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Low temperature X-Ray powder diffraction study of lead telluride doped with Yb

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The temperature and doping range dependences of the lattice constant of PbTe:Yb samples were studied. The concentration of the doping element C_{Yb} has varied between 0.5 and 2 at%. The temperature dependences of the lattice constant *a* of the cubic unit cell of the PbTe:Yb samples from room temperature down to 100 K were measured on a Scintag powder diffractometer equipped with He cryostat. It was shown that at room temperature the lattice constants of PbTe:Yb samples decrease approximately linearly with increasing the Yb content from *a*=6.4621(0)Å for C_{Yb}=0 to *a*=6.4591(3)Å for C_{Yb}=2,0. The lattice constants decrease linearly with decreasing of the temperature, the $\partial a/dT$ values are 0.000135 Å/K for PbTe and 0.000125 Å/K for PbTe:Yb<1.5%>. The accuracy of these measurements was better than 0.02%. The thermal expansion coefficient α of PbTe:Yb<2%> was measured in the temperature range from 300 to 80 K, using Netzch dilatometer. The experimental results showed that the thermal expansion coefficient α of PbTe:Yb<1%> remains constant in the studied temperature range from 300 to 80 K, and its value is $\alpha=19.73 \cdot 10^{-6}$ K^{-1}.

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Keywords: Lattice constant, Lead telluride, X-ray diffraction, Linear thermal expansion coefficient

1. Introduction

In recent years, the IV-VI semiconductors have been the object of considerable research due to their applications in IR technique. It was shown that lead telluride - based compounds group III – doped (In, Ga and Tl) acquire essentially new properties such as level Fermi stabilization, high photosensitivity at low temperatures, persistent photoconductivity, etc.

As these researches continue, the literature on these compounds increases, but there is insufficient information about lead telluride - based compounds doped with rare earth elements. It was observed that small amount of ytterbium considerable changes electric properties of lead telluride. Recent papers report that Yb forms an impurity band lower than the top of the valence band of PbTe. It means that we can stabilize the position of the Fermi level [1]. Besides, pronounced changes of the photoconducting properties of the compound were observed.

Our aim is to investigate the lattice parameters of the PbTe:Yb as a function of its composition and temperature.

2. Experimental results

Lead telluride single crystals were obtained using the Bridgman method. The YbTe compound was used as a source of the doping element during the synthesis processes. The samples were chemically polished in HBr + 5% Br_2 solution. The concentration of the doping element C_{Yb} has varied between 0.5 and 2 at %. Metallographic specimens were prepared of every compound. A chemical etch consisting of a concentrated solution of KOH, H_2O_2 and ethylene glycol has also been used. The average dislocation density in PbTe:Yb and PbTe crystals were less than 10^6cm^{-2}. The metal incorporations were not found.

The samples obtained were characterised by X-ray diffraction (XRD). The temperature dependences of the lattice constant *a* of the cubic unit cell of the PbTe and PbTe:Yb samples from room temperature down to 100 K were measured on a Scintag powder diffractometer equipped with He cryostat. X-Ray diffractograms for powdered samples, obtained using CuK_α radiation, for PbTe:Yb<2%> and PbTe are shown in Figs 1 (a) and (b), respectively. The scanning angle (2θ) range was from 10° to 100°. The temperature dependences of the lattice constants of PbTe and PbTe:Yb<1.5 %> measured at 100 K, 200 K, and 300 K are presented in Fig. 2. The accuracy of these measurements was better than 0.02 %. Detailed measurements of the lattice constant as a function of the doping range were made at room temperature (Fig. 3).

The thermal expansion coefficient α of PbTe:Yb<1%> was measured in the temperature range from 300 to 80 K, using Netzch dilatometer. The sample for thermal expansion measurements had cubic shape with dimensions of ca. 5 × 5 × 5 mm^3. The measurement sensibility was about 1 nm and several measurements of the thermal expanshion posses a good reproducibility.

The experimental results showed that the thermal expansion coefficient α of PbTe:Yb<1%> remains constant in the studied temperature range from 300 to 80 K, and its value is $\alpha=19.73 \times 10^{-6}$ K^{-1}.

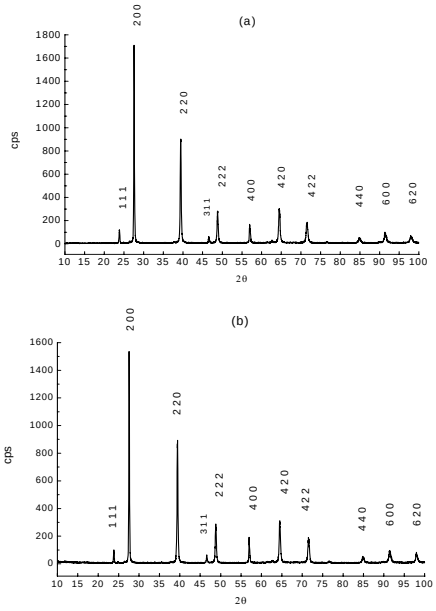

Fig. 1. (a) XRD pattern of PbTe, (b) XRD pattern of PbTe:Yb<2%>

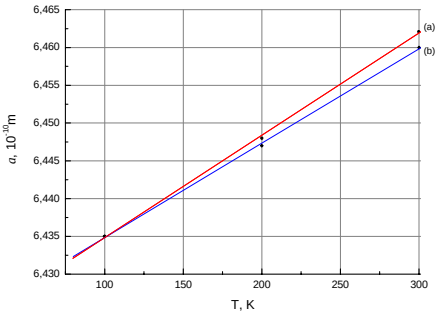

Fig. 2. The temperature dependences of the lattice constant of (a) PbTe, (b) PbTe:Yb<1.5%>.

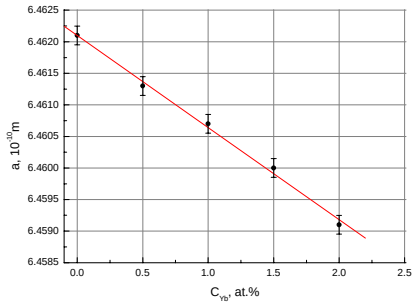

Fig. 3. The dependence of the lattice constant for PbTe as a function of the doping range for PbTe:Yb

3. Discussion

Typical XRD powder patterns of PbTe and PbTe:Yb<2%> obtained using CuKα radiation are given in Fig. 1. The XRD results show that our single crystal samples are of single phase with NaCl-type structure, the qualitative changes were not observed.

It was shown (Fig. 3) that at room temperature the lattice constants of PbTe:Yb samples decrease approximately linearly with increasing the Yb content from a = 6.4621(0) Å for C_{Yb}=0 to a = 6.4591(3) Å for C_{Yb}=2.0. Since the samples are *p*-type, we suppose that the Yb atoms are embedded in the Pb sublattice. Due to of the nearly equal values of ionic radii of Pb and Yb the change of the lattice constant is small (Table 1). Temperature dependences of the lattice constants of PbTe and PbTe:Yb<1.5%> are given in Fig. 2. There is a linear decreasing of the lattice constant with temperature down to 100K and its coefficient $\partial a/dT$ values are 0.000135 Å/K for PbTe and 0.000125 Å/K for PbTe:Yb<1.5%>.

We observed that temperature dependence of the thermal expansion coefficient α of PbTe:Yb<1%> remains constant, and its value is $\alpha=19.73\cdot10^{-6}$ K^{-1}. It means that temperature dependence of the lattice constant is linear. It is known that temperature dependence of the thermal expansion coefficient of polycrystalline PbTe has a non linear behavior [2]. We didn't observed a non linear dependence of the lattice constant for our single crystals of PbTe and PbTe:Yb.

Table 1. Lattice constant values for PbTe, PbTe:Yb measured at room temperatures.

a, Å	T=300K
PbTe	6.4621
PbTe:Yb<0.5%>	6.4613
PbTe:Yb<1.0%>	6.4607
PbTe:Yb<1.5%>	6.4600
PbTe:Yb<2.0%>	6.4591

4. Conclusion

Metallographic and XRD investigations show that the samples are of a single phase with rock-salt crystal structure. Temperature dependence of the thermal expansion coefficient of PbTe:Yb<1%> remains constant and temperature dependence of the lattice constant of this compound is linear. It was observed that temperature dependence of the lattice constant of PbTe and PbTe:Yb<0.5-2.0%> remains linear down to 100 K. The lattice constants of PbTe:Yb<0.5-2.0%> samples decrease approximately linearly with increasing the Yb content at room temperature.

Acknowledgements

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