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Thermoelectric Properties and a Defective Subsystem of Heterophasic Materials on the Basis of a Lead Telluride with Impurity of Antimony

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The results of the study of thermoelectric properties and the defective subsystem of lead telluride doped by antimony PbTe:Sb (8%), promising material for the creation of heat energy converters on their basis. The regularities in the behavior of the properties investigated, which are due to the biphasicity of the material and the significant influence of the technological factors of obtaining samples on their defective subsystem, are established. The modeling of the defect subsystem of PbTe:Sb crystals was carried out taking into account the presence of additional phase inclusions and it was found that dominant point defects are internode atoms of antimony.

Keywords: Lead telluride, doping, defects, heat energy.

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Introduction

The prospect of using an antimony impurity to improve the thermoelectric parameters of the lead telluride is due to the possibility of an increase in the Seebeck coefficient PbTe, due to the increase in the density of states at the edge of the conduction band [1]. Such an effect is studied, in particular, in papers [2-3]. In addition, in terms of increasing the thermoelectric figure of merit of a material, it may be more efficient to obtain a material with the inclusion of additional phases of the antimony, which will further contribute to the reduction of the thermal conductivity. Studies of polyphase materials, in particular solid solutions of PbSbAgTe [4-5], showed the presence of a strong dependence of the properties of materials on the technological factors of their obtaining. In this case, the dimensionless thermoelectric figure of merit of a material of the same chemical composition can vary in very wide limits (from $ZT \approx 0.6$ to $ZT \approx 1.6$) [6]. Such regularities are most likely due to the modification of a defective subsystem of materials in the process of thermal treatment. In view of this, the goal of this study is to determine the peculiarities of the behavior of point defects and the subsystem of the inclusion of additional phases of PbTe:Sb (8%) and their effect on the formation of a complex of properties of heterophasic materials.

I. Methods of obtaining samples and studying their properties

Detailed methodology of experimental studies is described in [7]. Materials synthesis was carried out in vacuumed quartz ampoules using high purity components (99.999 % by weight of base component). The resulting ingots were ground in an agate mortar and, having separated the fractions of a size (0.05 - 0.5) mm, compressed under pressure (0.5 - 1.5) GPa and obtain cylindrical samples with $d = (5 - 8)$ mm and $h \approx (5 - 8)$ mm with subsequent annealing in the range of temperatures (500 - 650) °C.

The phase composition and structure of the synthesized ingots and pressed samples were investigated by X-diffraction methods on automatic diffractometer STOE STADI P. Hall's measurements were carried out in constant magnetic and electric fields using a four-zone method. The current through samples was $\approx 100 - 500$ mA. The magnetic field was directed perpendicular to the longitudinal axis of the cylindrical samples at an induction of 1.5 T.

To measure the Seebeck coefficient α and specific conductivity σ , the sample was clamped with two copper rods placed in the furnace, which heated to a given measuring temperature. On one of the copper rods was

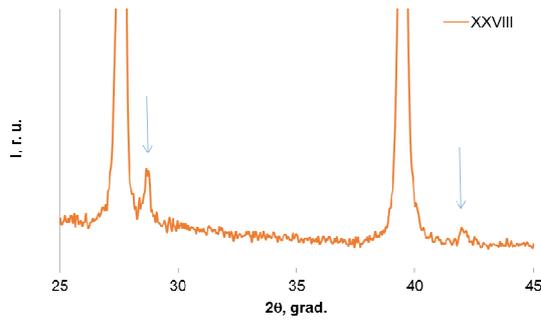
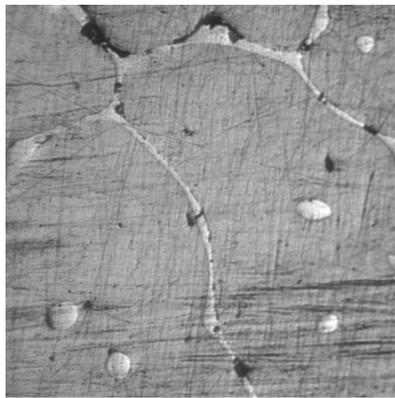


Fig. 1. X-ray diffraction pattern of lead telluride doped by antimony PbTe:Sb (8 %) in the region of reflexes of an additional phase of antimony.

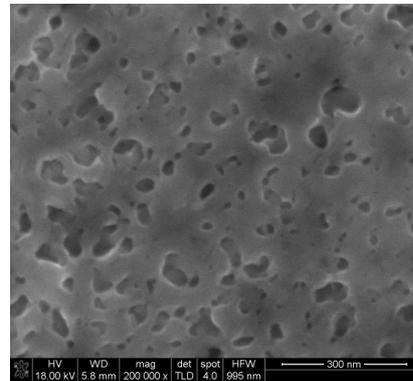
Table 1

Results of X-diffraction analysis of powder and pressed sample PbTe:Sb (8 at. %)

Investigated sample	Phase composition	Unit cell parameter a (Å) and the relative mass content of the phase
PbTe:Sb (8 at. %) powder	PbTe (ST NaCl, SG $Fm-3m$, $Z = 4$)	6.4581(2) 92.5(5) mass. %
	Sb (ST As, SG $R-3m$)	7.5(2) mass. %
PbTe:Sb (8 at. %) cold pressed & annealed	PbTe (ST NaCl, SG $Fm-3m$, $Z = 4$)	6.4577(2) 92.4(8) mass. %
	Sb (ST As, SG $R-3m$)	7.6(3) mass. %



a)



b)

Fig. 2. Microfilm of the surface of the sample PbTe:Sb (8 at.%) Obtained using optical (a) and scanning electron microscope (b) (image size 450x450 μm^2).

coil additional furnace to create a temperature gradient ($\approx 5 - 10^\circ\text{C}$) per sample. The conductivity was determined by measuring the voltage drop on the sample generated by the voltage source. The thermal conductivity of the samples was determined by the method of radial heat flux [7].

II. Thermoelectric properties of PbTe: Sb (8 at.%)

X-ray diffractometric studies of the lead telluride doped by antimony in an amount of 8 at.% confirmed the biphasicity of the material (Fig. 1). Reflexes from the phase of pure antimony have been recorded in the angles $2\theta \approx 29^\circ$ and $2\theta \approx 42^\circ$. The estimated size of the CDA (Coherent Dispersion Area) according to the Debye-Sherer formula of the additional phase at the peak $2\theta \approx 42^\circ$ is 55 nm. The unit cell parameter of the main phase is $a = 6.89 \text{ \AA}$ (Table 1).

The investigation of the surface of synthesized ingots of PbTe:Sb by optical and scanning electron microscopy also confirmed their two-phase nature. Additional phases

are present both in the form of micro- and nano-inclusions. The size of nano-inclusions is up to 100 nm (Fig. 2), which is well consistent with the data of X-ray analysis.

Figure 3 shows the temperature dependences of the main thermoelectric parameters of pressed samples. In contrast to the previously studied materials, in particular, the pure PbTe [7], the annealing of cold pressed samples at 500°C during 15 min leads to a significant decrease in specific conductivity at a practically constant Seebeck coefficient.

At annealing samples in argon at a temperature of 650°C , a significant increase in the coefficient of specific conductivity of the material with a constant Seebeck coefficient, and simultaneous growth of the coefficient of thermal conductivity is observed.

In researches of hot pressed samples it was established that after their annealing, the basic thermoelectric parameters do not differ from the analogous parameters for the samples obtained by the method of cold pressing with the subsequent annealing. The annealing of hot pressed samples at 650°C , as in the case of cold pressed, leads to a significant increase in specific conductivity and thermal conductivity.

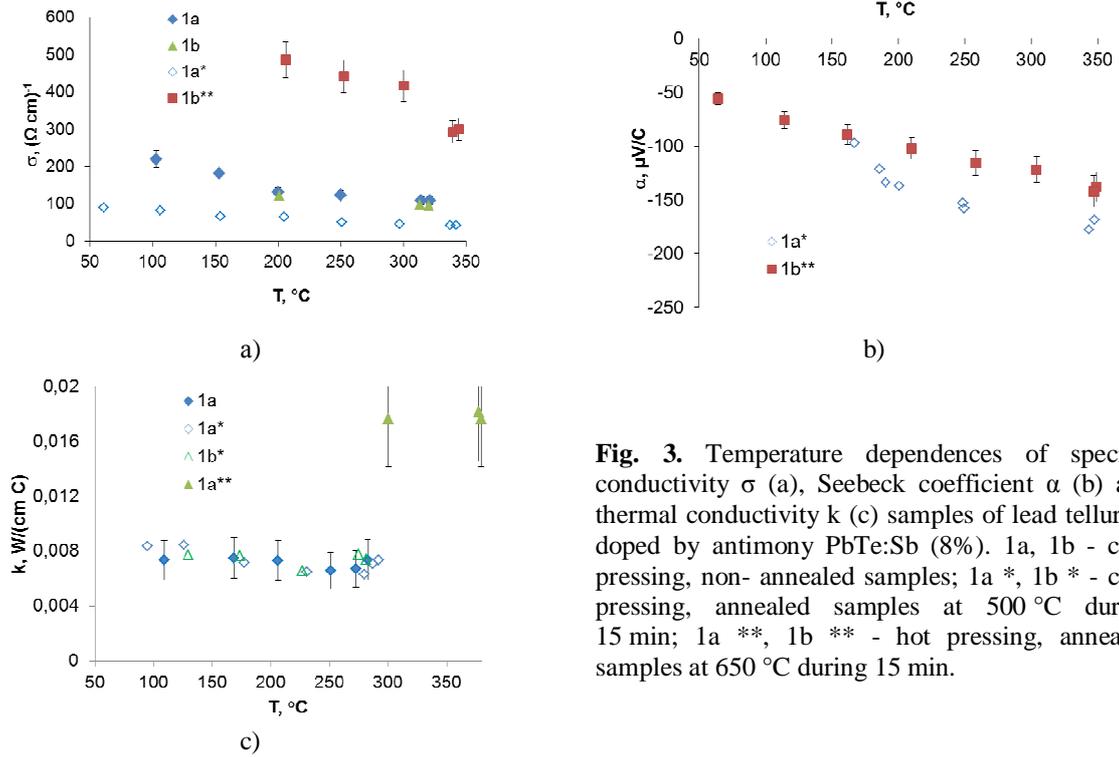


Fig. 3. Temperature dependences of specific conductivity σ (a), Seebeck coefficient α (b) and thermal conductivity k (c) samples of lead telluride doped by antimony PbTe:Sb (8%). 1a, 1b - cold pressing, non- annealed samples; 1a *, 1b * - cold pressing, annealed samples at 500 $^{\circ}\text{C}$ during 15 min; 1a **, 1b ** - hot pressing, annealed samples at 650 $^{\circ}\text{C}$ during 15 min.

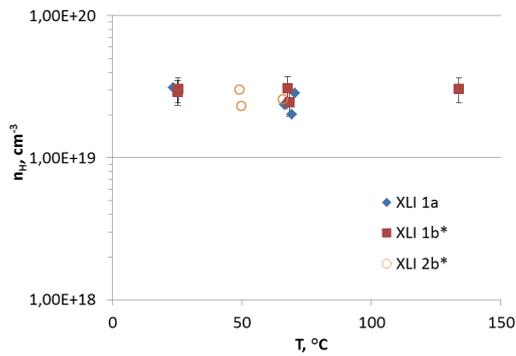


Fig. 4. Temperature dependences of the Hall concentration of carriers in samples PbTe:Sb (8 at.%) obtained under different technological conditions: XLI 1a - cold pressing; XLI 1b * - cold pressing, annealed samples at 500 $^{\circ}\text{C}$ during 15 min; XLI 2b * - hot pressing, annealed samples at 650 $^{\circ}\text{C}$ during 15 min.

On the basis of the Hall effect study, it was found that the pressed samples that annealed at a temperature of 500 $^{\circ}\text{C}$ or 650 $^{\circ}\text{C}$ did not change the concentration of carriers in them. In addition, the concentration of carriers in cold and hot-pressed samples is practically the same (Fig. 4). Thus, we can assume that the differences in thermoelectric parameters presented in Fig. 3, for samples with different technological parameters, is not due to the change in the concentration or type of dominant point defects. The advantage of this assumption is also evidenced by the fact that the unit cell parameter, as well as the relative mass content of the additional phase, non- annealed and annealed samples within the limits of the error, is identical (Table 1). That is, the annealing of the pressed sample does not lead to a change in the concentration of the dissolved impurity.

Instead, the study of the microstructure of the samples showed that the annealed samples at different temperatures led to the integration and growth of the inclusions of the additional phase (Fig. 5). Thus, the change, in particular, the decrease in the specific electrical conductivity of the samples, can be explained

by the dumping of antimony on the intergranular limits, which leads to a significant decrease in the mobility of free charge carriers. Instead, an increase in the thermal conductivity due to the agglomeration of the impurity may be due to the fact that the coefficient of thermal conductivity of the pure antimony ($k_{\text{Sb}} \approx 0.2 \text{ W}/(\text{cm} \cdot \text{K})$ (30 $^{\circ}\text{C}$)) is an order of magnitude higher than the coefficient of thermal conductivity of the base material ($k_{\text{PbTe}} \approx 0,02 \text{ W}/(\text{cm} \cdot \text{K})$ (30 $^{\circ}\text{C}$)).

III. Simulation of a defective subsystem of crystals

To determine the behavior of concentration of the free charge carrier, a simulation of the defective subsystem of PbTe:Sb crystals was performed. According to [3, 8], dominant point defects may be antimony atoms in cationic nodes, where they exhibit donor properties of $\text{Sb}_{\text{Pb}}^{1+}$, and in anion nodes, where they exhibit acceptor properties of $\text{Sb}_{\text{Pb}}^{1-}$. A smaller

amount of lattice parameter of the investigated material (6.458 Å), in comparison with the non-doped material (6.460 Å), confirms the probability that the atoms of the antimony are located in the nodes of the crystalline lattice, since the covalent radius of the antimony (1.46 Å) is less than the radius of the lead (1.53 Å) and equal to the radius of tellurium (1.46 Å) [9]. In addition, the probabilistic process may be the formation of inter-nodes atoms, both the own atoms of the matrix and the impurity atoms, and the antimony atoms of the inter-node positions can ionize to the state of 3+ [8]. The own atoms of the matrix can enter the inter-node position due to their displacement by the atoms of the antimony. Then lead in the inter-node position will exhibit donor properties, and tellurium is most likely to be neutral [10]. However, given that the electronegativity of telluride is greater than the electronegativity of a antimony, displacement Te from its node is unlikely. In the case of lead atoms, the difference in electronegativity can be both positive and negative, depending on the choice of the system of electronegativity [11]. For example, in the Pauling system, the electronegativity of these atoms is same. Thus, the most probable inter-nodes defects are the atoms of the antimony.

It is worth noting that in the works [12-13], in the study crystals of lead telluride doped by bismuth (bismuth, like the antimony, is element of the fifth group of the Periodic Table), the possibility of compensating the impurity by the vacancy of the lead, or their complexes with impurity atoms, or same complexes Bi₂Te₃. However, given that antimony is more prone to manifestation of amphoteric properties than bismuth, one can assume that the compensation in PbTe:Sb is more likely to be by antimony atoms in chalcogen nodes. In addition, at the investigated concentrations of impurities, vacancy formation is unlikely, as they should immediately be filled with impurity atoms. The formation of an electroneutral complex of type Sb₂Te₃, if any, does not have to affect the electrophysical properties. Firstly, because the complex is electroneutral, and secondly, because the antimony atoms for the formation of the complex will be taken not from dissolved in the crystalline lattice of electrically active defects Sb_{Pb}¹⁺, but from electroneactive inclusions. Although, it should be noted that, according to [14], such

complexes may have an effect on the microhardness of the material, and therefore the establishment of conditions for their formation may be a separate important application task.

Thus, the considered model of the defect subsystem of crystals PbTe:Sb takes into account the presence of antimony atoms in cationic (single charge donor) and anionic (single charge acceptor) nodes of crystalline lattice, as well as inter-nodes antimony atoms (triple ionized donor). Concentrations of defects can be determined by the method of minimizing the thermodynamic potential of the crystal (free energy) as a function of the concentration of defects.

$$F = F_0 + E_{Sb_{Pb}^+} [Sb_{Pb}^+] + E_{Sb_{Te}^-} [Sb_{Te}^-] + E_{Sb_i^{3+}} [Sb_i^{3+}] - TS_k + F_{el} \quad (1)$$

Here F_0 is the free energy of the crystal, which does not depend on the presence of defects, E is the energy of defect formation, S_k is the configuration entropy, F_{el} is the free energy of the electron subsystem. In case of neglecting the influence of holes, the last addition will be defined as:

$$F_{el} = (E_c + \mu)n$$

Here E_c is the energy of the bottom of the conduction band, μ is the chemical potential of the electrons, n is the electron concentration.

The configuration entropy is defined as the amount of entropy of the cationic and anionic sublattices, as well as of the inter-node positions.

$$S_{k,c} = k \cdot (N_c \ln N_c - [Sb_{Pb}^+] \ln [Sb_{Pb}^+] - (N_c - [Sb_{Pb}^+]) \ln (N_c - [Sb_{Pb}^+]))$$

$$S_{k,a} = k \cdot (N_a \ln N_a - [Sb_{Te}^-] \ln [Sb_{Te}^-] - (N_a - [Sb_{Te}^-]) \ln (N_a - [Sb_{Te}^-]))$$

$$S_{k,i} = k \cdot (N_i \ln N_i - [Sb_i^{3+}] \ln [Sb_i^{3+}] - (N_i - [Sb_i^{3+}]) \ln (N_i - [Sb_i^{3+}]))$$

Considering that the concentration of ionized impurities significantly exceeds its own, the equation of electroneutrality will have the form:

$$n = [Sb_{Pb}^+] - [Sb_{Te}^-] + 3[Sb_i^{3+}]$$

It was shown in [15] that the electrons concentration in PbTe, taking into account the dependence of the effective mass of electrons on their concentration, can be determined as

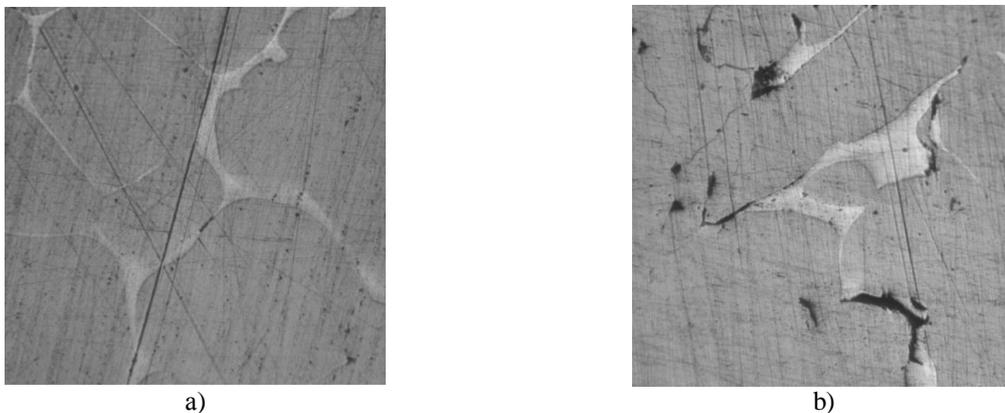


Fig. 5. Microfilm of the surface of the sample PbTe: Sb (8 atm.%) annealed at 500 °C during 15 min (a) and annealed at 500 °C during 60 min (b) (image size 450x450 μm²).

$$n = \alpha^3 \cdot a^2 \cdot N_{C,0}^2 \cdot e^{\frac{2b\mu}{kT}},$$

where

$$N_{C,0} = \left(\frac{2\pi m_{e,0}^* kT}{h^2} \right)^{\frac{3}{2}}.$$

Here α is correction that takes into account the concentration dependence of the effective mass of electrons in the conduction band PbTe. Then, from the equation of electroneutrality, one can determine the chemical potential of the electrons:

$$\mu = \frac{1}{2b} kT \cdot \ln \left(\frac{[Sb_{Pb}^+] - [Sb_{Te}^-] + 3[Sb_i^{3+}]}{\alpha^3 \cdot a^2 \cdot N_{C,0}^2} \right)$$

To calculate the concentrations of point defects in a crystal at a given temperature T, it is necessary to find derivatives of free energy (1) for each of the defects, and equating them to zero, solve the resulting system of equations. After performing the corresponding operations, this system will look like:

$$\begin{aligned} [Sb_{Pb}^+]([Sb_{Pb}^+] - [Sb_{Te}^-] + 3[Sb_i^{3+}])^{\frac{1}{2b}} = \\ = N_c \left(\alpha^3 \cdot a^2 \cdot N_{C,0}^2 \right)^{\frac{1}{2b}} \exp \left(- \frac{E_{Sb_{Pb}^+} + E_c + \frac{1}{2b} kT}{kT} \right) \end{aligned} \quad (2)$$

$$\begin{aligned} [Sb_{Te}^-]([Sb_{Pb}^+] - [Sb_{Te}^-] + 3[Sb_i^{3+}])^{\frac{1}{2b}} = \\ = N_a \left(\alpha^3 \cdot a^2 \cdot N_{C,0}^2 \right)^{\frac{1}{2b}} \exp \left(- \frac{E_{Sb_{Te}^-} - E_c - \frac{1}{2b} kT}{kT} \right) \end{aligned} \quad (3)$$

$$\begin{aligned} [Sb_i^{3+}]([Sb_{Pb}^+] - [Sb_{Te}^-] + 3[Sb_i^{3+}])^{\frac{3}{2b}} = \\ = N_i \left(\alpha^3 \cdot a^2 \cdot N_{C,0}^2 \right)^{\frac{3}{2b}} \exp \left(- \frac{E_{Sb_i^{3+}} + 3E_c + \frac{3}{2b} kT}{kT} \right) \end{aligned} \quad (4)$$

It is worth noting that no additional conditions for the connection of concentrations of various impurity defects are needed here, since the inclusion of additional phases is an additional source of impurity with a number significantly higher than that dissolved in the lattice.

IV. Power parameters of point defects

The energy of defect formation, according to [15], can be represented as

$$E_1 = E_0 - \frac{Z}{|Z|} \varepsilon_1 \pm \left\{ 3kT \ln \left(\frac{T_0}{T} \right) - kT \right\} + x \cdot 3kT \ln \left(\frac{\omega}{\omega_0} \right) \quad (5)$$

where E_0 is the energy of the formation of a neutral defect, Z is the charge state of the defect, ε is the ionization energy of the defect, and x is the number of atoms in the vicinity of the defect that have changed the frequency of their oscillations from ω_0 to ω . For the substitution atoms, the third addition in (5) will be absent, and for the inter-node atom before the third addition should be "+" sign.

Changes in the frequency of oscillations in the vicinity of the substitution atoms are determined by the

formula [16]: $\frac{\omega}{\omega_0} = \frac{T_{Sb} \theta_{PbTe}}{T_{PbTe} \theta_{Sb}}$. Given the data [11, 17, 18],

we will get: $\frac{\omega}{\omega_0} = \frac{904 \text{ K} \cdot 125 \text{ K}}{1191 \text{ K} \cdot 200 \text{ K}} = 0.47$. It was considered

that this value is the same for both defects of substitution. In the case of inter-node atom, the frequency change was considered as variation parameter.

According to [3], the impurity of antimony creates levels near the extreme points of the allowed zones. Respectively $\varepsilon(Sb_{Pb}^{1+}) = E_c$, and $\varepsilon(Sb_{Te}^{1-}) = E_v$. Given that the energy of the defect formation is much greater than the energy of its ionization, such an assumption should not significantly affect the result.

Quantum mechanical calculations using the FireFly 7 (PCGamess) and the limited Hartree-Fock method were used to generate point defects energy. In this case, a cluster of 27 atoms (one elementary cell of the NaCl structure) and valence basis are used. Establishing the correspondence of the model to the real structure of the crystal was carried out by comparing the interatomic distances and energies of interatomic bonds in the cluster after the process of optimizing its geometry to the corresponding experimental values. The task with the construction of the cluster was considered complete, if the crystallographic parameters of clusters after optimization of geometry no more than 1 – 2 % differed from the known experimental values. The energy of defect formation was defined as the difference between the energies of the defect-free cluster and the cluster in the center of which the defect was located. According to the results, the generation energy of the defects of Sb_{Pb} and Sb_{Te} is 3.19 eV and 3.21 eV respectively. The energy of the formation of the inter-node atom Sb is greater and is 4.33 eV.

V. Results of the calculations

The results of the calculations are presented in Fig. 6 separately for a model without inter-node antimony atoms (Fig. 6 a) and with their account (Fig. 6, b). Using calculating values of the energy of formation of defects substitutions for the calculating the concentrations of point defects, as well as the variation of the oscillation frequencies $\omega/\omega_0 = 0.47$, does not allow us to obtain the values of electron concentrations close to the experimental ($\approx 10^{19} \text{ cm}^{-3}$, Fig. 6, a) therefore, it is possible to assume that the probability of participation of inter-node antimony atoms in the formation of numerical values of n_H is high. On the other hand, the high energy of formation of the inter-node atom Sb should indicate the low concentration of such defects in crystals. However, given that the change in the frequency of oscillations of inter-node atoms is a variation parameter, one can estimate the maximum possible concentrations of these defects, assuming that $\omega/\omega_0 = 0.2$. According to [18-19] the frequency variation in the vicinity of point defects is more than 5 times unlikely.

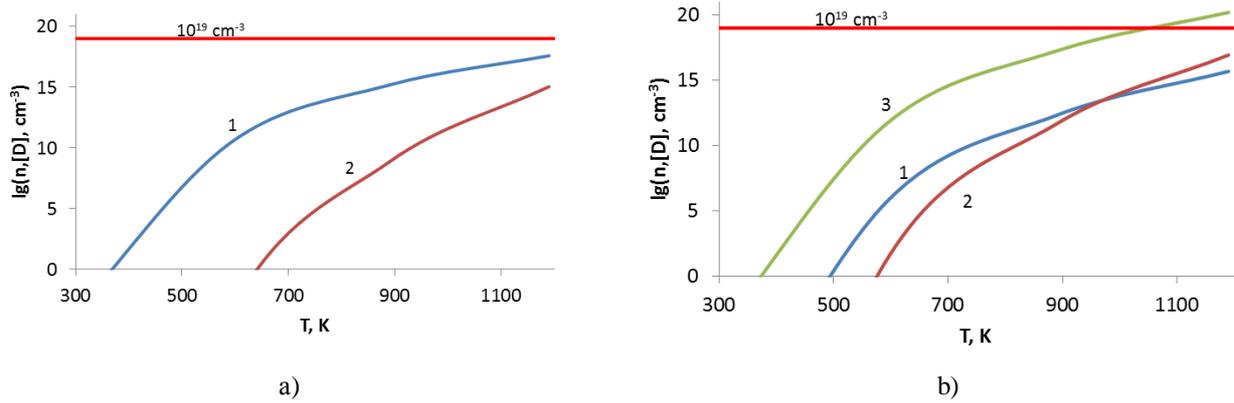


Fig. 6. Thermodynamically equilibrium concentrations of point defects in crystals PbTe:Sb depending on temperature: a - a model that does not take into account the possibility of formation of inter-node antimony atoms, b - a model that takes into account the possibility of formation of inter-node antimony atoms.
 1 - $\text{Sb}_{\text{Pb}}^{1+}$, 2 - $\text{Sb}_{\text{Te}}^{1-}$, 3 - Sb_i^{3+} .

For such parameters of calculation it is possible to obtain values n close to the experimental ones (Fig. 6, b). Concentrations of inter-node defects of order 10^{19} cm^{-3} , that is, the values of the order of the measured carrier concentrations, are observed at temperatures of $\approx 1100 \text{ K}$ (830°C). Consequently, it can be assumed that the measurements at temperatures up to 200°C the carrier concentrations (Fig. 4) are due to not equilibrium point defects, but due to hardening ones. Moreover, the investigated temperatures of annealing (500°C and 650°C) are significantly lower than the hardening temperature, which means that the concentration of carriers after annealing does not change.

It is worth noting here that at 1000 K its own carrier concentration is $n \approx 10^{18.9} \text{ cm}^{-3}$, that is, commensurate with the concentration of ionized defects. Consequently, in order to more accurately calculate in the region of these temperatures, it is necessary to consider own electrons and holes. It may also be worth considering the processes of hardening, which may give more accurate values of carrier concentrations at room temperatures. However, the result obtained quite satisfactorily explains the observed patterns in the properties of the samples studied, and therefore we can assume that the proposed model and parameters of point defects correctly reflect the features of the defect subsystem of crystals PbTe:Sb.

Conclusions

1. The complex of thermoelectric parameters (specific conductivity, Seebeck coefficient, thermal conductivity, Hall effect) of heterophase materials PbTe:Sb (8 at.%) is investigated.

2. It is shown that the significant dependence of the specific electrical conductivity of the material on the

technological conditions of obtaining experimental samples, in particular temperature and time of annealing, is caused by the formation in each case of inclusions of additional phases different in shape and size, which, accordingly, also determines a different influence on the mobility of carriers.

3. The temperature dependence of the Hall electron concentration in the temperature range under study is determined by the concentration of hardening electrically active point defects by temperatures of $\approx 1100 \text{ K}$ (830°C), which results in the absence of temperature dependence $n_H(T)$ in the temperature range up to 200°C .

4. On the basis of modeling a defective subsystem using the method of minimizing free energy of a crystal as a function of the concentration of point defects, it has been shown that dominant point defects in the investigated materials are inter-node atoms of antimony Sb_i^{3+} .

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Термоелектричні властивості і дефектна підсистема гетерофазних матеріалів на основі п्लомбум телуриду з домішкою сурми

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Представлено результати дослідження термоелектричних властивостей та дефектної підсистеми легованого сурмою п्लомбум телуриду PbTe:Sb (8%), перспективного матеріалу для створення на його основі перетворювачів теплової енергії в електричну. Встановлені закономірності у поведінці досліджуваних властивостей, що зумовлені двофазністю матеріалу та значним впливом технологічних факторів отримання зразків на їх дефектну підсистему. Проведено моделювання дефектної підсистеми кристалів PbTe:Sb з врахуванням наявності включень додаткової фази та встановлено, що домінуючими точковими дефектами є міжвузлові атоми стибію.

Ключові слова: п्लомбум телурид, легування, дефекти, тепла енергія.