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**PHASE ANALYSIS
AND ELECTROPHYSICAL
PROPERTIES OF *InGaTe₂***

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This paper presents the results of research on the temperature dependences of the electric conductivity, the Seebeck coefficient and the thermal conductivity in the temperature range of 300 to 900 K, and the results of calculation of the concentration, the Hall mobility of current carriers and the thermoelectric figure of merit of InGaTe₂ semiconductor compound. Based on the band structure of this phase, the unit cell parameters, the electron and hole effective masses have been calculated and it has been established that the unit cell parameters are in good agreement with the experimental data.

Key words: *InGaTe₂* compounds, band structure, effective mass, unit cell parameters, thermo-electric figure of merit.

Introduction

It is known that a search for new semiconductor materials is generally pursued toward the expansion of crystal structure group of already known materials.

In particular, crystal structure interpretation of *TlSe* has revealed that this phase is distinguished by extreme specific features. The lattice of *TlSe* proves to be composed of two independent structural units, namely an octagon with the ionic bond Tl^{1+}-*Se* and a tetrahedron with the covalent bond Tl^{3+}-*Se,* hence chemical formula of *TlSe* should be written as $Tl^{+}Tl^{3+}Se_2$ [1-3]. In subsequent works [4, 5], the substitution of indium and gallium atoms for a three-valence thallium atom in *TlSe* type lattices yilded a new class of semiconductor compounds of $A^{III}B^{III}X_2^{VI}$ type.

X-ray investigations have revealed that one part of these compounds has a chain structure and another part has a layered structure. Compounds with a chain structure are crystallized in tetragonal syngony, space group D_{4h}^{18} (I4/mcm) [2, 3].

The existence of the above compound type is also a reality from the standpoint of electronic structure of component atoms. With formation of $A^{III}B^{III}C_2^{VI}$ type compounds, the outer electron shells of two chalcogen atoms with electron shell $2(s^2p^4)$ at the cost of one $(6p^1)$ electron of univalent thallium (or indium) and one $(5s^2p^1)$ three-valence indium (or gallium) will be completed to a stable $2(s^2p^6)$ configuration.

In papers [3, 4] it was experimentally proved that *Tl* atoms interacting even with the elements of its subgroup (*In*, *Ga*) exhibit univalent state with the outer electron configuration $6s^26p^1$. Univalent state is also typical of indium and gallium elements, even though these elements competing with thallium show normal valence with the outer electron configuration $5s^25p^1$ and $4s^24p^1$, respectively.

The reality of this assumption follows from the fact that $5s^2$ shells of indium and $4s^2$ shells of

gallium as compared to $6s^2$ shell of thallium are less stable, i.e. the probability of univalent state appearance, hence of their occupying octahedral position in lattices of *TlSe* type, all other conditions being equal, is reduced in the sequence $Tl \rightarrow In \rightarrow Ga$. Thus, $TlInX_2^{VI}$, $TlGaX_2^{VI}$ and $InGaX_2^{VI}$ compounds, with their isotructurality, differ in respective anion radicals $[Tl^{3+}X_2^{VI}]^-$, $[In^{3+}X_2^{VI}]^-$ and $[Ga^{3+}X_2^{VI}]^-$ and the energy gap [4].

The existence of ternary compounds of $A^{III}B^{III}X_2^{VI}$ type was confirmed by the methods of differential-thermal, microstructural and *X*-ray phase analyses [6-9]. In later works their electrophysical, thermal, optical and photoelectric properties were studied and it was revealed that these compounds possess high photosensitivity, strain gauge factors and memory-switching properties [11-13], while tellurides and their solid solutions possess high coefficients of thermoelectric figure of merit [14-17]. The energy spectrum of $TlInSe_2(Te_2)$ $TlGaSe_2(Te_2)$ compounds was investigated [22-25], their optical functions were calculated, the origin of the valence band and conduction band, the energy gap, the electron and hole effective masses, the unit cell parameters were determined. However, the data on the research of $InGaSe_2(Te_2)$ compounds is insignificant, though the existence of these compounds was reported as far back as the mid of the last century [4]. In later works [4, 5] their electrophysical properties were studied. In paper [10], perfect crystals $InGaTe_2$ were grown, *X*-ray phase analysis was used to determine the unit cell parameters and it was revealed that $InGaTe_2$, as well as its other structural analogs is crystallized in tetragonal syngony.

In the same paper, the energy spectra were calculated and the origin of the energy gap, the valence band and conduction band was determined. Photoluminescence spectrum and photoelectric properties were investigated, the electronic structure of $InGaTe_2$ was calculated and it was revealed that the resulting data is in good agreement with the data of [22] where the band structure of this phase is interpreted. The optical functions of $InGaTe_2$ are calculated in [23]. However, the data on the investigation of the temperature dependences of the electrical and thermal properties, the results of calculation of the unit cell parameters, the electron and hole effective masses of $InGaTe_2$ is not available.

The purpose of this work is to study the electrophysical properties and calculate the electron and hole effective masses and the unit cell parameters of $InGaTe_2$.

Experimental

The electric conductivity σ, the Hall coefficient *R*, the Seebeck coefficient α and the thermal conductivity χ_p were measured by the procedure described in [24]. The errors of measurement of σ, *R*, α and χ were 5, 6, 7 and 4 %, respectively.

The $InGaTe_2$ compound was synthesized by melting the initial components taken in stoichiometric ratio in evacuated to 0.0133 Pa and sealed quartz ampoules.

For the synthesis of $InGaTe_2$ the elements of purity *In* – 000, *Ga* – 99.996, *Te* – 99.997 % were used. The ampoules were first cleaned with a mixture of HF and distilled water. After chemical cleaning the ampoules evacuated to 0.0133 Pa were placed into an oven at 1000 °C for 24 hours, following which they were cooled and filled with highly purified components. For homogenization of the alloy the mixture was held for 24 hours at a temperature of 970 °C. During the process of synthesis the ampoules were often shaken for better agitation of component parts. Them the ampoule with the substance at a rate of 1.33 mm/hour travelled from the high-temperature zone to crystallization zone with the respective temperature 700 °C. The obtained crystals, when cooled to room temperature, were subject to *X*-ray phase analysis. The results of *X*-ray phase analysis are given in Table 1.

Table1

Results of X-ray phase analysis of InGaTe₂

θ	d_{calc}, Å	d_{exp}, Å	Hkl	$I_{relative}$
$10^0 31`$	4.2300	4.2217	200	6
$13^0 42`$	3.2600	3.2554	211	100
$22^0 26`$	2.9911	2.020	220	14
$23^0 1`$	1.9685	1.9661	411	33
$23^0 22`$	1.9439	1.9442	332(402)	29
$24^0 39`$	1.8770	1.8662	420	18
$25^0 12`$	1.8102	1.8111	421	11
$27^0 20`$	1.6788	1.6784	340(500)	22
$30^0 46`$	1.5072	1.5140	502	10
$32^0 49`$	1.4227	1.4192	522	9

X-ray phase analysis has shown that *InGaTe₂* compound is crystallized in tetragonal syngony with the lattice parameters $a = 8.463$ Å, $c = 6.981$ Å. These values agree well with the data $a = 8.412$ Å, $c = 6.875$ Å from [10].

Discussion of the results

The results of investigation of the temperature dependences of the electric conductivity, the Hall coefficient, the Seebeck coefficient and the thermal conductivity, the calculated values of the Hall mobility, free-carrier concentration and the thermoelectric figure of merit of *InGaTe₂* compound are given in the Table and Fig. 1 – 3. As it follows from Fig. 1 *a*, the electric conductivity with a rise from room temperature to 400 K is relatively weak, and with the onset of intrinsic conductivity the intrinsic carriers quickly become dominant, and the conductivity is exponentially increased. The energy gap determined by the high-temperature slope of dependence $\lg \sigma = f(10^3/T)$ is equal to 0.74 eV.
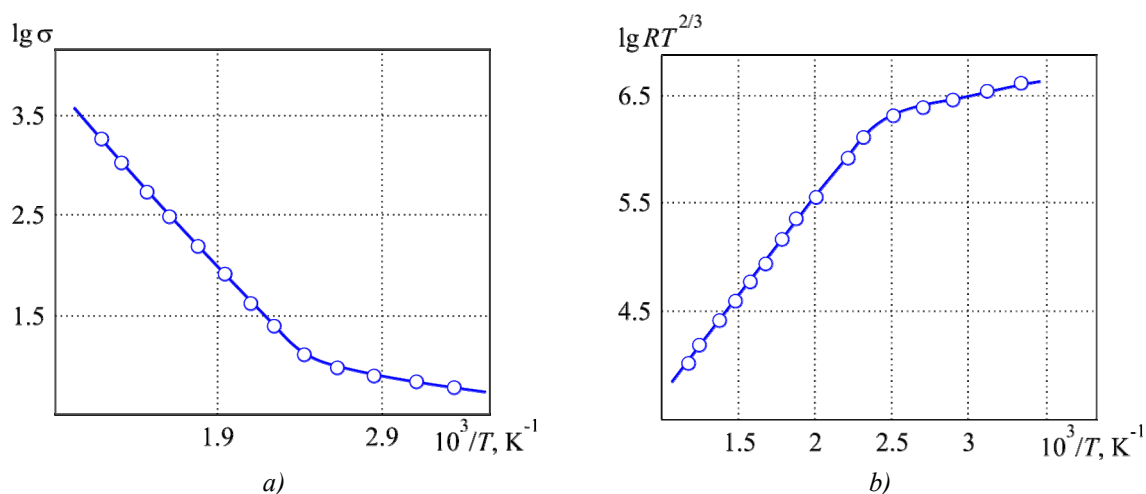
Fig. 1. Temperature dependences of the electric conductivity σ *(S/m) (a)*
and the Hall coefficient R (cm³/C) (b) of InGaTe₂.

The temperature dependence of the Hall coefficient is given in Fig. 1 *b*. As it follows from Fig. 1 *b,* the variation of the Hall coefficient with the temperature agrees well with the variation of the electric conductivity. The value of the energy gap determined by the Hall coefficient, i.e. by the high-temperature slope of dependence $\lg RT^{3/2} = f(10^3/T)$, is equal to 0.76 eV. It is noteworthy that the energy gap 0.56 eV thus defined is not in good agreement with the value found from the experiments with optical absorption or photoconductivity (0.56 eV) [10]. The reason for this discrepancy is that the energy gap itself is a function of temperature. Supposing that all the summands, except for the linear one, in Taylor series expansion of $\Delta E(T)$ with respect to temperature are negligibly small and writing $\Delta E(T) = \Delta E(T = 0) + \beta T$, it becomes apparent that the energy gap determined by the electric conductivity, to a first approximation, is the energy gap at $T = 0$ K and must increase with a rise in temperature.
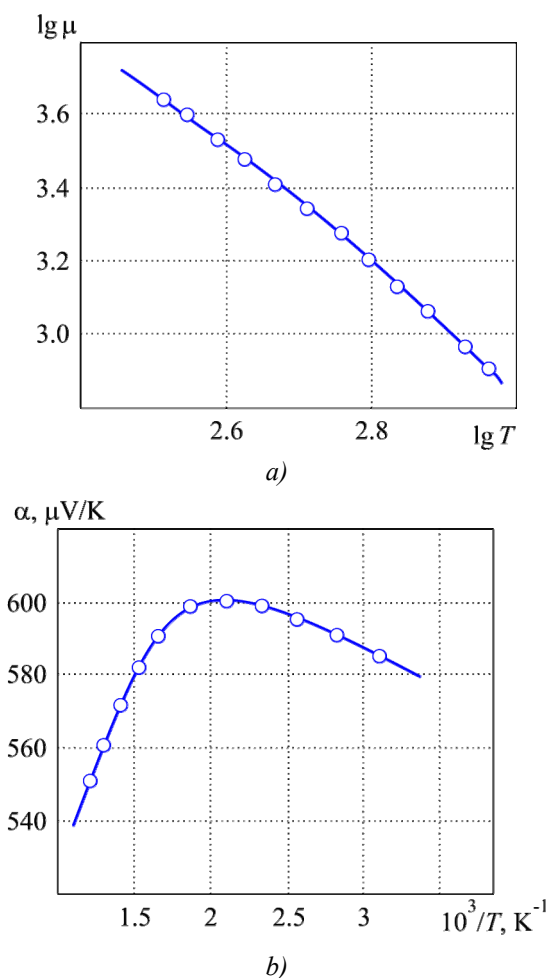
Fig. 2. Dependences of the Hall mobility of carriers μ *(cm²/V·s) (a)*
and the Seebeck coefficient α *(b) on the temperature T (K) of InGaTe₂.*

From the temperature dependence of the Hall mobility (Fig. 2 *a*) it is seen that within the investigated temperature range of 300 to 900 K the mobility drops with a rise in temperature as $T^{-3/2}$, i.e. in this case carrier scattering occurs on the longitudinal acoustic phonons. The temperature dependence of the Seebeck coefficient of *InGaTe₂* is given in Fig. 2 *b*. As it appears from Fig. 2 *b,* in the temperature range of 300– 500 K the thermoEMF is increased, and with the onset of intrinsic conductivity it is decreased which is a specific feature of ternary compounds of $A^{III}B^{III}X_2^{VI}$ type with a complex energy structure [4, 5, 18-22]. The variation of current carrier concentration with the

temperature in Fig.3a is in good agreement with the variation of the electric conductivity and the Hall coefficient with the temperature (Fig. 1).

Fig. 3 *b* shows the temperature dependence of the thermal conductivity of *InGaTe₂*. As it follows from Fig. 3 *b*, the variation of the thermal conductivity with the temperature occurs by the law T^{-1}.
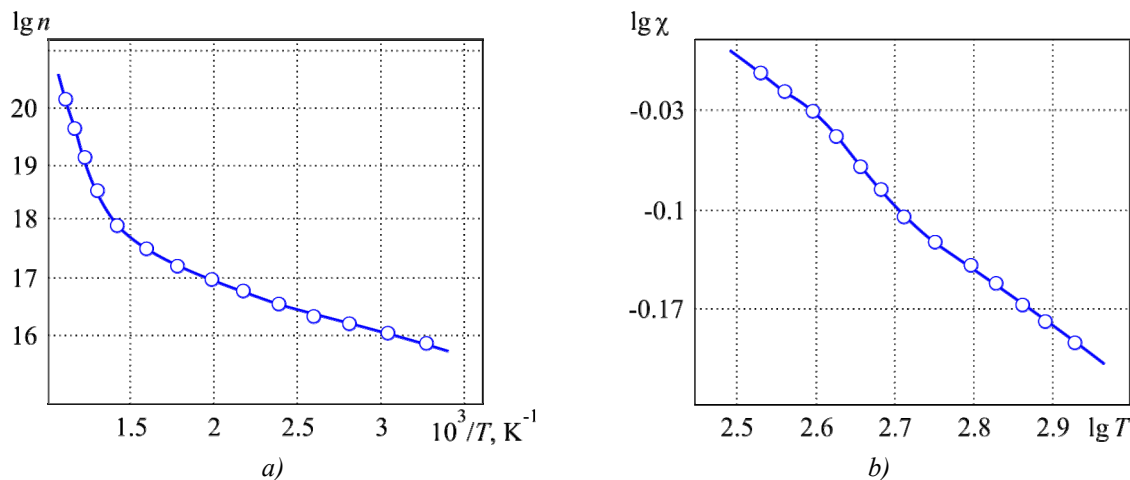

Fig. 3. Temperature dependences of charge carrier concentration n (cm⁻³) (a)
and thermal conductivity coefficient χ (W/m·K) (b) of InGaTe₂.

Based on the results of studying the electric parameters and thermal conductivity, the thermoelectric figure of merit of *InGaTe₂* was determined by the formula

$$Z = \frac{\alpha^2 \sigma}{\chi_p}. \qquad (1)$$

The values appearing in (1) are functions of temperature and carrier concentration, causing, accordingly, sharp temperature and concentration dependences of Z.

In the general form the temperature and carrier concentration dependence of *Z* is rather complex. However, with a number of simplifying assumptions of like-sign carriers, the absence of degeneracy, a low value of electronic thermal conductivity, we can establish a relation between Z_{max} and the characteristic parameters of crystals [25].

$$Z_{max} \sim N \frac{m*^{3/2} \mu T^{3/2}}{\chi_p} e^{r+\frac{1}{2}}. \qquad (2)$$

Here, *N* is the number of ellipsoids in the Brillouin zone, *m** is the effective mass of carriers, *T* is absolute temperature, *r* is parameter of scattering mechanism, χ_p is lattice thermal conductivity. For *InGaTe₂* $N = 4$ [4], conductivity is defined by *p*-type conductivity of carriers, the main mechanism is scattering on acoustic phonons with $r = -1/2$, i.e. exponential factor in (2) disappears.

The resulting data on the thermoelectric figure of merit of *InGaTe₂* is presented in the Table. It is seen that in the temperature range of 500 – 900 K the thermoelectric figure of merit is increased and reaches its maximum value at 900 K.

High thermoelectric figure of merit of *InGaTe₂* crystal (Table 2) in the specified temperature range is due to a low value of lattice thermal conductivity at mobility values 41 cm²/V·s.

The low values of χ_p are largely determined by a large mass of atoms forming *InGaTe₂*, and relatively high mobility values are caused by a low value of the effective mass of carriers. Apparently, increase in the thermoelectric figure of merit is promoted by a deeper scattering of phonons as

compared to electrons. However, a gain in μ/χ_p, as a rule, is reduced with a rise in temperature, since due to phonon-phonon scattering the temperature dependence of thermal conductivity is weakened.

Physical parameters of InGaTe₂ compound

T, K	σ, S/m	α, 10^{-6} V/K	χ, W/(m·K)	R, cm³/C	μ, cm²/(V·s)	n, cm⁻³	$Z \cdot 10^{-3}$, K⁻¹
300	6.3	580	0.84	794	780	$8 \cdot 10^{15}$	0.002
400	12	595	0.82	269	479	$2.3 \cdot 10^{16}$	0.005
500	31.6	600	0.79	72.4	160	$8.9 \cdot 10^{16}$	0.015
600	251	595	0.74	7.2	67	$8.7 \cdot 10^{17}$	0.12
700	646	590	0.69	2.02	58	$3 \cdot 10^{18}$	0.32
800	1260	570	0.66	0.98	41	$6.3 \cdot 10^{18}$	0.62
900	2512	540	0.63	0.112	22	$8.9 \cdot 10^{19}$	1.16

It is known that experimental determination of crystal unit cell parameters is a labor-consuming job. In this connection, here we have theoretically calculated the unit cell parameters of *InGaTe₂* using the results of calculation of *InGaTe₂* band structure [22]. The calculations were made by density functional method, using ABINIT software package, with the help of the Troullier-Martins pseudopotentials in the plane wave basis [27]. In the expansion of wave function we used plane waves with maximum kinetic energy 30 Ha[*]. The lattice parameters were determined by full energy minimization, and structure parameters were optimized using the Hellmann-Feynman forces. The process of forces minimization proceeded till scalar forces $\left| \vec{F} \right| < 3 \dfrac{\text{mRy}}{\text{a.u.}}$.

The external influence is known to cause crystal deformation. In this case, both lattice parameters and parameters that determine position of atoms (their coordinates) are changed as well. So, calculation of these parameters with a given deformation value is an important task. It is considered that pressure is determined by full energy derivative with respect to pressure at constant entropy S $P = -(\partial E/\partial V)_S$, and compression modulus – by pressure derivative with respect to volume at constant temperature $B = -V(\partial P/\partial V)_T$. In practice a derivative of compression modulus is found with small changes of pressure $B' = (\partial B/\partial P)_T$. Assuming that $B' = B_0'$, then $B = B_0 + B_0'P$

Then

$$\frac{dV}{V} = -\frac{dP}{B_0 + B_0'P}. \tag{3}$$

By integration of this expression we get

$$P(V) = \frac{B_0}{B_0'}\left(\left(\frac{V_0}{V} \right)^{B_0'} - 1 \right). \tag{4}$$

Whence we have

$$V(P) = V_0 \left(1 + B_0' \frac{P}{B_0} \right)^{-1/B_0'}. \tag{5}$$

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[*] Hartree energy

As is known, solid bodies have a certain equilibrium volume of the unit cell V_0, and, with a change in this volume by small value, full crystal energy is increased. The Murnaghan equation of state [26] describes the dependence of full energy E on the change in volume V of the unit cell.

$$E(V) = E_0 + \left[\frac{B_0 V}{B_0'} \left(\frac{(V_0/V)^{B_0'}}{B_0'-1} + 1 \right) - \frac{B_0 V}{B_0'-1} \right] \frac{1}{14703.6}. \tag{6}$$

Here $E_0 = E(V_0)$ is the energy corresponding to equilibrium volume V_0 (i.e. to energy minimum), $B = -V(\delta P/\delta V)_T$ is compression modulus, B_0 is the same parameter in equilibrium state corresponding to pressure $P = 0$, $B' = (\delta B/\delta P)_T$ is its first pressure derivative at constant temperature. Multiplier 1/14703.6 in the equation was introduced to obtain the value of full energy in Ry (volume is calculated in atomic units – a.u.).

To determine crystal lattice parameters, we changed the unit cell parameter within ±8 % and calculated the respective values of full energy. Parameters in the Murnaghan equation of state were selected such that a dependence of full energy on the unit cell volume $E(V)$ (Fig. 4), obtained from the equation (shown in Fig. 4 as a solid line) passed through the calculated points.
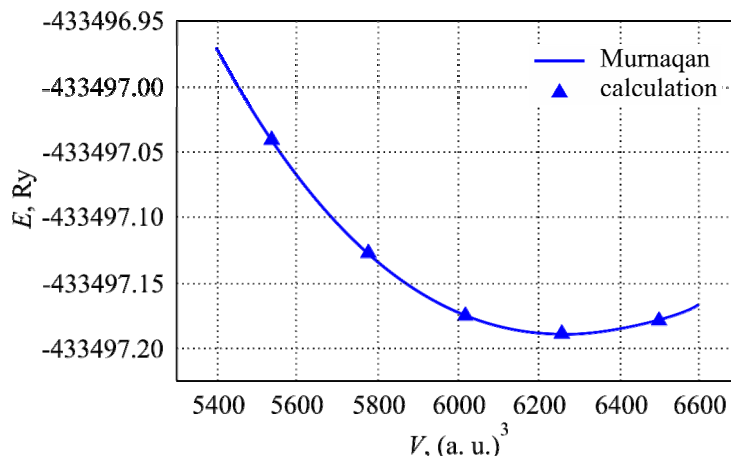

Fig. 4. Dependence of full energy on the unit cell volume of InGaTe2.

According to calculation results, the unit cell volume in equilibrium state $V_0 = 6268.1419$ a.u., compression modulus $B = 40.2392$ GPa, its pressure derivative $B' = 4.5588$.

These results are in good agreement with the calculations made according to the Birch-Murnaghan equation [28] (Table 3).

Table 3

Parameters of the Murnaghan and Birch-Murnaghan equations of state

Parameter	According to Murnaghan	According to Birch-Murnaghan
V_0, a.u	6268.1419	6267.8101
E_0, Ry	-433437.189425	-433497.189401
B, Gpa	40.2392	40.1350
B'	4.5588	4.7886

$$E(V) = E_0 + \frac{9V_0 B_0}{16} \left\{ \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3 B_0' + \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 \left[6 - 4 \left(\frac{V_0}{V} \right)^{\frac{2}{3}} \right] \right\} \frac{1}{14703.6}. \quad (7)$$

Owing to the fact that unit cell volume is $V = abc$ and the resulting equilibrium volume is $V_0 = 6268.1419$ a.u., calculations make it possible to find lattice parameters.

Crystal lattice parameters $a = 8.3945$ Å; $c = 6.8352$ Å that we calculated and coordinates of atoms $x = 0.1730$ in the unit cell agree well with our experimental data and the data in [10]. It should be noted that the results obtained allow further calculation of the phonon spectrum and to study the influence of deformation on the electron and optical properties of *InGaTe₂*, to calculate theoretically the unit cell parameters of other compounds with a known band structure.

The effective mass is known to be the main characteristic of the electron properties of semiconductors. The effective mass is used for studying the electric and magnetic properties, in the calculation of kinetic parameters and in the analysis of critical points of optical parameters.

The tensor components of the inverse effective mass are calculated by the formula:

$$\left[\frac{m_0}{m^*} \right]_{ij} = \delta_{ij} + \frac{2}{m_0} \sum_{n' \neq n} \frac{\langle n_1 k_0 | P_i | n_1' k_0 \rangle \langle n_1' k_0 | P_j | n_1 k_0 \rangle}{E_n(k_0) - E_{n'}(k_0)}, \quad (8)$$

m_0 is mass of electron at rest; δ_{ij} is Kronecker sign, $\langle n_1 k_0 | P_i | n_1' k_0 \rangle$ is magnetic element of momentum

operator, $P_i = -i\hbar \dfrac{\partial}{\partial x_i}$ at extreme point k_0. n, n' are electron bands. $|n_1 k_0\rangle$ is electron wave function.

$$\langle n_1 k_0 | P_i | n_1' k_0 \rangle = \frac{1}{\lambda} \int_{\lambda} \varphi_{n k_0}^*(r) P_i \varphi_{n' k_0}(r) d^3 r, \quad (9)$$

λ is unit cell volume.

The energy spectrum $E_n(k_0)$ and the respective wave function $\varphi_{nk0}(r)$ at extreme point k_0 are found from a one-electron Schrödinger equation. In the plane wave basis

$$\sum_{G'} \left[\frac{\hbar(k_0 + G')}{2m_e} \delta_{GG'} + V(k_0 + G_1 k_0 + G') \right] \phi_n(k_0 + G') = E_{nk_0} \phi_n(k_0 + G) - V(k_0 + G_1 k_0 + G') \quad (10)$$

is the Fourier image of crystalline pseudopotential.

In *InGaTe₂*, valence band maximum and conduction band minimum are at high-symmetry point T, $\kappa_0 = 0.5b_1 - 0.5b_2 + 0.5b_3 (b_1, b_2, b_3)$ are basic translations of the reciprocal lattice [22]. In our calculations, the tensor components of the inverse electron effective mass are calculated to an accuracy of $0.01m_0$

$$\left(\frac{m_0}{m_n} \right) = \begin{pmatrix} 3.09 & 0 & 0 \\ 0 & 3.09 & 0 \\ 0 & 0 & 4.59 \end{pmatrix}. \quad (11)$$

The tensor components of the inverse hole effective mass

$$\left(\frac{m_0}{m_{p\perp}^*} \right) = \begin{bmatrix} -2.31 & 0 & 0 \\ 0 & -2.31 & 0 \\ 0 & 0 & -0.11 \end{bmatrix}. \quad (12)$$

The tensor components of the inverse effective mass of both electrons and holes are of a

diagonal form, so constant-energy surfaces are ellipsoids of revolution. From the symmetry of *InGaTe₂* crystal it also follows that constant-energy surfaces must be ellipsoids of revolution.

Conclusions

1. In this paper, using experimental investigations of the temperature dependences of the electric conductivity, the Hall coefficient, the Seebeck and thermal conductivity coefficients, we have determined the energy gap, the concentration of charge-carrier Hall mobility and the thermoelectric figure of merit of *InGaTe₂* compound and established that the energy gap found by the electric conductivity (0.74 eV) and by the Hall coefficient (0.76 eV) are in good agreement.

2. For the first time, using the results of calculation of *InGaTe₂* band structure through use of ABİNİT software package, we have theoretically calculated the unit cell parameters of this phase and established that the the calculated and experimentally determined values of these parameters are in good agrement, and have calculated the tensors of the inverse effective mass of electrons and holes.

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