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POINT DEFECTS AND PHYSICO-CHEMICAL PROPERTIES OF CRYSTALS IN Pb-Bi-Te SYSTEM

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Abstract. Within crystalquasichemical formalism models of point defects of crystals in the Pb-Bi-Te system have been specified considering the amphoteric action of impurities in bismuth doped lead telluride PbTe:Bi, and solid solution formation mechanisms for PbTe-BiTe and PbTe-Bi₂Te₃ have been examined. Dependences of Hall concentration and the concentration of point defects on the composition and the initial deviation from stoichiometry in the basic matrix have been calculated.

Keywords: lead telluride, doping, solid solution, point defects, crystalquasichemical formula, defect formation.

1. Introduction

Lead telluride is promising semiconductor material for thermoelectric energy conversion devices that operate within high temperature range of 500–850 K. The important factors that determine the performance characteristics of device structures are point defects of the base material, which can be controlled

significantly by doping and solid solutions formation in the wide concentration range [1, 2].

Bismuth is one of the most important alloying elements in PbTe, input of which allows obtaining the concentration of electrons that provide the maximum values of thermoelectric figure of merit in the crystals.

In Pb-Bi-Te system there are two quasi-binary cross-sections: PbTe-Bi₂Te₃ and PbTe-Bi and non-quasi-binary cross-section PbTe-BiTe. It was established that less than 1 mol % of Bi [3] and BiTe [3, 4] and ~5 mol % of Bi₂Te₃ [4, 5] dissolve in PbTe. Research of the homogeneity region (GR) of PbTe in Pb-Bi-Te ternary system [5] showed that the introduction of Bi to ~3 at. % widens GR shifting it towards Te content increasing, and the maximal GR corresponds to PbTe-Bi₂Te₃ cross-section. According to [6-8], Bi in *p*-PbTe is distributed between cation and anion sublattices. Doping effect of Bi is more significant for PbTe-BiTe cross-section than the PbTe-Bi₂Te₃ one [4]. In the case of introduction of BiTe to ~0.1 at. % of Bi each Bi atom supplies one electron, and by further Bi content increase the carrier concentration growth rate slows [4, 9, 10].

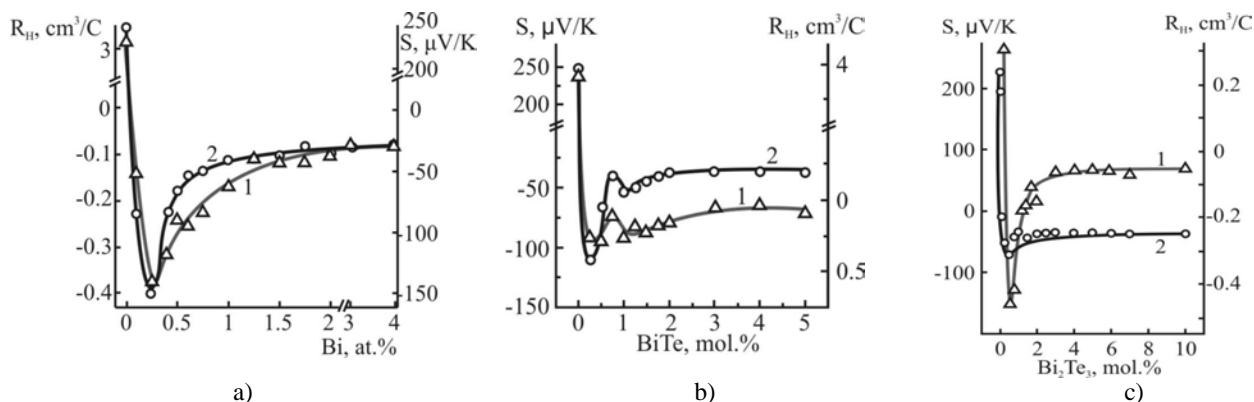


Fig. 1. Dependences of Hall coefficient R_H (1) and Seebeck coefficient S (2) on the composition of *p*-PbTe:Bi [11] (a), *p*-PbTe-BiTe [9] (b) and *p*-PbTeBi₂Te₃ [12] crystals (c)

Composition dependence of thermoelectric parameters for the investigated systems is shown in Fig. 1. It can be seen that at ~0.1 at. % of Bi (Fig. 1a) and 0.25 mol. % of BiTe (Fig. 1b) conversion of the conductivity from *p*- to *n*-type takes place [9, 11]. Conversion of conductivity type in *p*-PbTe-Bi₂Te₃ solid solutions comes at 0.1 mol % of Bi₂Te₃ (Fig. 1c) [12]. General regularity under the increase of dopant content in PbTe basic matrix is the decrease of Seebeck coefficient, reversal of its sign and some subsequent increase thereof (Fig. 1, curves 2). This hole concentration decreases initially and thermodynamic *p*-*n*-conversion comes with the following increase of electron concentration.

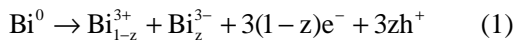
The purpose of this paper is behavioral analysis of bismuth in Pb-Bi-Te system and of its impact on the defect subsystem of crystal.

2. Crystalquasichemical Formulae

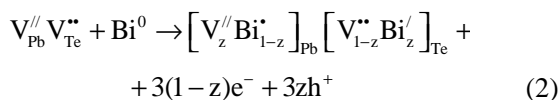
For the analysis of the defect subsystem in investigated crystals crystalquasichemical approach has been used. It is based on the concept of antistructure [13], which has the form of $V_{Pb}'' V_{Te}''$ for lead telluride, where V_{Pb}'' and V_{Te}'' – double-charged lead and tellurium vacancies, respectively; "'' and "•" – negative and positive charges, respectively. Crystal formula is written as a superposition of alloying cluster formed on the basis of basic matrix antistructure and crystal formula of basic compound.

2.1. Doped Crystals PbTe:Bi

In doped crystals PbTe:Bi bismuth, replacing lead in its sublattice, ionizes from the state of Bi⁰(6s²6p³) to the state of Bi³⁺(6s²6p⁰) + 3e⁻. Relative to cation sublattice impurity is in the state of Bi³⁺ → Bi_{Pb}⁺ (where it is a donor). In the tellurium sublattice bismuth ionizes Bi⁰(6s²6p³) → Bi³⁻(6s²6p⁶) + 3h⁺ (it is the acceptor), and is in the state of Bi³⁻ → Bi_{Te}⁻. The fact, that the impurity can occupy Pb and Te positions in PbTe crystal structure, can be described by disproportionation of its charge state:

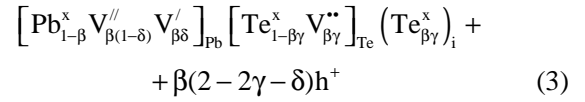


where *z* – the disproportionation value of Bi charge state. The relationship between Bi³⁺ and Bi³⁻ determines donor or acceptor action of impurities. Alloying cluster for bismuth looks like:

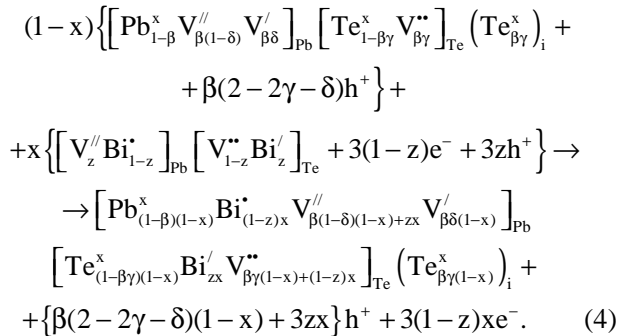


where e⁻ – an electron h⁺ – a hole, "x" – neutral charge.

Crystalquasichemical formula of *p*-PbTe with the complex range of point defects in the cation sublattice (single and double-charged Pb vacancies) is represented as [14]:



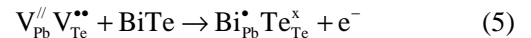
Its superposition with the alloying cluster (2) presents the crystalquasichemical formula of *p*-PbTe: Bi:



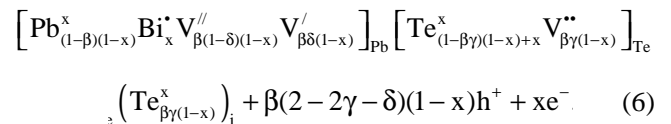
where *x* – atomic fraction of Bi, β – value of initial deviation from stoichiometry on Te side, δ – disproportionation coefficient of Pb vacancies charge state, γ – the fraction of interstitial tellurium atoms.

2.2. Solid Solutions PbTe-BiTe

Taking into account the substitution of Bi atoms Pb position in PbTe crystal lattice (Bi_{Pb}⁺) formula for alloying cluster looks like:



then crystalquasichemical formula of *p*-PbTe-BiTe is:



where *x* – molar fraction of BiTe.

2.3. Solid Solutions PbTe-Bi₂Te₃

There are two possible mechanisms of PbTe-Bi₂Te₃ solid solution formation: substitution of Bi ions Pb positions with the formation of cation vacancies (mechanism I) or the substitution of Bi ions Pb position with the formation of interstitial tellurium (mechanism II).

Mechanism I. At calculation per 1 tellurium atom and taking into account charge state of Bi³⁺ and Te²⁻ ions chemical formula for alloying component will look like:

Bi₂³⁺Te²⁻. Alloying cluster in this case is written as:



Then crystalquasichemical formula of p -PbTe- Bi_2Te_3 is:

$$\left[\text{Pb}_{(1-\beta)(1-x)}^x \text{Bi}_{\frac{2}{3}x}^{\cdot\cdot} \text{V}_{\beta(1-\delta)(1-x)+\frac{1}{3}x}^{\prime\prime} \right]_{\text{Pb}} \left[\text{Te}_{(1-\beta\gamma)(1-x)+x}^x \text{V}_{\beta\gamma(1-x)}^{\prime\prime} \right]_{\text{Te}} + \beta(2-2\gamma-\delta)(1-x)h^+ \quad (8)$$

where x – molar fraction of Bi_2Te_3 .

Mechanism II. At calculation per 1 Bi atom and taking into account charge state of Bi^{3+} and Te^{2-} ions chemical formula for alloying components is written as:

$\text{Bi}^{3+}\text{Te}_{\frac{2}{3}}^{2-}$, and its cluster:



Then crystalquasichemical formula of p -PbTe- Bi_2Te_3 is:

$$\left[\text{Pb}_{(1-\beta)(1-x)}^x \text{Bi}_{\frac{2}{3}x}^{\cdot\cdot} \text{V}_{\beta(1-\delta)(1-x)}^{\prime\prime} \text{V}_{\beta\delta(1-x)}^{\prime} \right]_{\text{Pb}} \left[\text{Te}_{(1-\beta\gamma)(1-x)+x}^x \text{V}_{\beta\gamma(1-x)}^{\prime\prime} \right]_{\text{Te}} \left(\text{Te}_{\beta\gamma(1-x)+\frac{1}{2}x}^x \right) + \beta(2-2\gamma-\delta)(1-x)h^+ + xe^- \quad (10)$$

The proposed mechanisms of doping and crystal formulae (4), (6), (8), and (10) make it possible to find analytical dependences of the concentration of individual point defects and current carriers on the magnitude of deviation from stoichiometric composition in the base compound (α , β) and impurity content (x). In particular for p -PbTe:Bi according to crystalquasichemical formula (4), total electroneutrality equation is written as follows:

$$n + |q_{\text{V}_{\text{Pb}}^{\prime\prime}}| [\text{V}_{\text{Pb}}^{\prime\prime}] + |q_{\text{V}_{\text{Pb}}^{\prime}}| [\text{V}_{\text{Pb}}^{\prime}] + |q_{\text{Bi}_{\text{Te}}^{\prime}}| [\text{Bi}_{\text{Te}}^{\prime}] = p + |q_{\text{V}_{\text{Te}}^{\prime\prime}}| [\text{V}_{\text{Te}}^{\prime\prime}] + |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| [\text{Bi}_{\text{Pb}}^{\cdot\cdot}], \quad (11)$$

where $n = 3A(1-z)x$, $p = A(\beta(2-2\gamma-\delta)(1-x) + 3zx)$, $[\text{Bi}_{\text{Te}}^{\prime}] = Azx$, $[\text{V}_{\text{Pb}}^{\prime\prime}] = A(\beta(1-\delta)(1-x) + zx)$,

$[\text{V}_{\text{Pb}}^{\prime}] = A\beta\delta(1-x)$, $[\text{Bi}_{\text{Pb}}^{\cdot\cdot}] = A(1-z)x$, $[\text{V}_{\text{Te}}^{\prime\prime}] = A(\beta\gamma \cdot (1-x) + (1-z)x)$, $[\text{V}_{\text{Te}}^{\prime}] = A(\beta\gamma(1-x) + (1-z)x)$

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| = |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| = |q_{\text{Bi}_{\text{Te}}^{\prime}}| = 1, \quad |q_{\text{V}_{\text{Pb}}^{\prime}}| = |q_{\text{V}_{\text{Te}}^{\prime}}| = 2.$$

where $A = \frac{2Z}{a^3}$, Z – number of structural units per unit cell, a – lattice parameter.

Hall concentration of current carriers n_H in this case is defined as:

$$n_H = A |3(1-z)x - \beta(2-2\gamma-\delta)(1-x) - 3zx|. \quad (12)$$

Similarly for p -PbTe- Bi_2Te_3 according to (6), total electroneutrality equation is:

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| [\text{V}_{\text{Pb}}^{\prime\prime}] + |q_{\text{V}_{\text{Pb}}^{\prime}}| [\text{V}_{\text{Pb}}^{\prime}] = p + |q_{\text{V}_{\text{Te}}^{\prime\prime}}| [\text{V}_{\text{Te}}^{\prime\prime}] + |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| [\text{Bi}_{\text{Pb}}^{\cdot\cdot}], \quad (13)$$

where $p = A\beta(2-2\gamma-\delta)(1-x)$, $n = Ax$,

$$[\text{V}_{\text{Pb}}^{\prime\prime}] = A\beta(1-\delta)(1-x), \quad [\text{V}_{\text{Pb}}^{\prime}] = A\beta\delta(1-x),$$

$$[\text{Bi}_{\text{Pb}}^{\cdot\cdot}] = Ax, \quad [\text{V}_{\text{Te}}^{\prime\prime}] = A\beta\gamma(1-x), \quad |q_{\text{V}_{\text{Pb}}^{\prime}}| = |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| = 1,$$

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| = |q_{\text{V}_{\text{Te}}^{\prime\prime}}| = 2.$$

Hall concentration is:

$$n_H = A |\beta(2-2\gamma-\delta)(1-x) - x| \quad (14)$$

In the case of the mechanism I in p -PbTe- Bi_2Te_3 , according to (8):

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| [\text{V}_{\text{Pb}}^{\prime\prime}] + |q_{\text{V}_{\text{Pb}}^{\prime}}| [\text{V}_{\text{Pb}}^{\prime}] = p + |q_{\text{V}_{\text{Te}}^{\prime\prime}}| [\text{V}_{\text{Te}}^{\prime\prime}] + |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| [\text{Bi}_{\text{Pb}}^{\cdot\cdot}], \quad (15)$$

where $p = A\beta(2-2\gamma-\delta)(1-x)$,

$$[\text{V}_{\text{Pb}}^{\prime\prime}] = A \left(\beta(1-\delta)(1-x) + \frac{1}{3}x \right), \quad [\text{V}_{\text{Pb}}^{\prime}] = A\beta\delta(1-x),$$

$$[\text{Bi}_{\text{Pb}}^{\cdot\cdot}] = \frac{2}{3}Ax, \quad [\text{V}_{\text{Te}}^{\prime\prime}] = A\beta\gamma(1-x), \quad |q_{\text{V}_{\text{Pb}}^{\prime}}| = |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| = 1,$$

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| = |q_{\text{V}_{\text{Te}}^{\prime\prime}}| = 2$$

Hall concentration in this case is:

$$n_H = A\beta(2-2\gamma-\delta)(1-x) \quad (16)$$

Similarly for p -PbTe- Bi_2Te_3 (mechanism II), according to (10), total electroneutrality equation is:

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| [\text{V}_{\text{Pb}}^{\prime\prime}] + |q_{\text{V}_{\text{Pb}}^{\prime}}| [\text{V}_{\text{Pb}}^{\prime}] = p + |q_{\text{V}_{\text{Te}}^{\prime\prime}}| [\text{V}_{\text{Te}}^{\prime\prime}] + |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| [\text{Bi}_{\text{Pb}}^{\cdot\cdot}], \quad (17)$$

where $p = A\beta(2-2\gamma-\delta)(1-x)$, $n = Ax$,

$$[\text{V}_{\text{Pb}}^{\prime\prime}] = A\beta(1-\delta)(1-x), \quad [\text{V}_{\text{Pb}}^{\prime}] = A\beta\delta(1-x),$$

$$[\text{Bi}_{\text{Pb}}^{\cdot\cdot}] = Ax, \quad [\text{V}_{\text{Te}}^{\prime\prime}] = A\beta\gamma(1-x), \quad |q_{\text{V}_{\text{Pb}}^{\prime}}| = |q_{\text{Bi}_{\text{Pb}}^{\cdot\cdot}}| = 1,$$

$$|q_{\text{V}_{\text{Pb}}^{\prime\prime}}| = |q_{\text{V}_{\text{Te}}^{\prime\prime}}| = 2$$

Hall concentration in this case:

$$n_H = A |\beta(2-2\gamma-\delta)(1-x) - x| \quad (18)$$

3. Results and Discussion

Some results of calculations of Hall concentration of current carriers and the concentration of the dominant point defects are presented in Figs. 2 and 3.

The calculation of Hall concentration in bismuth doped crystals p -PbTe:Bi (Fig. 2a, curve 1, Fig. 3a) shows that at value of $z < 0.5$ impurity acts as donor ($[\text{Bi}_{\text{Pb}}^{1+}] > [\text{Bi}_{\text{Te}}^{1-}]$): decrease of hole concentration, thermodynamic p - n -conversion and further increase of electron concentration take place. With the predominance of

bismuth ions in tellurium positions $z > 0.5$ ($[Bi_{Te}^{1-}] > [Bi_{Pb}^{1+}]$) the opposite relationship is observed. If $z = 0.5$ complete self-compensation of impurity occurs and Hall concentration varies slightly. The foregoing features are well illustrated in the 3d-diagram (Fig. 3a). Based on the experimental data [11] we can conclude that in practice realization of the case $z < 0.5$ takes place, i.e. the concentration of bismuth ions in the state of Bi_{Pb}^{1+} dominates the concentration of Bi_{Te}^{1-} . In particular, comparison of the experimental data [11] (Fig. 1a) with

the calculations (Fig. 2 and 3a) gives grounds to assert that the disproportionation value of Bi charge state (z) is equal to ~ 0.4 . Change of Hall concentration is associated with redistribution of the point defect concentration. The dominant defects are Bi ions, rooted both in Pb and Te sublattices of lead telluride crystal lattice, the concentration of which increases with the dopant content (Fig. 2, curves 2, 3). Also double-charged Pb and Te vacancies make significant contribution to the conductivity, and its concentration increases with the impurity content (Fig. 2, curves 4, 6).

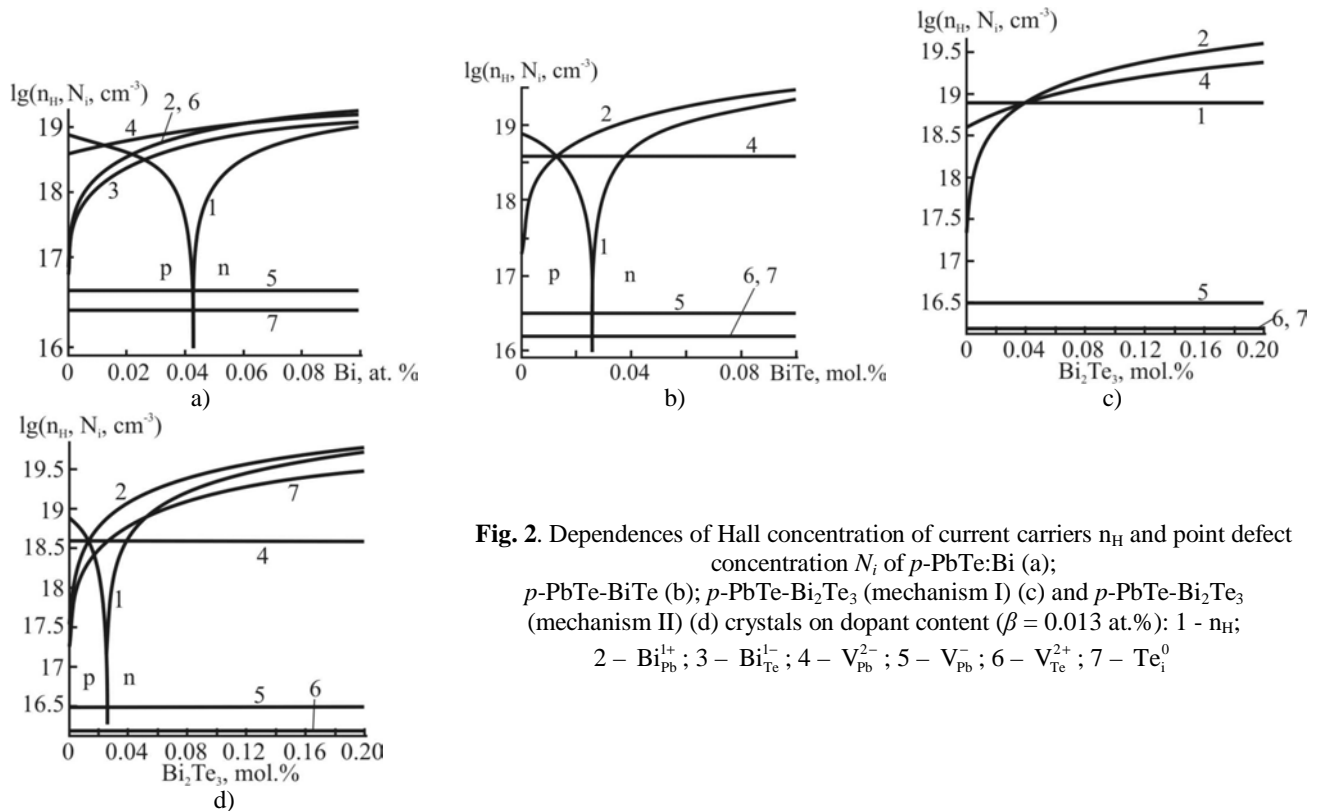


Fig. 2. Dependences of Hall concentration of current carriers n_H and point defect concentration N_i of p -PbTe:Bi (a); p -PbTe-BiTe (b); p -PbTe-Bi₂Te₃ (mechanism I) (c) and p -PbTe-Bi₂Te₃ (mechanism II) (d) crystals on dopant content ($\beta = 0.013$ at.%): 1 - n_H ; 2 - Bi_{Pb}^{1+} ; 3 - Bi_{Te}^{1-} ; 4 - V_{Pb}^{2-} ; 5 - V_{Pb}^- ; 6 - V_{Te}^{2+} ; 7 - Te_i^0

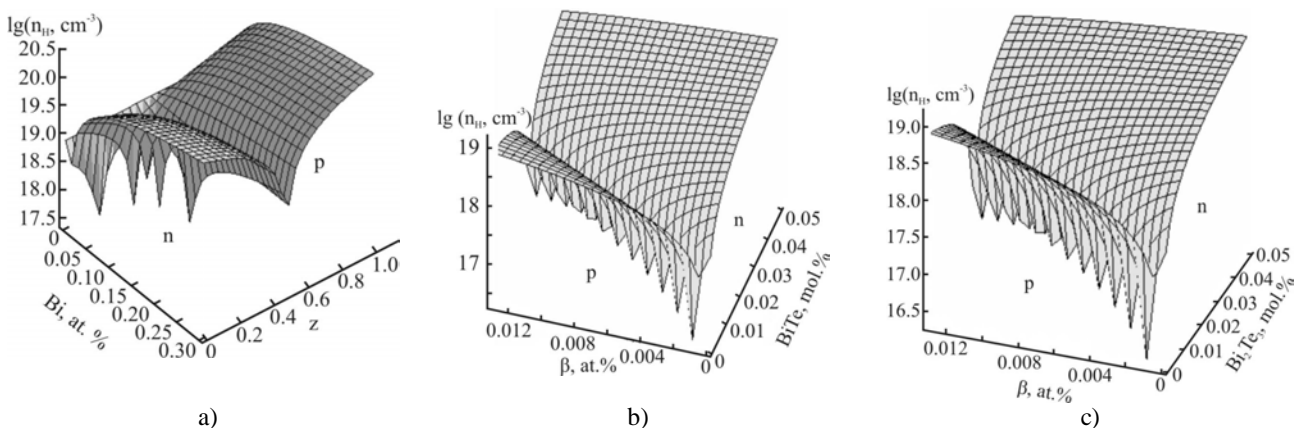


Fig. 3. 3d-Diagrams of Hall concentration (n_H) dependence in p -PbTe:Bi (a); p -PbTe-BiTe (b) and p -PbTe-Bi₂Te₃ (mechanism II) (c) crystals on the dopant content and the disproportionation value of charge state z (a) and the size of the initial deviation from stoichiometry β (b, c).

In PbTe-BiTe solid solutions dominant defects are Bi dopant atoms in cation positions Bi_{Pb}^+ (Fig. 2b, curve 2), the concentration of which increases with BiTe content. In the case of *p*-PbTe-BiTe cation vacancies $\text{V}_{\text{Pb}}^{2-}$ have sufficiently high concentration (Fig. 2b, curve 4), which is virtually unchanged. The concentrations of V_{Pb}^- , $\text{V}_{\text{Te}}^{2+}$, Te_i^0 point defects are low; their change with increasing content of BiTe is low as well (Fig. 2b, curves 5-7). Note that at low content of BiTe in *p*-PbTe-BiTe sharp decrease of the majority carrier concentration, conversion of the conductivity from *p*- to *n*-type and further increase of the electron concentration take place (Fig. 2b, curve 1; Fig. 3b). It should be noted that with the increase of the value of the initial deviation from stoichiometry in PbTe basic matrix on the tellurium side displacement the curve of thermodynamic *p-n*-conversion to the side of higher BiTe concentrations occurs, which is well illustrated in 3d-diagram (Fig. 3b).

Let us consider the detail analysis of the mechanisms of defect formation in *p*-PbTe- Bi_2Te_3 solid solutions. In the case of mechanism I (substitution of Pb position and formation of cation vacancies) there is a slight decrease of major carriers concentration with increase of Bi_2Te_3 fraction (Fig. 2c, curve 1). For *p*-PbTe- Bi_2Te_3 crystals under increasing Bi_2Te_3 content significant increase of concentration of the ionized Bi in Pb position (Fig. 2c, curve 2) and double-charged cation vacancy concentration (Fig. 2c, curve 4) take place. At the same time V_{Pb}^- , $\text{V}_{\text{Te}}^{2+}$, Te_i^0 concentrations are virtually invariable (Fig. 2c, curves 5-7). For mechanism II (Fig. 2d) the dominant defects are Bi_{Pb}^+ , Te_i^0 , $\text{V}_{\text{Pb}}^{2-}$. While the concentrations $[\text{Bi}_{\text{Pb}}^+]$ and $[\text{Te}_i^0]$ increase with the increase of impurity content (Fig. 2d, curves 2, 7), $[\text{V}_{\text{Pb}}^{2-}]$ decreases slightly (Fig. 2d, curve 4). V_{Pb}^- and $\text{V}_{\text{Te}}^{2+}$ point defects do not affect the conductivity significantly and their concentration does not change with the increase of Bi_2Te_3 content (Fig. 2d, curves 5, 6). Comparison the results of calculations with the experiment (Fig. 1c) on Bi_2Te_3 active donor influence, we can conclude that realization of mechanism II takes place. Increase of the initial deviation from stoichiometry on tellurium side (β) leads to the shift of thermodynamic *p-n*-conversion point to the side of higher Bi_2Te_3 concentration (Fig. 3c).

4. Conclusions

Experimentally determined dependences of thermoelectric parameters of crystals in Pb-Bi-Te system have been examined.

Crystalquasichemical formulae of *p*-PbTe:Bi nonstoichiometric crystals, which take into account the complex range of point defects in lead telluride ($\text{V}_{\text{Pb}}^{2-}$, $\text{V}_{\text{Pb}}^{1-}$, $\text{V}_{\text{Te}}^{2+}$, Te_i^0) and different charge state of dopant ions Bi^{3+} and Bi^{3-} have been developed. The impact of disproportionation value of bismuth impurity charge state on the implementation of the conductivity conversion for *p*-PbTe:Bi crystals has been determined. It was calculated that $z = 0.4$.

Crystal-chemical mechanisms of *p*-PbTe-BiTe and *p*-PbTe- Bi_2Te_3 solid solution formation have been introduced. It has been found that the dominant mechanism of defect formation of *p*-PbTe- Bi_2Te_3 solid solution is substitution of Bi for Pb position with the interstitial tellurium formation.

Dependences of Hall concentration of current carriers and the concentration of point defects on the composition and the initial deviation from stoichiometry of *p*-PbTe crystal basic matrix in Pb-Bi-Te system have been calculated.

It has been shown that new crystal approaches deepen the capabilities of scientific analysis of the defect subsystem in semiconductor crystals and determine the technological aspects of the property control.

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**ТОЧКОВІ ДЕФЕКТИ ТА ФІЗИКО-ХІМІЧНІ
ВЛАСТИВОСТІ КРИСТАЛІВ У СИСТЕМІ Pb-Bi-Te**

Анотація. У рамках кристалохімічного формалізму уточнено моделі точкових дефектів кристалів у системі Pb-Bi-Te з урахуванням амфотерної дії домішки в легovanому вісмутом плумбум телуриді PbTe:Bi та розгля-

нуто механізми утворення твердих розчинів PbTe-BiTe і PbTe-Bi₂Te₃. Розраховано залежності холлівської концентрації та концентрації точкових дефектів від складу і початкового відхилення від стехіометрії в основній матриці.

Ключові слова: плумбум телурид, легування, твердий розчин, точковий дефект, кристалохімічна формула, дефектоутворення.