.This work was performed using the equipment of Unique Scientific
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Studying the structure and dynamics of water within the main binding phase of cement using neutron scattering

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Background

During cement hydration different mineral hydrates nucleate and grow, of which calcium silicate hydrate (C-S-H) is the most important binding phase. Understanding structural and dynamical properties of different types of water (interlayer, adsorbed, pore water) within the C-S-H phase is crucial, as water plays a key role in cement dissolution-recrystallization, carbonation, diffusivity of ionic species and it partially controls the mechanical properties of cement.

Aims

To study the structure and dynamics of distinct types of water within the main binding phase of cement.

Methods.

The protocol based on water sorption isotherms was developed to synthesize and isolate samples with a confined interlayer, adsorbed and bulk pore water within the C-S-H phase by careful conditioning under inert controlled humidity atmospheres. The structure of these distinct types of water within the C-S-H phase has been investigated using Neutron Diffraction with Isotopic substitution. Two identical sets of samples were analysed; one half was conditioned using light water and the other half was conditioned using heavy water. The first-difference method was applied to obtain partial Pair Distribution Functions centered on the hydrogen atom. The vibrational density of states for interlayer, adsorbed and pore water was probed using Incoherent Inelastic Neutron Scattering. Finally, the atomistic-level models simulations will be executed to interpret collected experimental data.

Results.

The Incoherent Inelastic Neutron Scattering technique confirmed the presence of at least three types of water within the C-S-H phase. The vibrational dynamics for bulk pore water differ clearly from the ones of interlayer water and water adsorbed on the external surfaces. The extracted structure factors for hydrogen atoms will be used together with vibrational density of states data to construct an atomistic model of C-S-H with water molecules within the structure. Furthermore, a close study of an interlayer water indicated the swelling and collapse of an interlayer space of C-S-H varying depending on Ca/Si ratio and drying conditions. The temperature regime mimicking natural summer weather conditions revealed overall dehydration of C-S-H and collapse of an interlayer space. Tests are being carried out to verify the reversibility of swelling and shrinkage for varying Ca/Si ratios and drying conditions.

Conclusions.

The structure of disordered C-S-H phase and the structure and dynamics of water within the C-S-H phase and are being studied using a combination of neutron, X-ray and simulation techniques. Preliminary results demonstrate the presence of at least three distinct types of water within C-S-H phase in terms of vibrational properties. Their distribution showed the dependence on temperature, relative humidity atmosphere and the initial Ca/Si of the C-S-H phase.

New organic compounds as materials with nonlinear optic properties

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Over the past two decades, the synthesis of molecules with nonlinear optical properties (NLO) and their hyperpolarizabilities have become the focal point of extensive research efforts. Currently much attention has been paid to organic NLO materials owing to their substantial first (β) and second (γ) hyperpolarizabilities and high laser damage resistance compared to inorganic materials [1].

In searching for new organic materials with ability to be applied in non-linear optics an attention was paid to 3,9-dinitro-5a,6,11a,12-tetrahydro[1,4]benzoxazino[3,2-b][1,4]benzoxazine (DNBB) which appeared to be highly efficient non-linear crystal with largely expressed phase – matching characteristics [2,3].

We have previously reported the synthetic and structural study of propellanes derived from 1,2-cyclohexanedione and o-aminophenols while searching for new and efficient materials for nonlinear optics[4,5,6].

Miniewicz *et al* [7] describe a molecule, earlier described by Nowicka-Scheibe *et al*[5], 16,20-dinitro derivative of 10-diaza[4.4.4] propellane, which belongs to a large family of heteropropellanes. These studies demonstrate that among the molecules of the propellane family, there exist very promising crystals for second-order, and possibly for third-order, NLO applications.

In the present work, we are investigating the condensation reaction between 1,2-cyclohexanedione, D,L-camphoroquinone and a variety of substituted pyridine. Depending on the ratio of the reagents used and the structures of 1,2-diketone and N,O-binucleophile or reaction conditions the condensation reaction leads to propellanes, adduct or Schiff base. These studies demonstrate that among the molecules of the propellane family, there exist very promising crystals for second-order, and possibly for third-order, NLO applications.

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DEPENDENCE OF THE PHONON SPECTRUM OF NARROW-GAP SEMICONDUCTOR FeSi FROM ATOMIC VOLUME

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The analysis of experimental data on the evolution of the spectrum of thermal vibrations of iron atoms in the FeSi monosilicide is presented as function of two external parameters – temperature (range T= 46 – 297 K, at P= 0.1 MPa) and pressure (P= 0.1 MPa – 43 GPA, at T=297 K). The spectra are measured by nuclear inelastic scattering of synchrotron radiation with high energy resolution [1, 2, 3]. It was found that the decrease the atomic volume, resulting from decreasing temperature as well as increasing pressure causes a strong modification of the phonon spectrum. The modification is manifested particular, in splitting of the low-energy phonon peak, and in increasing of the energies of all spectral peaks. The dependences of the mean energy of the vibrational spectrum of iron atoms and Debye energy on decreasing of the atomic volume have been obtained and analyzed. Two possible scenarios of changes in the electron spectrum of FeSi are proposed, which allow us to explain the observed phonon anomalies. Under normal conditions, the compound behaves like a metal and turns into a narrow-gap semiconductor upon a decrease of the atomic volume. According to the first scenario, a further decrease of the atomic volume leads to metallization of the compound, while in the second scenario, this decrease broadens of the bandgap in the electron spectrum and, hence, leads to the formation of a semiconductor state with a broad bandgap. In any case, FeSi ceases to be a narrow-gap semiconductor, and all anomalies associated with the presence of a narrow gap disappear. The results obtained generally allow us to distinguish the electron-phonon interaction in the iron sublattice as a physical mechanism linking the change in the atomic volume with the manifestations of anomalies in the phonon spectrum of FeSi.

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A Tungsten-based nano-laminated ternary carbide: (W,Ti)4C4−x

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Nano-laminar transition metal carbides are important as precursors for 2D derivative materials and due to their promising applications. We report a new nano-laminated tungsten based structure, $(W,Ti)_4C_{4-x}$ (Fig. 1). The crystallographic symmetry, specific site occupancies and crystallographic out-of or in-plane ordering were investigated using x-ray and neutron diffraction, supplemented by contrast scanning electron microscopy. Only a simultaneous refinement of the x-ray and neutron profiles is found to generate a stable solution and its details are discussed.

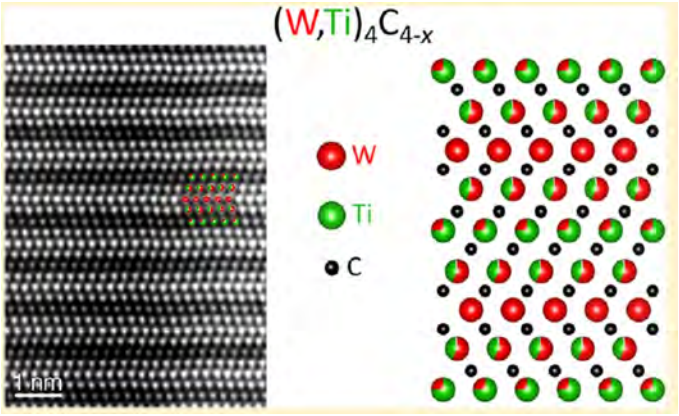

Fig. 1. Atomic ordering of $(W,Ti)_4C_{4-x}$. Left) HRSTEM image along the [1120] direction. Right) Structure model and stacking sequence of $(W,Ti)_4C_{4-x}$, where W, Ti, and C are shown by red, green, and black spheres, respectively.

How do the graphenic domains terminate in activated carbons? An INS & DFT study

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Inelastic neutron scattering (INS) spectroscopy is a powerful technique widely employed in the study of several carbon-based materials such as activated carbons, coals, carbon blacks, glassy carbons or reduced graphene oxides. These materials display very different chemical and physical properties, but their structure at the atomic scale is actually very similar: small graphenic domains, terminated by C-H groups, featuring variable amounts of functional groups containing other heteroatoms (O, N) and displaying high disorder and defectivity. Thanks to the high sensitivity toward the vibrations of hydrogen-containing species of INS spectroscopy, the spectra of these classes of carbon-based materials can provide important information regarding the nature of the terminations of the regular graphenic domains responsible for their chemico-physical properties.

With this contribution, I will focus on the case study of a series of activated carbons of industrial interest having different origin studied by a combination of INS spectroscopy and DTF simulation. The aim is to locate the fingerprints of different C-H terminations on the INS spectra and quantify their relative abundance, and consequently identify the most likely border geometry for each sample.

All the samples employed for this study have been provided by Chimet S.p.A, in the frame of a long-lasting collaboration, and have been extensively explored by means of INS spectroscopy, with measures performed on the TOSCA instrument at ISIS [1-2] and on LAGRANGE at ILL [3-4]. The obtained INS spectra display evident differences among samples, ascribable to significant differences in their C-H border geometries.

The assignment of the bands observed in the experimental INS spectra to vibrational modes of specific border geometries is a challenging task. The simulation of INS spectra by means of DFT calculations has the potential to shade new light on several details otherwise impossible to point out [5]. In the frame of our simulation work, we demonstrated that the main features of the experimental spectra can be well simulated by using simple models consisting in polycyclic aromatic compounds. By simulating the spectra of a large number of different models, it was possible to understand the contributions to the overall spectrum of several border geometries, and to quantify the relative abundance of different termination geometries within each sample.

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Correlation of Local Structure and Oxygen Transport in Oxide Ion Conductors

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There are many open questions over the relationship between the average perovskite structure composed of a network of ABO_3 corner-shared BO_6 octahedra and its local atomic arrangement, and it has been found in many cases that short-range order of materials can have a significant impact on their properties [1]. Our group recently used neutron total scattering measurement to aid in the understanding of the impact of local structure on the oxygen transport properties of $CeNbO_{4.25}$ at room temperature [2]. In our present study, this was carried further by analysing the total scattering data collected at high temperatures, which is of particular significance given the potential applications of cerium niobates in high-temperature electrochemical devices.

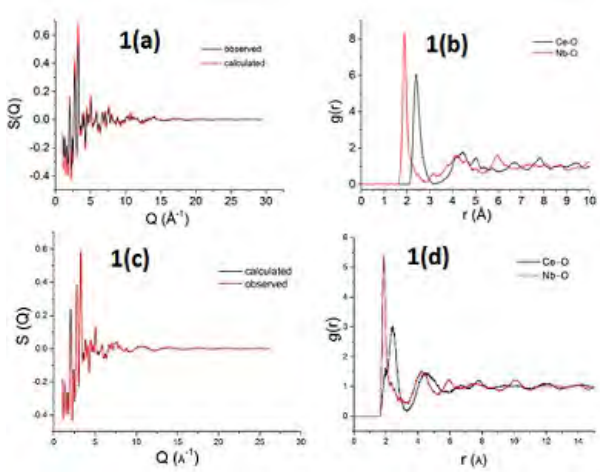

Figure 1. PDF analysis of $CeNbO_{4.25}$ powders showing 1(a) total scattering structure factor S(Q) and 1(b) partial pair correlation functions g(r) of $CeNbO_{4.25}$ at 273K and 1(c) S(Q) and 1(d) g(r) of $CeNbO_{4.25}$ at 923K.

The neutron diffraction data for Bragg scattering were analysed using GSAS [3] and the total scattering data correction was performed using Gudrun [4] before applying Reverse Monte Carlo analysis as adopted in RMCProfile [5]. The pair distribution function [G(r)] of $CeNbO_{4.25}$ analysed at different temperatures showed Nb−O peaks were sharp whereas the Ce−O peaks were broader, which suggests that Ce−O bond distance has slightly greater distribution {Fig. 1; 1(a) and 1(b) were adopted from ref. 2}. This data was later fitted with RMCProfile and it indeed was found that the partial pair correlation function g(r) for Ce−O was broader. This result fits well with the reported existence of mixed Ce^{3+} and Ce^{4+} ions in the $CeNbO_{4.25}$ system, resulting in a distribution of Ce-O bonding environments. It was also observed that there was extended coordination of Nb−O from 4+2 (in $CeNbO_4$) to 7 and 8 in $CeNbO_{4.25}$, which is due to the insertion of three interstitial oxygen ions per formula unit [2]. This is expected to have a direct influence over oxygen transport mechanisms in these materials. Furthermore, it was observed that the bond length distribution widens with the increase in temperature from 273K to 923K.

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Visualizing hydrogen atoms and protons in proteins

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Neutron crystallography is an important technique in Structural Biology since it provides details of hydrogen (H) atom and proton (H^+) positions in biological macromolecules. Knowledge of these positions are important as they allow details of protonation and hydration to be determined that are often necessary for understanding many biological processes, such as elucidation of enzyme mechanisms. Moreover, since H-atoms are involved in drug binding via directional H-bonding and non-directional hydrophobic and electrostatic interactions, visualization of these key interactions in enzyme-drug complexes can help guide structure-based drug design. Here I will describe examples of recent neutron crystallography studies performed at the Institut Laue-Langevin, including HIV-1 protease [1-2], an essential enzyme for the life-cycle of HIV; galectin-3 [3], a sugar-binding protein implicated in heart disease and breast cancer; cAMP- and cGMP-dependent protein kinases [4, 5], enzymes that drive many diseases including cancers, diabetes and neuropathies; aspartate aminotransferase [6], a vitamin B_6 dependent enzyme involved in amino-acid metabolism; carbonic anhydrase II [7], an enzyme implicated in glaucoma; and transthyretin [8], a highly amyloidogenic transport protein. These examples illustrate how results from neutron crystallography advance our comprehension of enzyme catalytic mechanisms and protein-ligand/drug binding, thereby allowing us to suggest new ways to improve the design of drugs that inhibit or activate their target proteins.

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Keywords.
Neutron crystallography, hydrogen, deuterium, protonation, hydration, enzyme mechanisms, drug design

Structural flexibility of thylakoid membranes revealed by small-angle neutron scattering

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Biological organisms capable of oxygenic photosynthesis developed highly organised structures to convert light energy into chemical energy. Small-angle neutron scattering (SANS) is a non-invasive technique, free of radiation damage – ideally suited for characterising complex biological macro-assemblies on the mesoscopic scale. Earlier SANS measurements have provided statistically and spatially averaged information about the structure of multilamellar thylakoid membrane systems in different photosynthetic organisms [1-2]. SANS has also revealed light-induced reversible structural changes on a time scale of seconds to minutes - small but well discernible variations in the characteristic repeat distances of the thylakoid membranes in isolated chloroplasts, living unicellular organisms and intact leaves [3-5]. Some of these reorganisations have been shown to be associated with key regulatory mechanisms of photosynthesis. In my poster presentation I will summarize the present state of this field, and outline my proposed contribution to better understand the nature of thylakoid membrane reorganisations elicited by different biotic and abiotic stress conditions in algae and plants.

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Human dystrophin structural changes upon binding to anionic membrane lipid

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Scaffolding proteins play important roles in supporting the plasma membrane (sarcolemma) of muscle cells. Among them, dystrophin strengthens the sarcolemma through protein-lipid interactions, and its absence due to gene mutations leads to the severe Duchenne muscular dystrophy. Most of the dystrophin protein consists of a central domain made of 24 spectrin-like coiled-coil repeats (R). Using small angle neutron scattering (SANS) and the contrast variation technique, we specifically probed the structure of the three first consecutive repeats 1-3 (R1-3), a part of dystrophin known to physiologically interact with membrane lipids. R1-3 free in solution was compared to its structure adopted in the presence of phospholipid-based bicelles (Figure 1). SANS data for the protein/lipid complexes were obtained with contrast-matched bicelles [1] under various phospholipid compositions to probe the role of electrostatic interactions. When bound to anionic bicelles, large modifications of the protein three-dimensional structure were detected. R1-3/anionic bicelle complexes were further analyzed by coarse-grained molecular dynamics simulations. From these studies, we report an all-atom model of R1-3 that highlights the opening of the R1 coiled-coil repeat when bound to the membrane lipids (Figure 1). This model is totally in agreement with SANS and click chemistry/mass spectrometry data. We conclude that the sarcolemma membrane anchoring that occurs during the contraction/elongation process of muscles could be ensured by this coiled-coil opening [2]. Therefore, understanding these structural changes may help in the design of rationalized shortened dystrophins for gene therapy. Finally, to probe the membrane interaction more accurately, we performed recently specular neutron reflectivity measurements on R1-3 in interaction with phospholipid monolayers (in Langmuir trough) or supported bilayers (on silicon wafer).

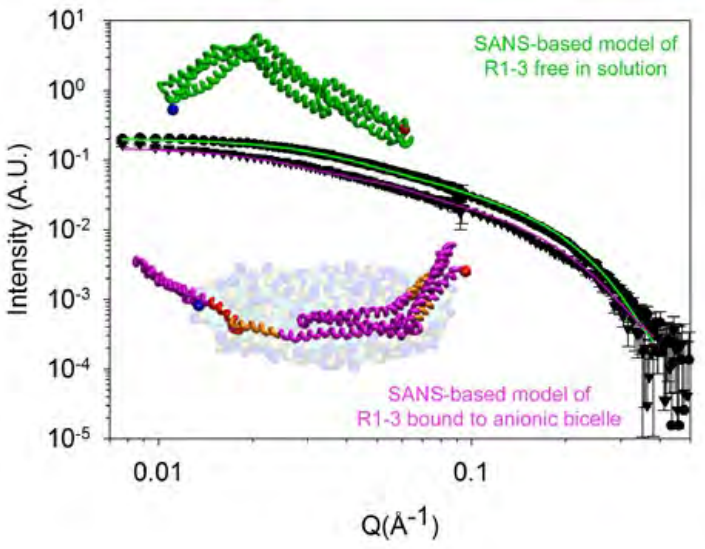

Figure 1. Experimental SANS intensities (circles and triangles for R1-3 alone or bound to contrast-matched anionic bicelles, respectively) fitted with the theoretical CRYSON curves generated from the R1-3 model free in solution (green) and the R1-3 model bound to anionic bicelles (purple), showing an opening of repeat 1. The corresponding all-atom models are represented with the same color code. From [2].

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Are proteins dynamcially heterogeneous? A rotation-translation model combining elastic, time domain and multiple neutron scattering.

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We address the question, whether proteins as 'complex systems' can be characterized dynamically by specific spatial motions, instead of resorting to heterogeneous diffusion in energy space (1,2). The neutron scattering spectra of dry and hydrated proteins are analyzed in the time domain based on a generic dynamic model with two major components, rotational transitions of side chains, mainly methyl groups and local translational diffusion of non-methyl side chains (3). The significance of the fits is based on data covering a wide range in time, momentum exchange and temperature. The translation-rotation model applies the established theory of space time correlation functions successfully, which is compatible with the idea of homogeneous quasi-elastic spectra (4,5). Dynamical heterogeneity on a small scale can be deduced from the rate distributions of the motional components. The temperature dependent elastic intensity is shown to support the dynamic analysis. The puzzeling change of the intensity at zero momentum exchange is easily explained by multiple scattering effects, without resorting to energy landscape models (5, 6, 7).

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Chromatin Structural Organization And Protein-Oleic Acid Complexes

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Multimeric alpha-lactalbumin oleic acid and lactorerrin oleic acid complexes are known to exhibit antitumor effects in some tumor cell cultures. Complexes featuring oleic acid (OA) with human alpha-lactalbumin (hAl), bovine alpha-lactalbumin (bAl), and human lactoferrin (hLf) were investigated using small-angle neutron scattering (SANS).

We show that the artificially created complexes featuring multimeric alpha-lactalbumin formed in the presence of oleic acid contain a stable suspension of oleic acid with particles of various sizes (up to tens, and possibly hundreds, of nanometers). Alpha-lactalbumin molecules are localized on the surfaces of such particles. Lactoferrin/oleic acid complexes, on the other hand, do not contain large micelles, and they can be considered a monodisperse system of small (~20 nm) particles.

When applied to isolated HeLa nuclei, both hAl-OA and hLf-OA complexes lead to changes in small-angle neutron scattering pattern of chromatin. These changes indicate a likely effect of these complexes on the large-scale structure of chromatin and may point to the possible mechanism involved in their anticancer activities.

DEMAX: The Deuteration and Macromolecular Crystallization Support labs for the European Spallation Source.

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DEMAX is the Deuteration and Macromolecular Crystallography support lab for soft condensed matter, chemistry, and life science users of the European Spallation Source (ESS). DEMAX offers three areas of support: Biological deuteration (e.g. cell paste, soluble proteins, lipids, membranes), Chemical deuteration (e.g. small organic molecules, surfactants, phospholipids), and Crystallization (biological macromolecules e.g. proteins).

We kicked off our first call for proposals in Q1 of 2019 and will conclude with delivering materials during Q3 2019. This gives us a chance to practice and refine our procedures while we are still establishing the labs and our methodological capabilities. Access to DEMAX is proposal-based and is granted on a technical/safety/feasibility and scientific peer review basis. We are running three pilot cycles and accepting 12-15 proposals per cycle during 2019-2021. During this pilot phase we will not limit access to DEMAX to ESS member countries and materials are provided to user free of charge (S&H fees may apply for dangerous goods).

We have well-equipped chemistry and life science labs and offer service for specific classes of deuterated organic small molecules (e.g. lactic acid, fatty acids, alcohols, surfactants, detergents), deuterated biomass from algae & bacteria, deuterated recombinant proteins, and access to our crystallization labs for large crystal growth. To enable our biological deuteration and protein crystallization activities we have established a partnership with Lund University's Lund Protein Production Platform (LP3), a cross-faculty support lab for the production and crystallization of proteins. DEMAX and LP3 are co-located in the Biology Department of Lund University. For the chemical deuteration activity we are located in labs in the Medicon Village campus in Lund. ESS is also the organizing node for DEUNET, a network of deuteration facilities around Europe, more information and news can be found at: http://www.deuteration.net.

Biohybrid entities with potential applications in biomedical field

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Hybrid entities based on biogenic nanosilver (bio-AgNPs) chitosan, bioinspired membranes labelled with chlorophyll *a* were prepared by "green" approach. The new silver nanoparticles were eco-synthesized from different vegetal sources. In order to get deep inside about the structure of the bio-AgNPs alone, and incorporated into the assemblies with liposomes and chitosan, and also about the interaction between the components of the biohybrids, spectral methods have been used: UV-Vis absorption and emission spectroscopy. The internal structural of the bio-AgNPs in presence of liposomes and chitosan has been studied by Small-angle neutron scattering, Small-angle X-ray scattering, and X-ray diffraction. The size and morphology of the biohybrid systems were studied by AFM and SEM analysis. The bioperformances are closely related to the structure of the biohybrids. Thus, the obtained biohybrid entities exhibited: good antioxidant properties (up to 98.5%, *in vitro* tested through chemiluminescence method) and good antibacterial activity against the pathogenic bacteria: *E. faecalis*, *Escherichia coli* ATCC 8738 and *Staphylococcus aureus* ATTC 2592.

The obtained bio-based hybrids could be used in biomedical field, as antioxidant and biocide materials.

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Complementarity of SAXS and SANS investigations of large protein complexes: SAXS/SANS EID and SEC-SAXS methods

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The method of small angle scattering (SAS) is widely used in the field of biophysical research of proteins in aqueous solutions. Obtaining low-resolution structure of proteins is still a highly valuable method despite the advances in high-resolution methods such as X-ray diffraction, cryo-EM etc. SAS offers the unique possibility to obtain structural information under conditions close to those of functional assays, i.e. in solution, without different additives, in the mg/mL concentration range. SAS method has a long history, but there are still many uncertainties related to data treatment. We compared 1D SAS profiles of large protein complex (d = 120Å) apoferritin that consists of twenty four subunits, obtained by X-ray diffraction (XRD) and SAS methods. It is shown that SAS curves for X-ray diffraction crystallographic structure of apoferritin differ more significantly than it might be expected due to the resolution of the SAS instrument. Extrapolation to infinite dilution (EID) method does not sufficiently exclude dimerization and oligomerization effects and therefore could not guarantee total absence of dimers account in the final SAS curve. In this study, we show that EID SAXS, EID SANS and SEC-SAXS methods give complementary results and when they are used all together, it allows obtaining the most accurate results and high confidence from SAS data analysis of proteins. It also might be useful for accurate structure determination of other large protein complexes.

The studies by SEC-SAXS method were supported by RFBR according to the research project № 18-34-00256\18. EID SAXS and SANS studies were supported by the Ministry of Education and Science of the Russian Federation (grant no. 6.3157.2017).

Structural determinants for secondary nucleation pathway in Amyloid-beta fibrils formation by contrast variation SANS

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Alzheimer's disease is the most common form of neurodegeneration in which the brain shows accumulation of insoluble fibrillary deposits and neuronal death is caused by co-existing smaller aggregates. The formation of those aggregates involves the misfolding of two major forms of Amyloid-β peptide: Aβ40 and Aβ42. The co-existence of several Aβ length variants motivates our interest to investigate the cross-seeding behaviour among Aβ40 and Aβ42. We define cross-seeding as the contribution of pre-formed fibrils of one variant to induce the aggregation of other variants. A recent study has demonstrated the presence of three steps in the aggregation mechanism of pure Aβ40 or Aβ42. The primary nucleation process creates aggregated species from monomer only, while the growth process involves the elongation of existing β-sheet-rich fibrils by monomer addition (Cohen et al, PNAS 2013, Meisl G. et al., PNAS, 2014). Above a critical fibril concentration, the majority of oligomers are generated from monomers by secondary nucleation catalysed by the larger fibrils. (Cohen et al., PNAS 2013). Only at the very earliest time points of a reaction starting from pure monomer, before the first fibrils are formed, all oligomers have to be generated through primary pathway. The identification of secondary nucleation as the major source of toxic oligomers makes it important to elucidate the structure of the mature amyloid fibrils and the nuclei formed on their surface with an aim to understand the molecular basis of the surface catalytic activity.

Here we will present our most recent Small Angles Neutron Scattering data to provide for the first time structural insights into the cross-reaction between the recombinant species of Aβ40 and Aβ42 polypeptides with the contract variation method.

Novel crystallization device for large protein crystal growth.

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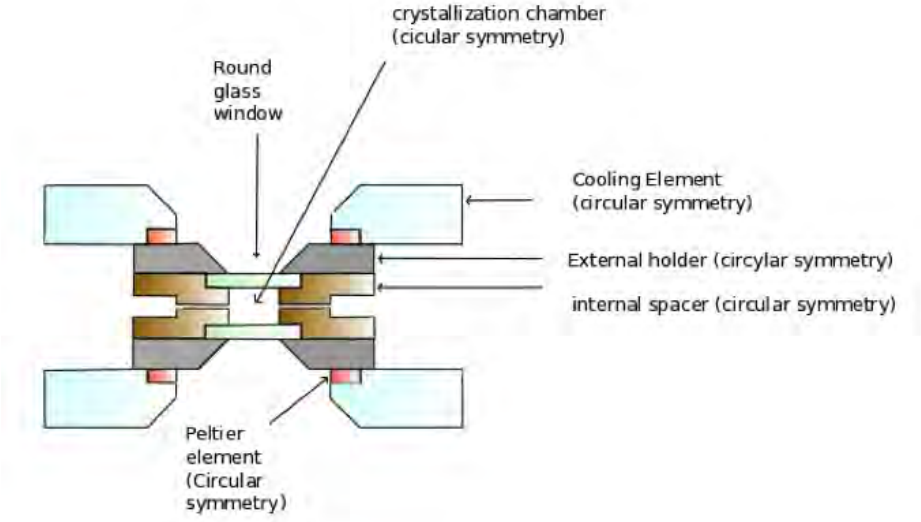
The achievement of sufficiently large protein crystals is the main obstacle for a successful neutron diffraction experiment. Even by using perdeuterated protein, a minimum crystal volume of about 0.1 $mm^3$is necessary. The crystallization process is composed of two main steps: the nucleation and the crystal growth, which occurs in the nucleation and the metastable zone of the phase diagram, respectively. The phase diagram of a specific protein is a multidimensional graph as a function of temperature, pH, protein and precipitant concentration. Depending on the values of these parameters, the protein solution can be either in the undersaturation zone, where there is no crystallization, or in the supersaturation zone, where either nucleation or crystal growth occurs. To initiate the crystallization process, all the parameters have to be selected in order to set the protein solution in the nucleation zone. After the development of the first nuclei a natural decreasing of the protein concentration, due to the consumption of the protein for the formation of initial aggregates (the nuclei), will drive the protein solution into the metastable zone, where the nuclei can grow during time. In this context, an increase of the final protein crystal volume can be achieved by keeping the protein solution in the metastable zone as long as possible. With this goal we designed and built a crystallization apparatus based on the possibility to choose the crystallization method (batch and vapour diffusion) and control fundamental parameters such as the temperature, the precipitant and the protein concentration in the same crystallization experiment. The crystallization chamber is connected with the external environment by means of capillaries, which allow a replacement of the mother liquor around the crystal for the batch crystallization case or the reservoir solution in case of the vapour diffusion method. A first test of the crystallization apparatus has been performed by using lysozyme as model system, which has the advantage that the phase diagram is well known and crystals form readily and fairly reliably. The crystallization apparatus will be tested with other model systems in the future. Additional measurement techniques as for example dynamic light scattering to monitor the aggregation status of the proteins in solution phase or UV-visible spectroscopy to control the concentration of the protein in solution will be discussed.



Lipid bilayer covered nanoweiers studied with GISANS

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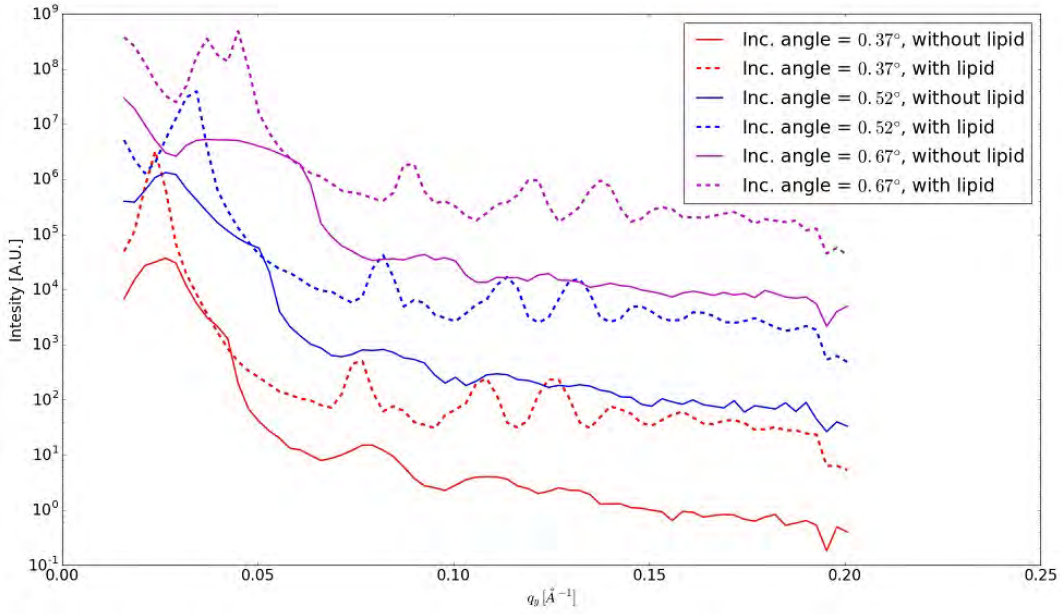
Semiconductor nanowires are increasingly used in life science as nanometer probes and to manipulate living cells. When interfacing high aspect ratio nanowires with cells, the first point of contact is the cell membrane which forms a locally highly curved membrane around the nanowires [1]. The mechanisms of the formation of this type of structures are not fully understood. We have previously demonstrated the formation of a supported phospholipid bilayer as a proxy to curved membranes on gallium phosphide (GaP) nanowires via vesicle fusion. Based on fluorescence recovery after photobleaching, FRAP, measurement, the phospholipid bilayers were found to follow the contours of the nanowires as continuous and fluid, locally curved bilayers [2]. However these data do not reveal the coverage, composition and the dimensions of the bilayer. In this project we aim to revel this using grazing incident small angle neutron scattering (GISANS).

Curved cell membranes are important for the function of the cell, both for compartmentalization in organelles within the cell as well as for cellular mitosis. It has also been shown that the curvature of a lipid membrane can affect the concentration of membrane bound proteins. We have studied bilayer covered nanowires as a way to model to study how curvature affects a cell membrane and how it influences the binding of proteins.

For this purpose we have performed a GISANS experiment at the KSW-1 beam line at FRM II in Garching with phospholipid covered nanowiers. The nanowiers were covered with a phospholipid bilayer obtained from deposition from vesicular dispersion of mixture of 20mol% DOPE in DOPC, as described in detailed by Dabkowska et.al [2]. The figure below shows a comparison between bilayer covered (dashed lines) and bare nanowires in D_2O. The figure shows a cut along $q_x = 0$ at three incident angles at 8 m sample to detector distance with a 5 Å wavelength. When the nanowiers are covered with the phospholipids, three Bragg peaks appears more clearly. The peaks also seem to be narrower and a bit more intense than the bare nanowiers.



Experiments are planed at ISIS and NCNR (NIST) during the year to further investigate the system.

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Effects of Stressors on the Macroorganisation of Thylakoid Membranes

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Thylakoid membranes, the site of oxygenic photosynthetic light reactions, in most photosynthetic organisms are organised into multilamellar membrane assemblies with remarkable structural and functional plasticity, associated with different regulatory mechanisms [1]. When the organisms are subjected to stress conditions, monitoring the nature and extent of stress-induced membrane reorganisations is a key step towards the understanding the mechanism of stress responses *in vivo*. In a series of experiments, we exposed different photosynthetic organisms to abiotic and biotic stresses and used small-angle neutron scattering (SANS) to reveal the stress-induced changes in the thylakoid membrane ultrastructures. SANS is a non-invasive technique, which has been demonstrated to be capable of providing statistically and spatially averaged structural information about the structure and structural flexibility of multilamellar membrane systems of different photosynthetic organisms [2,3].

Unicellular algae are highly sensitive to heavy-metal ions, such as cadmium and chromium. Cadmium is one of the most toxic aquatic contaminants. The inhibitory effects of Cd on both the dark and light reactions of photosynthesis have been studied in several laboratories [4,5]; however, a general model is yet to be formulated. Chromium is also highly toxic for photosynthetic organisms [6]; due to its extensive industrial use, large quantities of Cr compounds are present as pollutant in the environment. Here we report on the effects of these two heavy metal ions on the thylakoid membrane systems of the green alga *Chlorella variabilis*, at different concentrations and lengths of the treatments [7].

The trace element selenium, while being an essential nutrient for animals, also poses an environmental hazard at larger concentrations – a duality that depends on multiple factors such as the chemical form and concentration of selenium [8]. While the influence of Se on photosynthesis is highly relevant to environmental pollution and soil remediation, the production of Se-rich crops is also of interest. Our investigations on cultured tobacco plantlets revealed adverse effects of different forms and concentrations of selenium, selenate and nano-Se, on the granum thylakoid membranes of young tobacco leaves [9].

We also studied the effects of strong illumination, a key biotic stress factor, on the rainforest vine *Monstera deliciosa* – a plant which can survive both the low-light environment of the rainforest floor and the high-light environment on the sunlit canopy. We used this model plant, with giant grana and an outstanding capability for the photoprotective, ΔpH-dependent non-photochemical quenching (NPQ), to study the hypothesized correlation between membrane reorganizations and NPQ. Our results revealed a close correlation between the time courses of NPQ and major reversible reorganizations in the periodic multilamellar organization of the grana in these leaves [10].

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Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum MLZ

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Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules, thus providing important complementary information to that gained by X-ray crystallography. At the FRM II neutron source in Garching near Munich the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is dedicated to structure determination of proteins. Typical scientific questions address the determination of protonation states of amino acid side chains, the orientation of individual water molecules and the characterization of the hydrogen bonding network between the protein active centre and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behaviour of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal. Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography.

Protein and water dynamics at the atomic level: realistic atomic displacement parameters using neutron crystallography

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Protein biological function is tightly regulated by dynamical changes in protein structure. In structural biology, the mechanism of action of a protein is usually inferred from a set of different conformational states captured in the presence of co-factors, substrates, inhibitors or products of the studied reaction. The most prolific method to decipher the structure of a protein, and subsequently its reactional mechanism, is X-ray crystallography. Despite of the overwhelming success of this technique in unravelling the function of proteins, there's still relevant information buried in the diffraction data that has been overlooked due to limitations both inherent to the technique and to the methods of model refinement [1]. The atomic displacement parameters (ADPs) incorporated in the Debye-Waller factor represent an unexplored pathway, in the case of proteins, toward the description of local and global dynamics. The ADPs derived from X-ray diffraction data suffer from the unrealistic assumption of the nuclear position and motion, based on the spherical model of the electron density [2]. Also, H/D atoms, which play a central role in protein function [3], are usually "invisible" to X-rays, and radiation damage is a constant concern, leading often to structural and functional misinterpretations [4]. On the other hand, neutron scattering poses as the fundamental technique to describe the atomic thermal motion, routinely in the case of small molecules [5]. Our work aims at pushing the boundaries of neutron crystallography by determining realistic and unbiased ADPs of partially deuterated and perdeuterated hen egg white lysozyme (HEWL).

Since the description of anisotropic ADPs relies on very high-resolution and complete neutron diffraction data, we are aiming at obtaining triclinic HEWL crystals that will be measured in D19, at ILL. A protocol for perdeuterated protein expression, purification and refolding was successfully devised and optimized. Preliminary tests on hydrogenated recombinant HEWL showed that it was possible to obtain native-like refolded protein, as proven by data collected up to 1.1 Å in ID30-b, at ESRF. As a consequence, we adapted the procedure to obtain refolded perdeuterated HEWL, resulting in folded and stable protein, as shown by the thermal shift assay results, with a ΔT_m of only 5º C, compared with the native hydrogenated commercial HEWL. Furthermore, a crystal of refolded perdeuterated protein was obtained in analogue conditions, as for the hydrogenated form, in D_2O, however it didn't diffract in the X-ray beam, suggesting that optimization of the crystallization conditions is still required.

An exciting opportunity to understand the impact of the aforementioned limitations of X-ray data, compared with neutrons, is present in the research we are conducting. The analysis of X-ray and neutron data collected on hydrogenated and perdeuterated HEWL may reveal systematic discrepancies between the derived ADPs that could change the interpretation of these parameters in future research. Furthermore, the comparison between diffraction data on HEWL crystals with different deuteration levels will provide answers regarding the effect deuteration on protein structure and dynamics.

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Inelastic neutron scattering study of gallic acid and its monohydrate

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Gallic acid i.e. 3,4,5-trihydroxybenzoic acid in its lowest energy state has three hydroxyl OH groups on the ring oriented in the same direction [1]. It is widely found in plants such as hardwood oak and chestnut trees, as well as grape, berries and nuts [2,3]. Gallic acid exhibits biological activity as it shows cytotoxicity against cancer cells, antifungal and antiviral properties, and is used as an antioxidant [2,3]. Motivated by its biological effects and pharmaceutical applications number of studies of its structure, properties, and interactions in the solid state and in solution have been performed in the past. A number of crystal structure conformations of gallic acid in monohydrate and anhydrous forms are known [1,4,5].

Previously, infrared and Raman spectra of gallic acid have been measured for the monohydrated and anhydrous solids and the spectra have been interpreted with the help of density functional theory [6-10]. Difficulties occurred in the assignment of the spectra of the polycrystalline gallic acid monohydrate due to the strong intermolecular hydrogen bonds present, which caused broadening and mixing of vibrational modes.

In this work we will present inelastic neutron scattering (INS) spectra of the title compounds, including the low wavenumber region below 450 cm^{-1} (200 cm^{-1}) that was not measured with infrared (Raman) spectroscopy up until now. INS is a useful and established technique to explore vibrational spectra of solid state samples that offers better resolution at low wavenumbers (< 1200 cm^{-1}) and thus is particularly suited for studies of low energy modes, a spectral region that is not easily accessible with laser spectroscopy of high enough resolution. The low temperature of 10 K at which these studies have been performed simplified the spectra in comparison with the previous measurements. Indeed the vibrational studies of the gallic acid are important for better understanding of its biological function.

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SANS study of the NpSRII/NpHtrII complex

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The complex of Sensory rhodopsin II (SRII) with its cognate transducer (HtrII) from *Natronomonas pharaonis* is a representative of archaebacterial photoreceptors, which along with chemoreceptors and sensor histidine kinases comprises the class of two-component signaling systems (TCS), which is the most common signaling system in archaea. SRII/HtrII is a widely used model system for studying how TCS transfer signals across the membrane.

Despite the structure of the truncated construct is available [1], for complete understanding of the molecular mechanisms of the signal transduction, it is necessary to have full-length complex structure. Since the task of the full-length complex crystallizing is so difficult, we can use mall-Angle X-ray and Neutron Scattering (SAXS and SANS) to solve a low-resolution structure of the full-length [2].

In work [3] it was shown that the structure and oligomerization state of the HtrII cytoplasmic part are different in 150 mM and 4 M KCl.

We conducted an analysis how salt concentration influences to the structure of the trimer-of dimers of the full-length SRII/HtrII complex. The SRII/HtrII were prepared in four salt concentrations: 150 mM, 1.4 M, 2.8 M and 4 M NaCl. As these samples were prepared for SANS measurements, buffers were prepared with heavy water (D_2O). SANS measurements were done on the YuMO spectrometer (IBR-2, Dubna, Russia) [4].

It is shown that length of *ab initio* models corresponds to the full-atomic coarse-grained model [5] only for salt concentrations 2.8 and 4 M NaCl, which are close to natural *N. pharaonis* salt concentration 3.5 M. Length was smaller ror 150 mM and 1.4 M NaCl, that can be explained by disordering of the HtrII cytoplasmic part, which do not have a secondary structure in low salt concentration. This conclusion is confirmed by CD-spectroscopy: the protein in 150 mM NaCl has a typical for α-helix CD spectrum, because transmembrane part includes α-helixes, however, CD signal increases with increasing salt concentration.

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Small angle scattering study of Aspergillus awamori glucoamylase

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Glucoamylase (α-1,4-glucane-glucohydrolase, EC 3.2.1.3, GA), a glycoprotein of the GH15 glycoside hydrolase family, catalyses hydrolysis of α-1,4- and α-1,6-glycoside bonds in starch and oligosaccarides. GA from *Hypocrea jecorina, Rhizopus* and *Aspergillus* species are known to consist of the catalitic and starch-binding domains connected by glycosylated peptide chain. The structure of the catalytic domain of GA from *A. awamori* and *A. niger* has been obtained by X-ray crystallography [1-3]. The structure of the starch-binding domain of GA from *A. niger* has been determined by NMR [4]. The full structure of the enzyme has not been resolved, but a low-resolution structure of the entire GA1 from *A. niger* has been reconstructed from SAXS [5].

For investigation of the *A. awamori* glucoamylase, an expression system in *Pichia pastoris* has been developed, yielding an enzyme with more uniform glycosylation as compared to the native species. The expressed protein has been found to have very similar enzymatic activity as the natively glycosylated GA. This recombinant GA was studied by SAXS, SANS and cryo electron mycroscopy.

Comparison of SANS data obtained for H_2O and D_2O solvents show that the shape of the scattering spectra strongly depend on contrast. The gyration radii obtained by Guinier approximation ranged from ca. 31Å for the solvent with high D_2O content to 33–35Å in low D_2O solvent. The intensities to zero angle I_0 were determined for six contrast points and could be approximated by a second-degree polynomial function with a minimum at ca. 45% D_2O buffer. The results obtained are a strong indication that we observe a multi-component system, with components of different scattering densities (corresponding to peptide and sugar residues) present in the enzyme.

The gyration radius obtained in D_2O is close to that expected for a monomeric form of enzyme. A significantly higher value obtained in H_2O and 0.2 D_2O contrast points, where the non-peptide component has a higher weight. SAXS experiments (MIPT, Russia and ESRF, France) have yielded an intermediate value of R_g ~ 33 Å, which is likely due to a different contrast conditions of X-ray scattering.

Based on the data of small angle scattering and cryo electron microscopy, a GA model was constructed using homologous modeling and molecular dynamics methods. The gyration radius of GA dynamic model was 33.4 ± 0.6 Å, which correlates with the experimental results. Calculated SANS spectra of glucoamylase model for each contrast point were consisted with experimental data.

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A new method for calculating the SANS spectra including H2O/D2O contrast contribution estimation directly using all-atom molecular dynamics trajectories

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SANS is a common method that can be used to study various types of biological systems in solution. In the case of large molecular complexes, using only SANS methods, it is possible to obtain limited information about the structure of such systems (for example, the global geometric parameters of the system). In this case, using hybrid methods such as molecular dynamics with the involvement of the SANS data, even limited information obtained by the SANS method can be used to build full-atom models of biological systems. Another factor is the use of SANS data for verification of models of biological systems obtained using molecular dynamics. Taking into account the two methods, we can create and test atomic level models even for a large and complex molecular system.

The method for calculating the SANS [1] and NSE [2] curves from MD trajectories was developed and implemented as modules for the GROMACS molecular dynamics software package. Previously, other groups proposed contrast assessment methods for small systems, such as fatty acids in organic non-polar solutions [3]. We have created a universal method that allows us to estimate the contrast of D_2O/H_2O directly from molecular dynamics trajectories. This new technique has been applied to systems containing DNA and protein parts.

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PROBING STRUCTURE AND MOBILITY OF PROTEINS IN THE AMORPHOUS STATE AT LOW HYDRATION

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The characterization of proteins in the dry state has implications for the pharmaceutical industry, since it provides deeper understanding of the effect of lyophilisation on the stability and biological activity of bio-macromolecular drugs. We have performed structural and dynamical analyses on a series of lyophilised and hydrated bio-macromolecules with varying degrees of structural complexity by means of Molecular Dynamics (MD) simulations; the simulated dynamical results being compared to experimental findings obtained from neutron scattering.

Atomistic simulation of lyophilised proteins is still a challenge since the available force fields, and water molecule topology, used for the modelling have to be carefully correlated with experiment. Fortunately, the outputs from Molecular Dynamics simulations, and the time and length scales probed, align directly with those accessed by neutron scattering. In particular, the method of Quasi-Elastic Neutron Scattering (QENS) can be used to investigate picosecond to nanosecond dynamics of macromolecular species and thus help validate the efficacy of the MD protocols applied.

Here we report on the simulated effect of temperature and hydration on the structural features of the proteins, focusing particularly on the predicted changes in secondary structure and radial distribution. We also present a comparison of the temperature dependence of the mean squared displacement (msd) parameter, obtained by analysing the MD trajectories, with those resulting from experimental QENS measurements.

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The enhancement of the proton therapy efficiency with PBCT

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Depending on the density of the tissue and the beam energy protons penetrate into the body to a depth up to 38 cm. Heavy charged particles (HCP) such as protons practically do not lose energy due to weak scattering on the way to the affected area (tumor) and also can be focused by electromagnetic fields, which provides the maximum energy transfer to the tumor at the end of its path. At the same time, there is no radiation influence on the areas located behind the tumor [1].

A significant increasing of the effective dose at the end of the HCP-path (Bragg peak) due to ionization losses with slowing down of the HCP causes the main advantages of using protons instead of X-rays in the treatment of deep-seated tumors. Modulation of the beam energy leads to a change of the particle penetration depth resulting in a flat distribution of the radiation dose covering the entire tumor region (plateau on the Bragg curve). It is possible to achieve a sharp decrease of the healthy tissue radiation damage by uniformly changing the direction of irradiation at the same dose absorbed by the pathological focus.

The nuclear fusion reaction $p + {}^{11}B \rightarrow 3\alpha$ amplifies the therapy effect by generation of three alpha particles with higher radiobiological exposure (proton boron capture therapy, PBCT), [2]. Sodium borocaptate (BSH) with a natural isotopic content of ${}^{11}B$ (80%) and ${}^{10}B$ (20%) is used for localization of boron atoms in the tumor. The target dose increasing at 2.5 to 3 times with the addition of boron isotope (compared with conventional proton therapy) is expected [3].

The ongoing experiments are aimed at determining the effectiveness of the PBCT methodology by irradiating biological targets on the SC-1000 synchrocyclotron (NRC KI PNPI) with a proton beam energy of 200 MeV in order to obtain experimental Bragg curves of samples with boron isotopic content and without it.

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Small-angle diffraction study of proteoglycan structures of mucins and extracellular matrix of biological tissues

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The X-ray patterns of epithelial tissues and mucins from different sources are very similar and display a large number of sharp diffraction rings at spacings 4.5 nm and its higher orders. We attribute them to highly ordered proteoglycan structures which due to the interchain spacing of polysaccharides. The intensity and the width of 4.5 nm reflection changed within a wide range, whereas the spacing varied insignificantly. A correlation between an integral intensity of X-ray pattern and elemental content in tissue was observed. The peculiarity of X-ray pattern for intact tissues can reversibly be transformed by salt solutions and chelating agents. It was shown that the proteoglycan structures of mucus are very stable in a wide temperature range (0 – 130°C). Note, that it did not reveal any changes of the 4.5 nm spacing during stretching of hair tissue about 50%, while 6.7 nm spacing of intermediate keratin filaments of the cytoskeleton shifts towards small angles up to 8.0 nm.

Various normal and tumor transformed human and animal epithelial tissues were studied. *A variety of changes in X-ray patterns of tumor transformed tissues were observed.* In terminal stages of tumor transformation no discrete reflections are observed, increasing of intensity of diffuse small-angle scattering is displayed, specific density and rigidity of tissue increase, Ca-content is significantly higher. It is necessary to consider mobile proteoglycan structures of the extracellular matrix as the universal scaffolding providing structural homeostasis of biological tissues. *The 4.5 nm spacing is a structural invariant in the nano-dimensional scale of the proteoglycans of mucus and the extracellular matrix of biological tissues*. The 4.5 nm reflection should be considered as a marker of solely structural modifications of intact tissue under various exogenous influences.

The report also will analyze structural dynamics of three fibrillar protein systems of living muscle during contraction using a time-resolved technique. A 3D nanoscale morphological model of titin strand, a giant protein of the third fibrillar system of muscle, is suggested. Pulling is determinative factor in formation of heterophase-separated states in in aperiodic multidomain proteins of immunoglobulin superfamily.

High-Throughput SANS characterization of lipidic in meso phases

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Experiments of high-throughput characterization of lipidic *in meso* phases by small-angle X-ray scattering were described by (1). However, the method has severe limitations on materials, for example, glass material is not transparent for X-ray irradiation. In this work we measured monoolein with different polymeric supplements in glass plates by small angle neutron scattering on D16 instrument, ILL, Grenoble, France(2, 3).

The results showed the possibility of investigations of lipid *in meso* phases using high-throughput SANS technique. The measurements were done with monoolein with polymeric supplements in 200 uL pcr tubes. The diameter of neutron flux was 8 mm. The time per one measurement was approximately 30 sec. The samples were characterized and had Im3m and Pn3m types of symmetries. Some samples contained a mixture of Im3m and Pn3m.

The accuracy of data is sufficient for further investigations of lipid *in meso* phases by high-throughput SANS technique.

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Neutron component of radiation background at Mars

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Introduction.

High Energy Neutron Detector (HEND) onboard orbital Mars Odyssey mission (operating on Mars orbit from February 2002) and Dynamic Albedo of Neutrons (DAN) onboard Curiosity rover (operating on Mars surface from August 2012) are measuring neutron albedo of Mars produced by Galactic Cosmic Rays (GCR), see for example [1,2].

Mars is a future ambitious target for the human expansion will strongly requires as much as possible information and analysis about the Martian radiation environment. The radiation environment on Mars is very complex. It is mainly composed by energetic charge particles of GCR but also their secondary products (secondary charge particles, neutrons and photons) via interactions with nucleus in Martian atmosphere and in the top layer of surface material.

Previous studies have shown that during a direct and return flight to Mars plus staying on surface for 500 days astronaut can get total dose up to 1 Sv [3,4], which is about the astronaut life time limit defined by different space agencies. It could be even higher during an intense solar activity period. While the charge particles are the main contributor of radiation dose, the effect from secondary particles (primarily from secondary neutrons) should be also taken into account due to its higher biological impact and difficulties with radiation protection. The neutron component of the radiation background presents quite significant factor since the dose equivalent from neutrons can vary from 1% to tens of percent of the total dose, depending on the design and type of the spacecraft and selected protection method against ionizing radiation. Thicker body of a spacecraft decreases the flux of charged particles but enhances the production of secondary radiation and its subsequent contribution to the total dose.

The numerical simulations of HEND/Odyssey and DAN/MSL and comparison between model predictions and experimental data has been implemented to unfold Mars neutron spectra both on orbit and surface and evaluate biological impact contributed by neutrons. It was found that maximal neuron equivalent dose rate in energy range below 10 MeV approaches to 500 Sv per day providing up 7% of the expected charged-particle dose equivalent rate.

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Active neutron sensing of the Mars subsurface onboard the NASA's Marsrover Curiosity

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Description of the experiment for measurements of Dynamic Albedo of Neutrons (DAN) is presented, which is the part of scientific program of NASA's Mars Science Laboratory mission with the marsrover Curiosity. The instrument DAN contains the unit of Pulsing Neutron Generator (PNG), which radiates pulses of 14.1 MeV neutrons for irradiation of subsurface material below the rover, and the unit of Detectors and Electronics (DE), which operates the instrument and measures the die-away time profiles of epithermal and thermal neutrons after each pulse.

The experimental results of DAN investigation are presented for the content of water, chlorine and iron within a top layer of about 60 cm along the traverse of the rover.

The application of the method of active neutron sensing are also discussed for future space mission for studying Moon and Mars.

Neutron spin rotation at Laue diffraction in a transparent weakly deformed noncentrosymmetric crystal

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The effect of neutron spin rotation at Laue diffraction in a weakly deformed neutron-transparent noncentrosymmetric crystal has been described theoretically and studied experimentally. The effect is due to the bending of a Kato trajectory of the neutron in the deformed crystal. At a certain type of deformation, one of two neutron waves excited at Laue diffraction, which propagate in opposite crystal fields in the crystal with no center of symmetry, leaves the crystal. As a result, the spin of the remaining neutron wave will rotate by a certain angle with respect to initial direction due to the interaction of the magnetic moment of a moving neutron with the intracrystalline electric field. This effect is absent in an undeformed perfect crystal, where only the depolarization of a beam takes place because both waves moving in opposite electric fields have the same amplitude. A method has been developed for controlled deforming the perfect single crystal by means of creating a temperature gradient in it. Thereby, a new possibility of measuring electric fields acting on a neutron in noncentrosymmetric crystals, as well as a method of controlling these fields in experiments on studying the fundamental properties of the neutron, has been implemented.

Spontaneous breaking of time-reversal invariance at magnetic phase transitions

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The symmetry of crystals is usually considered as a starting point for the study of their physical properties. The relationship between the phenomenon and the symmetry of a medium is determined by the Curie principle*: A phenomenon can exist in a medium possessing its characteristic symmetry or that of its subgroups*. However, in conventional physics of magnetic phenomena the question about the symmetry of magnetic phases G_m is practically ignored because the possible answers give rise to the fundamental problem, which for the first time was marked by Landau and Lifshits. Indeed, the time reversal invariance (*t*-parity) was considered as one of the basic physical postulates. On the other hand, the use of this postulate for the definition of the symmetry G_m [1] gives the result, which conflicts with Curie's principle. Such a situation looks rather strange, while there is no comprehension that its origin is directly related to one of the central problems of natural sciences known as a dissymmetry of material world [2]. For magnetic crystals, this means a strong violation of the *T*-invariance principle (parity and invariance are different concepts). Modern theories do not allow justifying this hypothesis, but its experimental verification seems to be quite realistic.

Use of the symmetry principles allowed us to explain the nature of induced magnetic anisotropy [3,4], a classic example of which is a permanent magnet. The Curie's principle should, of course, be taken into account when determining magnetic structures by neutron diffraction. Other results of our research can be found in the brief overview [5].

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Interaction of Dirac particles with two-dimensional materials in models of quantum electrodynamics with a singular background.

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A method is proposed [1] for developing a model for the interaction of fields of quantum electrodynamics (QED) with two-dimensional materials in the framework of the Symanzik approach [2]. It is based on the modification of the QED Lagrangian by adding to it an additional contribution (the Lagrangian of the defect) concentrated in a two-dimensional region of space. The requirement to satisfy with the basic principles of QED (renormalization, locality, gauge invariance) makes significant restrictions on the type of defect Lagrangian, and as a result of the modification of QED, a small number of new dimensionless parameters, which describe the material properties of defect, appear in the model . The Dirac spinor fields in this approach can be used to describe the processes of interaction of ½ spin particles (electrons, protons, neutrons) with two-dimensional objects. The talk presents the results of the study of the scattering of Dirac particles on a homogeneous isotropic plane, as well as bound states arising from the interaction of the spinor field with the plane [3]. It is shown that the choice of specific values of the seven dimensionless parameters in the model can achieve significant differences in the quantitative characteristics of the studied physical effects. Theoretical investigations within the framework of the proposed approach may be useful both for improving the methodology of experiments with two-dimensional materials, and for analyzing the possibilities of technical devices created on their basis.

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Test of a new technique for ultra-precise neutron spectrometry

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A well-known effect of dynamical diffraction in perfect crystals is the enhancement of angular deviation of neutron trajectory inside the crystal, when the angle of neutron incidence on the crystal is slightly varied. The enhancement can reach values of the order of 10^5 - 10^6 [1]. Moreover, there is an additional gain factor $\tan^2(\theta_B)$ that becomes significant in the case of large diffraction angles. This factor is due to the fact that the neutron propagation time inside the crystal is becomes larger with an increase of the diffraction angle [2]. Combining both effects, the joined gain factor of the angular neutron trajectory deviation can reach values 10^7 - 10^8. This might give a chance to build an experimental setup with a sensitivity to external force effect on the neutron in order of 10^{12} - 10^{13} eV/cm.

Such ultra-precise spectroscopy technique could be used for a broad range of experiments:

1. The accuracy of the neutron electric charge experiment could be improved by one order of magnitude compared with the current experimental limit [3];
2. A test of the equivalence of inertial and gravitational neutron masses can could be done with an accuracy of 10^5 (compared with the current experimental value $1.7 \cdot 10^{-4}$ [4]);
3. Neutron scattering amplitudes can be measured with high accuracy both for solid materials and gases;
4. Neutron diffraction in perfect crystals and crystal properties on the inter-planar distance homogeneity about $\Delta d/d \sim (10^{-6} - 10^{-8})$ can be studied.

A double-crystal setup [5] made of highly-perfect silicon crystals was used to implement this technique. The results of experimental test of this technique at PF1b beam of ILL (Grenoble, France) reactor will be presented.

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A multidisciplinary non-destructive study of historical pipe organ fragments

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The so-called tin plague is often related to the progressive decay of metal organ pipes. A non-destructive methodology has been applied to the study of historical pipe organ fragments. Our aim was a bulk material characterization mainly in the altered regions, combining different non-destructive techniques:

- by neutron diffraction we could derive tin beta phase and several tin oxide phases;
- by neutron imaging we could map hydrate phases;
- by Raman spectroscopy we could for example associate romarchite phases with the border of crater regions.

The detection of oxidative phases is important for an archeometallurgical characterization and for conservative issues, since these phases could be in principle treated. Although we used well-established techniques, we took advantage from their combination inferring relevant indications, also in the form of mapping (both through Raman spectroscopy and through energy selective neutron imaging).

The results will guide restorers and conservators in the choose of the best practices in the preservation, but may be useful to a broader audience [1]. Indeed, many artefacts or unique samples may be tested by combining neutron based techniques and Raman spectroscopy, using a similar protocol for an in-depth non-destructive material characterization.

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Neutron imaging study of preservation of metal in the cultural heritage artefacts

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In the study of objects of cultural heritage, one of the main tasks is to determine their preservation. This is especially true for metal artifacts that have been exposed to factors such as fire and moisture, leading to a significant chemical transformation of the material. The present work describes the results of experiments on neutron tomography of metal objects from the collections of the A.S. Pushkin State Museum of Fine Arts, State Historical Museum and the Institute of Archaeology RAS, Moscow. Bronze and iron objects are investigated. It is shown that in the projections obtained on a monochromatic neutron beam, the metal manifests itself in diffraction on grains, so that it is possible to determine the areas of its preservation. Examples of inhomogeneous corrosion of archaeological objects detected using neutron and synchrotron tomography are also considered.

This work was performed using the equipment of Unique Scientific Facilities «Research reactor IR-8» and «Kurchatov Synchrotron Radiation Source».

Small Angle Neutron Scattering analysis of early medieval pottery wares

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Small Angle Neutron Scattering (SANS) measurements on archaeological and experimental control ceramic samples have been performed at the Yellow Submarine and FSANS instruments at Budapest Neutron Centre. The main objective of the research was to deepen our knowledge about the utility and limitations and of SANS method on obtaining information about the firing conditions of ceramic samples, and to use this knowledge for examining the firing technique of archaeological objects from the Late Roman / Early Medieval settlement in Keszthely (Hungary).

Three series of control samples have been prepared from different geological origin and composition (Keszthely yellow, Hollád yellow and Hollád grey clay): These samples have been fired at temperatures from 500°C to 1000°C, in steps of 50°C.

The samples have been measured on a wide scattering vector (Q) range, and after a proper data calibration, the intensity versus scattering vector (Q) curves were obtained. The fractal like behaviour of the nano-inclusions – crystallites, pores, voids, amorphous inclusions – present in the pottery matrix proved to correlate with the firing temperature, as shown in the Figure 1.

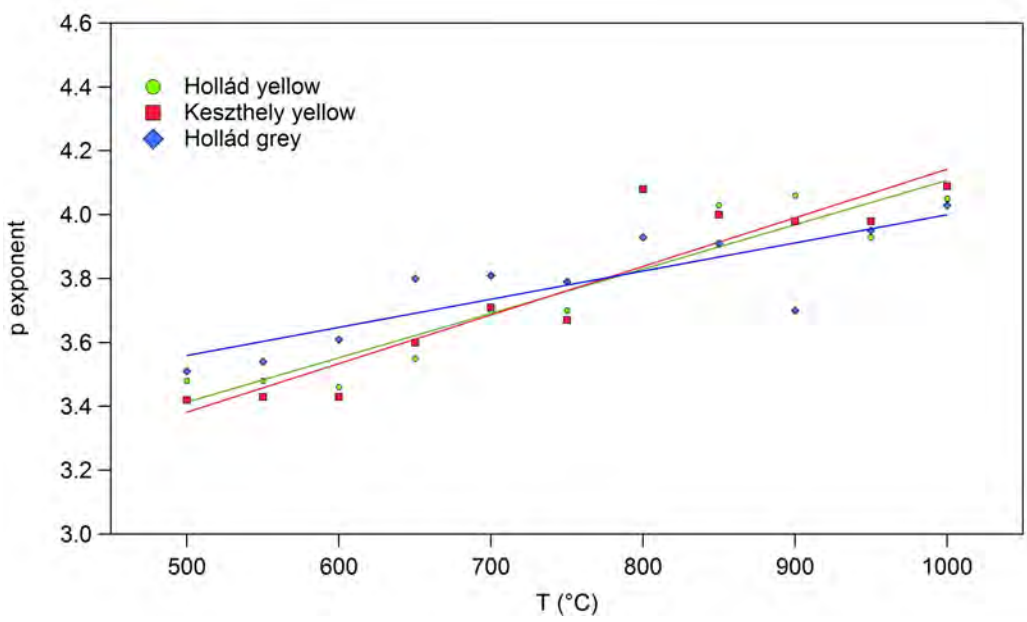

Figure 1. p exponent (obtained from the model fitting of SANS curves) versus the firing temperature for the three series of samples, prepared from different origin raw material

Additional measurements on the effect of the samples thickness on the p exponent (obtained from the model fitting of the SANS curves) have been performed.

The present work discusses the applicability of the non-destructive small angle neutron scattering method on obtaining information about the environment of the production (namely firing) of pottery wares; and based on the control series measurements draws conclusions about the firing temperature of the archaeological samples from Keszthely.

Complex neutron studies of the cross-enkolpion of the XVI century from the Novodevichy Convent

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In 2017, in the territory of the Novodevichy Monastery, during the security work by the IA RAS, a relief cast bronze cross-encolpion of the second quarter of the 16th century (reign of Vasily III, before the era of Ivan the Terrible) was found in a pit at a depth of 1.75 m. In 2018, at the Kurchatov Institute at the research reactor IR-8, complex neutron studies of this cross encolpion were carried out using the method of neutron tomography and neutron diffraction.

In the course of research, small (up to 12 mm in length) separate objects scattered over the area of various shapes (elongated, filiform, lumpy), mainly distributed along the edges of the valves, some of which are of organic origin, were found in the encolpion cavity. The presence of an upper and lower locking pin was confirmed, the upper one is parallel to the sash, and the lower one is perpendicular. The presence of pins indicates that the cross was not opened. Neutron tomography made it possible to find cast inscriptions (differing in content) under a thick layer of oxides. It was determined that all the parts of the cross-enkolpion from the Novodevichy Convent (both wings, loop) are made of the same bronze alloy based on Cu-Sn-Pb copper.

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This work was performed using the equipment of Unique Scientific Facility "NRC IR-8".

Study of artifacts from the Chernaya Mogila burial mound (X CE) by neutron tomography and complementary methods

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Comprehensive study of several iron artifacts from the collections of State Historical Museum (archaeologic site Chernaya Mogila burial mound, Chernigov, modern Ukraine, 10th century) was carried out in National Research Center "Kurchatov Institute". The aim of the study was to get information on their structure, decoration and preservation.

Due to the fact that the objects under study are the museum exhibits, the study was conducted by using complementary non-destructive methods - neutron and synchrotron radiography and tomography, scanning electron microscopy with X-ray energy dispersive microanalysis, and thermal-neutron diffraction.

The most interesting results were obtained in the study of fragments of objects of unknown use. They are iron plates with scalloped edges, one of them has a handle. An ornament hidden by a layer of oxides and "mastic" was found on two of them. The ornament is a ribbon weaving (Scandinavian style), made using silver wire inlay. 3D reconstruction of objects based on the synchrotron and neutron imaging suggests that the two fragments are parts of the same object.

An arrowhead and spearheads were also studied. These items revealed complex decor: a floral ornament was revealed on the arrowhead, a geometric ornament was revealed on the the spearheads.

It was shown that the artifacts currently consist mainly of iron oxides and hydroxides. The funeral fire had a significant impact on their preservation. The areas of the remaining metal were identified by the effects associated with the grain structure observed in neutron tomography and diffraction.

This study shows the promise of using the non-destructive methods of neutron and synchrotron radiography and tomography, in combination with other methods, in the study of artifacts from museum collections.

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Neutron methods for Heritage Science

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Scientific tools and, in particular, research infrastructures have become to play an essential role in exploring objects of Cultural Heritage in the past decade. Distributed infrastructures with a wide range of experimental techniques – often with mobile access to artefacts or monuments – or archives with large data-base mostly in digital form provide comprehensive information to answer questions regarding the identification of workshops or manufacturing techniques, provenance or authenticity of an object as well as to enable conservation or preservation. Another class of experimental tools is offered by large scale facilities (accelerators, neutron sources), which are used to reveal unique or very complex information on analytical and structural features of artefacts. Neutrons are perfect tools of archaeometrical studies due to their non-destructive and non-invasive nature, while able to deeply penetrate into the bulk of materials. Neutron methods can be used to explore compositional, structural and topological features of the samples. Intense neutron beams are produced in nuclear reactors or accelerator based neutron sources. The usefulness and complexity of investigations with neutrons is based on the interaction of neutrons with matter by three major ways: 1) Imaging by passing neutron beams through objects – neutron radiography and tomography; this can reveal internal parts or hidden objects inside bulky materials. 2) Absorption of neutrons by nuclear reaction with atoms of studied materials – radiative capture via (n,γ) reaction; this technique gives information on the elemental composition of objects. 3) Week interaction with atoms - neutron scattering (elastic or inelastic); measuring intensity variation of scattered neutrons from the sample reveal information on atomic, molecular or nano-scale structures.

The Budapest Neutron Centre (BNC) is a research organisation based on a 10 MW reactor and 15 experimental stations offers open access to its facilities in science and technology [1]. BNC has long traditions in archaeometrical research, it has made part of the FIXLAB access programme within the CHARISMA and IPERION-CH EU projects. The unique feature of BNC is to offer a complex approach of studying artefacts by utilising the ensemble of its experimental stations, thus the 3 types of the above described neutron techniques might provide complementary information on the investigated objects. Moreover, the scattering instruments (diffractometers, small angle scattering machines), activation techniques (e.g. prompt-gamma activation analysis devices) and neutron imaging facilities are complemented by measurement possibilities offered by the use of External Milli-Beam PIXE and compact XRF spectrometers, microscopes, optical spectroscopy methods etc. – also at the BNC campus.

We present recent studies, BNC highlights as comprehensive analysis of artefacts by combined neutron techniques. For example, in 2017-18 the famous small bronze statute attributed to Leonardo da Vinci was investigated and new information on the inside of both parts, the horse and the rider was obtained to prove and learn more details about the casting as supposed to be the indirect lost wax technique [2]. High resolution tomography images revealed inside details of the cast, while neutron diffraction and elemental composition analysis results of the bronze alloy on the horse, rider and the horse tail proved unambiguously that the horse and the rider were cast from the same bronze material, but the casting process was different. Laser-Raman spectroscopy results revealed that the patina (black and green stain on the surface of both the horse and rider) is the result of natural formation during centuries.

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Scientific Investigations regarding Ancient and Byzantine ceramics in Dobrudja, Romania

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Scientific Investigations regarding Ancient and Byzantine ceramics in Dobrudja, Romania

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A lot of ceramic fragments discovered in the excavations from archeological sites from Dobrudja, southeastern Romania, dated to the 4^{th}-11^{th} centuries AD, were subjected to archaeometric research in order to obtain data on raw materials and techniques production. The samples selected for analysis were initially grouped according to stylistic criteria. Later was used Optical Microscopy (OM) to detail fabric characteristics, and for some fragments micro-PIXE analyzes were performed to obtain the chemical composition of the paste. In a previous project, fragments of the Roman amphorae discovered in Constanța were analyzed by the neutron tomography method, a non-destructive method that provides detailed information about the internal structure of objects. Other fragments will be subject to this analysis. The results of the investigations will be compared to obtain scientific evidence on the Black Sea West Coast trade networks in the Roman and Byzantine periods.

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Trace elemental composition of Palaeolithic mammoth ivory as a valuable record of ancient human behaviour

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Aurignacian ivory tools and symbolic artefacts dating back to about 35000 years represents a high point in the rich material culture of the Upper Palaeolithic. Until now chemical analyses of these ivory artefacts was limited due to the exceptional status of these objects. New technological developments using external microbeam Proton-Induced X-ray and gamma-ray analyses (PIXE/PIGE) now allow non-invasive study of such artefacts. Our research pursues three main goals:

1. the evaluation of the state of preservation of mammoth ivory from the Aurignacian
2. the measurement of trace elements as an indication of the provenience of mammoth ivory
3. the measurement of F-content to establish relative ages within individual sites.

Here we present new results from the study of mammoth ivory artefacts from five key Palaeolithic sites in France and Germany. Our initial results document site-specific patterns of trace element that are in part the consequence of local diagenetic processes. These observations allow us to draw reliable conclusions about the provenience of ivory and to provide new insights into procurement and use of mammoth ivory during the Early Upper Palaeolithic [1-3].

This talk addresses both the potential and limitations of these analyses and highlights the importance to merge natural science approaches with those of the field of the humanities to obtain new insights in ancient human behaviour.

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STRUCTURE AND PHASE STUDIES OF HIGHLY IRRADIATED DISPERSED U-Mo/Al FUEL BY THE NEUTRON DIFFRACTION METHOD

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A performance capability of the U-Mo/Al dispersion fuel depends on a stability of fuel composition and a condition of its components. It was found that the structure of the fuel particles and matrix were changing during a fuel operation life and new phases were observed to form in the fuel. In order to predict the safe operation life-time of fuel elements with the U-Mo/Al dispersion fuel under irradiation the relationships of the changes in the structure and phase condition of the components of the dispersion fuel as dependent of burn–up and temperature were studied.

This paper presents the results of the structure and phase studies on the dispersed U-Mo/Al fuel after irradiation in the IVV-2M reactor to different burn up levels from 33 to 97% and one-hour annealings within temperatures of 150 to 580 ^{o}C by the neutron diffraction method. It was found that in the U-Mo/Al irradiated up to 97% burn up at temperatures less than 100 ^{o}C the (U,Mo)Al_x layer was the amorphous phase containing less than 0.5% UAl_3 phase. The irradiated fuel composition U-Mo/Al remained stable when heated to 300-350 ^{o}C and after that a recrystallization of the amorphous phase (U,Mo)Al_x with a formation of UAl_3 was observed with increasing temperatures.

The investigation revealed three regions, where the lattice parameters of γ-(U-Mo) and Al were changing with fuel burn–up. In the first region of the fuel burn-up the lattice parameter increases, the interval of the change in the γ-(U-Mo) lattice parameter is within 0 to ~50 % fuel burn–up and that of the Al lattice parameter is within 0 to ~78 % burn-up. The rate of changing in γ-(U-Mo) lattice parameter is $(3.9)\cdot10^{-4}$ Å per 1 % burn–up and that of Al lattice parameter is $(2\text{-}2.7)\cdot10^{-4}$ Å per 1 % burn–up. In the second region of the fuel burn where the intervals are from 50 to 75 % for γ-(U-Mo) and from ~75 to 95 % for Al the lattice parameters of both phases do not practically change. In the third region of the fuel burn-up being > ~75 % for γ-(U-Mo) and > ~95 % for Al the decrease of the lattice parameter of both phases is observed.

It was found that the change in the lattice parameter of both phases was due to the changes in their structure, accumulation of the radiation defects and fission products.

It was revealed that the irradiated U-Mo/Al dispersion fuel annealed within the range 150 to 550 ^{o}C resulted in the decrease of the lattice parameter of both γ-(U,Mo) and Al. The decrease of the γ-(U,Mo) lattice parameter depends on burn–up value; and the decrease in the specimen with ~55 % burn–up proceeds in two phases, the decrease in the specimen with ~97 % has only one phase. The Al lattice parameter decreases with the annealing temperature in two stages irrespective of the burn–up value.

Structure and magnetic properties of the SiO2(Co)/GaAs and SiO2(Co)/Si interfaces

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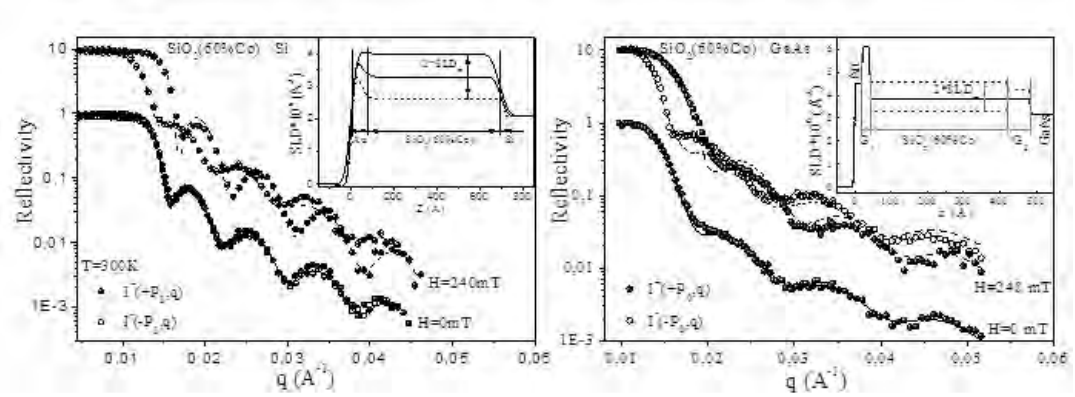
Granular films SiO_2(Co) exhibits unusual magnetic and magnetotransport properties which are strongly dependent on the composition of the film and material of a substrate. Coefficient of the giant injection magnetoresistance reaches a value of 10^5% at the room temperature in the films on n-GaAs substrate. However, this effect is negligible in the case of similar granular films deposited on n-Si substrate. In this report the structural and magnetic properties of the granular films SiO_2(Co) on Si and GaAs substrates were investigated by the complementary methods of Polarized Neutron Reflectometry (PNR), Grazing Incidence Small-Angle X-ray Scattering (GISAXS), and SQUID magnetometry.



Both systems have the specific layer of Co nanopartilces at the interface granular film/substrate. The interparticle distance of this layer is larger than that in the main part of the granular film. Moreover, the layers thicknesses, intergranular distances, layer magnetization values of the SiO_2(Co) films on GaAs and Si substrates are also very similar. Thus, one can conclude that the giant injection magnetoresistance caused by the effects taking place not in the granular film, but by the localized electron levels near the surface of GaAs. High values of the GIMR effect can be explained by the spin-dependent potential barrier formed in the accumulation electron layer (G_2 on Figure) in the semiconductor GaAs near the interface. Such an accumulation electron layer does not form in a Si semiconductor substrate, which is most likely due to the formation of a chemical bond between the silicon substrate and cobalt granules. As a result, metallic conductivity is formed and the tunnel effect necessary for electron injection is absent. Therefore, the magnetotransport properties of a granulated SiO_2(Co) film on a silicon substrate in the form of a giant injection magnetoresistance do not manifest themselves.

The proton linac for DARIA compact neutron source

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The 13 MeV 162.5 MHz 5mA CW proton linac is under development at ITEP. The linac is designed for DARIA [1] compact neutron source and based on linac for BELA project [2] which is also under development at ITEP.

The different linac layouts were considered. The most perspective linac layout is one when the linac includes RFQ and DTL sections with 6D-beam matching between them. The DTL section has modular structure and consists of separated individually phased IH-cavities with beam focusing by magnet quadrupoles between the cavities. This DTL structure provides linac compactness, tuning and commissioning cavity by cavity.

Results of beam dynamic simulation and RF parameters of linac cavities are presented.

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Combining rheology and small-angle scattering of neutrons and X-rays for dynamic assessment of microfibrillated cellulose under shear

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Cellulose fiber is a natural food component present in fruits and vegetables. Presence of the cellulose fiber in the diet aids digestion and helps in preventing a variety of diseases. Cellulose fibers also provide texture to food products. The texturing capacity of cellulose fibers can be enhanced by defibrillation under high shear. Dispersions of microfibrillated cellulose form a 3D soft space-filling network, which can, for example, mimic the texture of fat-based products. Critical for the consumer perception of microfibrillated cellulose networks are spreadability and mouthfeel. The microstructural features that underly these rheological parameters are poorly understood. Small-angle scattering of neutrons (SANS) and X-rays (SAXS) provides structural information in a wide range of length scales. Combination of rheological data with SANS/SAXS measurements of the samples under shear, conditions shed light on the mesoscale structural dynamics that underlies the peculiar flow of microfibrillated cellulose under industrial processing conditions and during consumer use and consumption.

Recent studies [1] have shown nonlocal flow behavior of microfibrillar cellulose suspensions. Based on Rheo-MRI data two different hypotheses to explain such nonlocality were suggested: flocculation of cellulose microfibrils and formation of a liquid-crystal like a phase in these suspensions. To validate these hypotheses we constructed a special sample cell, which allows for SANS/SAXS on the materials under shear with a spatial resolution (100 µm) across the velocity gradient direction of the cell [2]. No alignment of microfibrils was observed at shear rates from 1 to 300 s^{-1}. The scattering invariant calculation indicates a homogeneous density distribution of cellulose microfibrils across the gap at all applied shear-rates. This implies that no shear-induced aggregation and concomitant migration of cellulose over the gap occurs. The shear-SAXS experiments are in line with the flocculation hypothesis with the flock sizes much larger than 200nm (maximal accessed in the performed experiment).

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