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Temperature effects in $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ solid solutions

Alloys of the $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ system were synthesized, and single crystals were grown by the Bridgman method. X-ray diffraction studies established the solubility range of TlGdS_2 in TlInS_2 . The linear thermal expansion coefficient (α_L) and isothermal compressibility (χ_T) of TlInS_2 and the solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ ($0 \leq x \leq 0.10$) were investigated over the temperature range of 80–400 K. Based on the experimental α_L and χ_T values, the Debye temperature, mean-square atomic displacement, Young's modulus, shear modulus, Poisson's ratio, and the difference between C_p and C_V were determined. The band gap was calculated from the temperature dependence of electrical conductivity and compared with values obtained using thermal and optical methods. The anomalous behavior of electrical conductivity was attributed to hopping conduction associated with stoichiometric vacancies and localized states within the band gap. Unlike TlInS_2 , no phase transitions were observed in the investigated solid solutions over the temperature range of 80–400 K. Increasing the TlGdS_2 concentration resulted in higher thermal expansion and compressibility coefficients, indicating weaker interatomic interactions and enhanced anharmonicity of lattice vibrations. The obtained results reveal correlations among crystal structure, chemical bonding, and physical properties in layered chalcogenide semiconductors.

Keywords: solid solutions, linear thermal expansion, isothermal compressibility, shear modulus, anharmonicity, band gap, photoconductivity, single crystals, Bridgman method, X-ray diffraction

Introduction

Interest in semiconductor compounds of the type $\text{TlA}^{\text{III}}\text{B}_2^{\text{VI}}$ ($\text{A} = \text{In, Ga}; \text{B} = \text{S, Se, Te}$) and solid solutions based on them is initially due to the fact that the crystals represent a promising material for use in optical electronics [1–3]. The crystal structure of TlInS_2 is solved in [4]. It is established that TlInS_2 belongs to the monoclinic syngony and has the following crystal lattice parameters: $a = 10.95$; $b = 10.95$; $c = 15.14 \text{ \AA}$, $z = 16$, pr.gr. $\text{Cc} - \text{C}_s^4$.

A characteristic feature of the crystals of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ is the presence in their crystal lattice of a high concentration ($10^{20} \div 10^{22} \text{ cm}^{-3}$) of stoichiometric vacancies and associated localized states in the band gap [5, 6], and this value increases with the growth of the molar fraction of gadolinium in the composition of solid solutions. With an increase in the concentration of solid solutions, the average distance between the atoms of the dissolved substance TlGdS_2 reaches values at which the inter-impurity interaction begins to make a significant contribution to the energy of the TlGdS_2 solvent crystal [7, 8], and this leads to the appearance of fundamentally new properties that are not characteristic of the original material.

Temperature and concentration dependences of thermal and electrophysical properties of alloys of the TlInS_2 – TlGdS_2 systems are studied in the work [9]. However, these data are insufficient to clarify the nature of the bond and the strength of interatomic interaction in the TlInS_2 compound and solid solutions of the TlInS_2 – TlGdS_2 system, which is of particular interest for the analysis of thermal and elastic properties of this object.

To obtain additional information about the chemical bond in the crystal lattice, its influence on the nature and magnitude, the temperature dependence of the heat capacity of thermal expansion (α) and isothermal compressibility (χ_T) are studied in a wide temperature (80–350 K) and concentration ranges.

The aim of the present work is a comprehensive investigation of the temperature and concentration dependences of the coefficient of linear thermal expansion (α_L) and isothermal compressibility (χ_T) of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ ($0 \leq x \leq 0.10$) in the temperature range 80–400 K. The specific objectives include: establishing the solubility region of TlGdS_2 in TlInS_2 by X-ray diffraction analysis; calculating the Debye temperature, mean-square atomic displacements, Young's modulus, shear modulus, Poisson's ratio, and the difference $C_p - C_v$ from experimental α_L and χ_T data; determining the band gap E_g from temperature dependences of electrical conductivity; and comparing the band gap values obtained from thermal, electrical, and optical measurements to verify the consistency of the applied approaches.

Experimental

Alloys of the $\text{TlInS}_2 - \text{TlGdS}_2$ system are studied using differential thermal, X-ray phase, and microstructural analysis methods. DTA of the samples is carried out using a low-frequency thermal recorder NTR-73 with a Pt-Pt/Ph thermocouple at a heating rate of 10 K/min. X-ray fluorescence analysis is carried out using a DRON-1.5 apparatus (Ni filter, 35 kV, 10 mA). The radiographs are decoded using the IZA-2 comparator with an error of 0.01–0.05 mm. The swing radiographs are obtained in the RKOP-A chamber. The intensity of the lines is determined visually using a ten-point scale. The lattice parameters are determined by the

extrapolation method using the function $\frac{1}{2} \left(\frac{\cos^2 \theta}{\cos \theta} + \frac{\cos^2 \theta}{\theta} \right)$ with an accuracy of 0.001 Å. Single crystals of

the samples are grown by the Bridgman method in evacuated quartz ampoules with a diameter of 20–25 mm with different bottom forms. The best homogeneity of samples is obtained with a conical shape of the ampoule bottom and a growth rate of single crystals of 0.5 mm/h. The monocrystalline of the grown crystals is judged by the recorded Lauegrams. To conduct a temperature X-ray diffractometry study, plane-parallel plates are separated from the obtained monocrystal along the cleavage plane and installed on the goniometric head of the DRON-1.5 diffractometer [5]. Measurements of electrical conductivity and the Hall effect are carried out on samples with ohmic contacts at direct current [10] in constant magnetic fields up to 1200 A/m. The measurement error did not exceed 4–5 %.

To measure the all-round compression of the alloys of the $\text{TlInS}_2 - \text{TlGdS}_2$ system in the range of 77–420 K, the setup described in [11] is used. In order to increase the accuracy of measuring the frequency of sinusoidal signals with different interferences, an integrated Schmidt trigger is used in the registration circuit. The setup is calibrated according to the compressibility of reference samples of copper and aluminum. Helium gas is used to compress the sample, the pressure of which varied from 10^5 Pa to 10 MPa. With a small modification, on the same installation, without removing the sample, measurements of thermal expansion are also carried out. The rate of temperature rise did not exceed 2 K/min. The samples had the shape of a cylinder with a cut of 30 mm and a diameter of 5 mm. The error in measuring thermal expansion is ~1.45 %, and in measuring isothermal compressibility ~4.5 % [12]. Synthesis and X-ray diffraction of samples.

Solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ are synthesized in quartz ampoules by melting the starting materials. The starting materials are high-purity elements (Tl — 99.99 wt.%, Gd — 99.5 wt.%, In — 99.999 wt.%, S-oc.4.16-5). From these data, with the exception of gadolinium, it follows that the purity of the initial elements is satisfactory. It is found that 8–10-fold zone purification allows increasing the purity of the element gadolinium to 99.7 mass %. The alloys are synthesized as follows. The initial elements, loaded into an ampoule evacuated to 0.01 Pa, are placed in a furnace. Depending on the gadolinium content, the furnace is heated to a temperature of (1100–1200) K. The time the ampoule with the substance is kept at this temperature also depended on the gadolinium content and increased from 2 to 3 hours as it increased. After which the temperature of the ampoule with the substance is cooled to room temperature at a rate of 15–20 K/h. The obtained samples had a golden-orange color. The alloys synthesized are $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ where $0 \leq x \leq 0.10$.

To conduct an X-ray study using the Bridgman method, single crystals of the $\text{TlInS}_2 - \text{TlGdS}_2$ system alloys are grown. The speed of movement of the ampoule with the melt is 3 mm/h. When growing single crystals of the $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ alloys, the temperature of the high-temperature zone varied from 1000 to 1300 K. In particular, for the composition $x = 0.05$, the zone temperature is 1130 K, and for $x = 0.10$, 1300 K. To establish the solubility region based on TlInS_2 , the obtained single crystals are subjected to X-ray phase analysis. X-ray analysis of crystals $x = 0.05$ and $x = 0.10$ showed that these phases crystallize in the monoclinic syngony based on the TlInS_2 lattice. Calculations of the diffraction patterns of powders of the composition $x = 0.05$ and $x = 0.10$ are given. Laue grams are taken from the obtained sample to determine

the quality of monocrystalline. It appeared that the obtained samples are perfect monocrystals. The quality of the monocrystals worsens with increasing gadolinium concentration in the studied compositions. Based on the rocking X-ray diffraction pattern in three crystallographic directions $[h00]$, $[0k0]$ and $[00l]$, the following lattice parameters of the monoclinic syngony are established for single crystals $x = 0.05$ and $x = 0.10$; $a = 10.843$; $b = 10.90$; $c = 15.145$ Å; $\beta = 100^\circ$; $z = 16$; $a = 10.964$; $b = 10.848$; $c = 15.167$ Å; $\beta = 100^\circ$; $z = 16$.

The calculated numbers of molecules per unit cell confirm that $(\text{TlInS}_2)_{0.95}(\text{TlGdS}_2)_{0.05}$ and $(\text{TlInS}_2)_{0.9}(\text{TlGdS}_2)_{0.1}$ as well as alloys (0–10) mol% TlGdS_2 are substitution solid solutions.

From the above crystal along the $[00l]$ plane is obtained in clear diffraction reflections corresponding to the angles: $\theta = 5^\circ 55'$ (002), $11^\circ 55'$ (004), $24^\circ 23'$ (006), $31^\circ 03'$ (008), $38^\circ 15'$ (00,10), $46^\circ 14'$ (00,12) based on the temperature study conducted, in the temperature range of 320–800 K, curves of the dependence of the lattice parameter “C” on temperature are constructed. It turned out that with an increase in temperature along the $[00l]$ plane, a linear expansion of the crystal $(\text{TlInS}_2)_{0.95}(\text{TlGdS}_2)_{0.05}$ is observed. Thus, as a result of the conducted X-ray study of single crystals $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$, it is established that when TlGdS_2 atoms are replaced by TlInS_2 in the range of (0–10) mass%, the structure does not change and substitution solid solutions are formed (Table 1).

Table 1

Calculation of diffraction patterns of powders of composition $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$

№	$x = 0$	$x = 0.05$	$x = 0.1$	hkl
	$d_{\text{theo.}}, \text{\AA}$	$d_{\text{exp.}}, \text{\AA}$	$d_{\text{exp.}}, \text{\AA}$	
1	7.4550	7.4576	7.4681	002
2	3.8417	3.8176	3.8230	220, 212
3	3.7275	3.7282	3.7283	004
4	3.4554	3.4400	3.4531	311
5	3.0116	3.0232	2.9958	105
6	2.8661	2.8628	2.8610	321, 224
7	2.7545	2.7563	2.7568	323
8	2.5202	2.5191	2.4957	305
9	2.3904	2.3891	2.3820	404
10	2.1347	2.1351	2.1295	151
11	1.9902	1.9875	1.9902	414
12	1.9262	1.9342	1.9271	252
13	1.8643	1.8688	1.8664	208, 008
14	1.7712	1.7716	1.7672	155
15	1.7199	1.7181	1.7184	614
16	1.6867	1.6846	1.6900	317
17	1.6009	1.6037	1.5977	328, 319
18	1.5006	1.4944	1.4903	721

Results and Discussion

The temperature dependences of the electrical conductivity (σ) of the solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ turned out to be complex. It is evident that the electrical conductivity maxima are observed at temperatures of ~795, 810, 830 K for $x = 0.01$; 0.05; 0.10, respectively. With a further increase in temperature, σ decreases, reaches a minimum, and again sharply increases (the region of intrinsic conductivity). This behavior of electrical conductivity in solid solutions of the $\text{TlInS}_2 - \text{TlGdS}_2$ system can be associated with hopping conductivity (Fig. 1a, b).

In this region, the temperature dependence $\lg \sigma \sim AT^{-1/4}$ is typical for such jumps. According to, even in specially undoped crystals TlInS_2 , TlGaSe_2 , TlGaS_2 there is hopping conductivity $T = 200$ K [13]. The nature of uncontrolled defects in TlInS_2 is most likely associated with anion vacancies, which lead to hopping conductivity, at relatively high temperatures can be different. The reason for this may be both anionic and cationic.

onic vacancies disordered in the layer joints and other defects. However, as noted in, these defects do not lead to the state of ferroelectric glass [14].

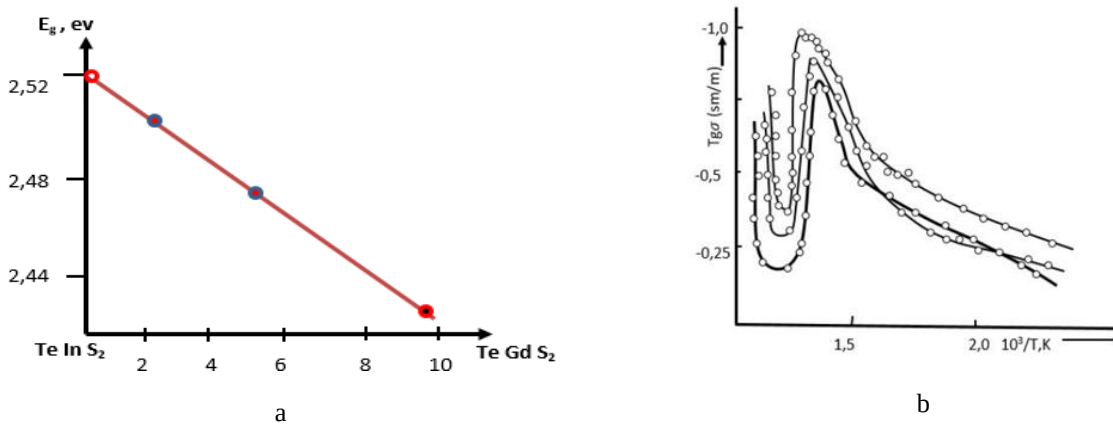


Figure 1. Temperature dependence of electrical conductivity (a) and concentration dependence of the bandgap (b) of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ (1 — $x = 0.02$; 2 — $x = 0.05$; 3 — $x = 0.10$)

The bandgap widths of the indicated phases are determined from the high-temperature slope of the temperature dependence of electrical conductivity and the Hall effect and are in good agreement. Figure 1b shows the dependences of the band gap of the solid solutions $[\text{TlInS}_2]_{1-x}[\text{TlGdS}_2]_x$, determined by $\lg \sigma = f\left(\frac{10^3}{T}\right)$. It is evident that with an increase in TlGdS_2 in TlInS_2 the value of E_g decreases. Based on

the band structure of TlInS_2 , the valence band is mainly formed by the split $3p$ levels of sulfur and partially by the $5p5s$ levels of indium ions, as well as the $6p$ levels of thallium. The conduction band is formed by the $5p5s$ levels of indium ions and the $6p^1$ levels of thallium. When substituting atoms in the $\text{TlInS}_2 - \text{TlGdS}_2$ system, the valence electrons of the latter ions partially pass into a collectivized state, which leads to strong electronic interactions and a “loosening” of the lattice ($R_{\text{In}} = 0.92 \text{ \AA}$; $R_{\text{Gd}} = 0.96 \text{ \AA}$). As a result, during the transition from TlInS_2 to solid solutions based on it, the valence band undergoes a certain shift towards higher energies due to the overlap of the sulfur $3p$ states with the higher-lying gadolinium $4f$ states. At the same time, the lattice parameters increase and the band gap decreases.

Figures 2, 3 show the results of the study of the temperature dependence of the coefficient of linear thermal expansion (α_L) and isothermal compressibility (χ_T) in the range of 80–400 K in TlInS_2 .

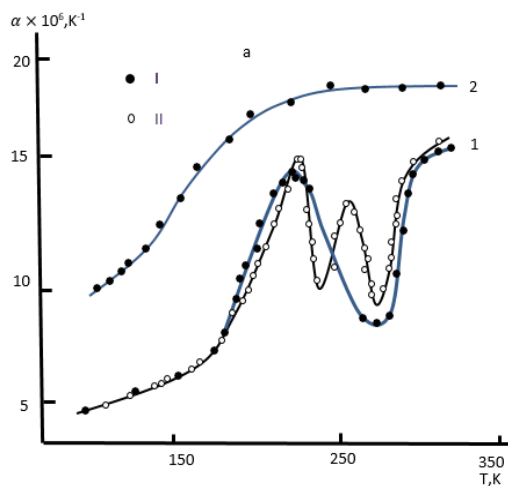


Figure 2. Temperature dependence of the coefficient of linear thermal expansion of 1 — TlInS_2 ; 2 — TlGdS_2 compounds (○ — monocrystalline, ● — polycrystalline)

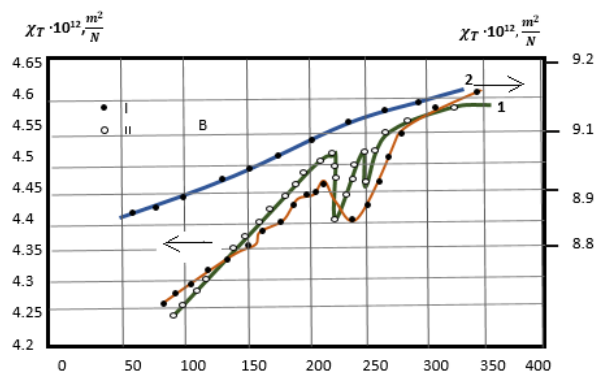


Figure 3. Temperature dependence of the isothermal compression coefficient of TlInS_2 and TlGdS_2 compounds (symbols are the same as in Figure 2)

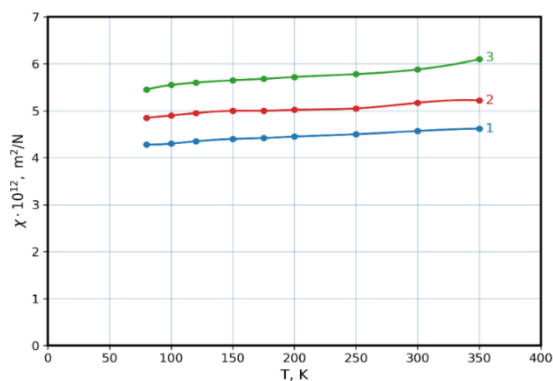


Figure 4. Temperature dependence of the coefficient of linear thermal expansion of $[\text{TlInS}_2]_{1-x}[\text{TlGdS}_2]_x$ solid solutions (markings are as in Figure 1)

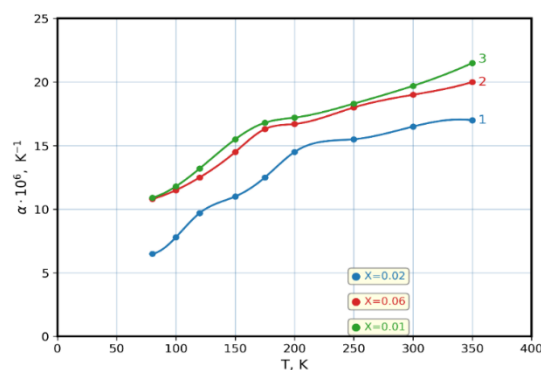


Figure 5. Temperature dependence of the isothermal compressibility coefficient of $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ solid solutions (the symbols are the same as in Figure 1)

It follows from the figure that for the single-crystal sample of TlInS_2 , two anomalies are observed, which correspond to the temperature range of the ferroelectric and incommensurate commensurate transitions [15]. For polycrystalline TlInS_2 , only one anomaly is observed on the curve, covering a wider temperature range, and the even boundary of anomalies observed in the case of a single-crystal sample disappears. The changes in the anomaly in the single-crystal and semi-crystalline samples of TlInS_2 that we have discovered can also be associated with the influence of the “random field” and “random temperature” defects, since these defects create non-zero values of the order parameter independent of symmetry. In this connection, an electric field is created that strongly affects the incommensurate-commensurate phases.

From the standpoint of interatomic interaction mechanisms, the anomalies observed in TlInS_2 reflect the softening of certain phonon modes associated with the structural instability of the layered monoclinic lattice near the ferroelectric transition. The high concentration of stoichiometric vacancies ($\sim 10^{20} - 10^{22} \text{ cm}^{-3}$) inherent to TlInS_2 plays a decisive role: these point defects generate local electric fields and random strain fields that couple to the order parameter of the incommensurate modulation. The complete suppression of anomalies in solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ can be attributed to the disruption of long-range structural order upon substitution of In^{3+} by Gd^{3+} ions. The larger ionic radius of Gd ($R_{\text{Gd}} = 0.96 \text{ \AA}$) compared to In ($R_{\text{In}} = 0.92 \text{ \AA}$) introduces local lattice distortions that pin the incommensurate modulation and prevent the cooperative atomic displacements required for the phase transitions observed in the parent TlInS_2 compound. The monotonic increase of α_L and χ_T with growing TlGdS_2 content is consistent with the progressive weakening of interatomic bonding and the increase in anharmonicity confirmed by the observed decrease in the Debye temperature.

The results of the studies of the temperature dependence of the linear thermal expansion and isothermal compressibility (α_L and χ_T) of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ where $0 \ll x \ll 0.1$ at $80 - 400 \text{ K}$ are shown in Figure 4, 5. It is evident that no anomalies are observed in the temperature dependences of α_L and χ_T in the studied temperature range. This indicates that there are no phase transformations in the specified temperature range. As follows from Figure 4, 5, in all the crystals studied, the nature of the temperature dependence of both α_L and χ_T is almost the same, i.e., at relatively low temperatures, α_L increases with increasing temperature and, starting from $\sim 210 \text{ K}$, the growth of α_L somewhat weakens and gradually comes to a constant value. This behavior of α_L and χ_T in solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ is explained by the identity of the types of crystal structure and chemical bonds between atoms. In order to identify the temperature, increase of α_L , the degrees of temperature dependence of α_L are determined graphically at different temperature ranges $80 \leq T \leq 200 \text{ K}$. At $x = 0$, $\alpha_L \sim T_{0.81}$; $x = 0.02$, $\alpha_L \sim T_{0.86}$; $x = 0.05$, $\alpha_L \sim T_{0.92}$; $x = 0.10$, $\alpha_L \sim T_{0.95}$. Such a large change in the degree of temperature dependence of α_L in solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ is explained by the fact that during thermal expansion, along with a change in the size of the unit cell, the amplitude of oscillations of atoms in the crystal lattice also changes, which in turn leads to a change in the anharmonicity value.

The experimental data obtained by us on the values of α_L TlInS_2 and various compositions of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ are used to calculate the Debye temperature (θ_D) and the root-mean-square dynamic displacements of atoms ($\sqrt{\bar{u}^2}$) according to the following equations:

$$\theta_D = \frac{14.37}{(\bar{A} \cdot V^{3/2} \cdot \alpha)^{1/2}}; \quad (1)$$

$$\sqrt{u^2} = \frac{4.3 \cdot 10^{-14} [D(\theta_D / T)(\theta_D / T) + 1/4]}{\bar{A} \theta_D}, \quad (2)$$

where α_L is the coefficient of linear thermal expansion, $\bar{A}$ is the average atomic mass, V is the average atomic volume, $D(\theta_D / T)$ is the Debye function. The calculation data for the values of (θ_D) and $(\sqrt{u^2})$ using expressions (1) and (2) are presented (Table 2).

Table 2

The value of the Debye temperatures and the root-mean-square dynamic displacements of atoms in the crystal lattice of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$

T, K	x = 0		x = 0.02		x = 0.05		x = 0.10	
	θ_D , K	$\sqrt{u^2}$, Å	θ_D , K	$\sqrt{u^2}$, Å	θ_D , K	$\sqrt{u^2}$, Å	θ_D , K	$\sqrt{u^2}$, Å
80	335	0.066	392	0.072	323	0.080	313	0.084
100	314	0.075	353	0.081	306	0.091	300	0.093
120	290	0.085	325	0.092	292	0.101	283	0.104
140	266	0.098	302	0.103	280	0.111	269	0.115
160	240	0.113	285	0.115	270	0.120	260	0.126
180	206	0.139	272	0.126	263	0.131	252	0.137
200	182	0.166	264	0.136	257	0.141	245	0.148
220	178	0.177	259	0.145	253	0.149	240	0.160
240	220	0.115	256	0.153	250	0.158	236	0.168
280	174	0.120	255	0.167	248	0.172	232	0.185
310	171	0.122	254	0.175	247	0.179	230	0.196
350	170	0.123	253	0.187	246	0.194	228	0.210

It is evident that when replacing indium atoms with gadolinium atoms, the mean square dynamic displacement of atoms in the crystal lattice increases, and the Debye temperature decreases by $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$. The change in the Debye temperature with temperature indicates a deviation of the phonon spectrum from the Debye model.

Based on the experimental data on the isothermal compressibility coefficient, some elastic parameters for solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ are also calculated using the formulas given: Young's modulus (E)

$$E = \left(\frac{\theta_D \cdot m^{1/3} \cdot \rho^{1/6}}{1.6818 \cdot 10^3} \right)^{1/2}, \text{ shear modulus } (\mu) \mu = \frac{E}{2(1+\sigma)}, \text{ Poisson's ratio } (\sigma) \sigma = 1 - \left(\frac{E}{3K} \right) \text{ and the velocity of propagation of longitudinal ultrasonic waves } (\vartheta_e) \vartheta_e = \sqrt{\frac{E}{\rho}}, \text{ where } \theta_D \text{ is the Debye temperature, } \rho \text{ is the density, } m \text{ is the mass.}$$

ty of propagation of longitudinal ultrasonic waves $(\vartheta_e) \vartheta_e = \sqrt{\frac{E}{\rho}}$, where θ_D is the Debye temperature, ρ is the density, m is the mass.

The calculation results are given. It is evident from Table 3 that with the increase of the TlGdS_2 content in TlInS_2 the elastic parameters E , μ , ϑ_e . (σ -slightly changes) decrease. This allows us to conclude that with the increase of the TlGdS_2 content in TlInS_2 the chemical bond between the atoms in the solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ changes significantly, which leads to a large change in the degree of anharmonicity of thermal vibrations (Table 3). The uncertainties in the calculated elastic parameters are determined primarily by the measurement errors of the experimental quantities: the error in α_L is $\sim 1.45\%$ and in χ_T is $\sim 4.5\%$, as indicated in the Experimental section. Error propagation through formulas (1) and (2) yields an estimated uncertainty of $\sim 3\%$ for θ_D and $\sim 5\text{--}6\%$ for $\sqrt{u^2}$. For the elastic moduli, the combined uncertainty is approximately $5\text{--}8\%$. These values are consistent with the typical accuracy reported for similar chalcogenide systems in the literature [16]. A comparison of the obtained Debye temperatures (228–392 K depending on composition and temperature) with values reported for structurally related compounds TlGaSe_2 (~ 220 K) and TlInSe_2 (~ 240 K) [17] confirms the physical reasonableness of the calculated parameters.

Table 3

Values of Young's modulus, shear modulus, Poisson's ratio and the velocity of longitudinal ultrasonic waves of solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$

T, K	$x = 0.02$				$x = 0.05$				$x = 0.10$			
	E, GPa	σ	μ , GPa	ϑ_e , m/c	E, GPa	σ	μ , GPa	ϑ_e , m/c	E, GPa	σ	μ , GPa	ϑ_e , m/c
80	513.1	0.458	176.0	9479	349.6	0.470	118.9	7800	331.2	0.472	112.7	7541
90	459.6	0.463	157.1	8972	330.4	0.472	112.3	7583	316.6	0.473	107.8	7373
100	416.1	0.466	141.9	8537	313.8	0.473	106.5	7390	304.3	0.475	103.6	7228
120	352.7	0.471	110.9	7859	285.7	0.475	96.8	7051	270.8	0.476	91.9	6819
140	304.6	0.475	97.1	7304	262.8	0.477	89.0	6763	244.7	0.479	82.9	6482
160	271.2	0.478	87.3	6892	244.3	0.479	82.6	6520	228.6	0.480	77.7	6265
180	247.1	0.479	82.4	6578	231.8	0.480	78.3	6351	214.7	0.482	72.6	6072
200	232.7	0.480	78.6	6384	221.5	0.480	74.8	6209	203.0	0.483	68.6	5904
210	227.5	0.481	76.8	6312	217.9	0.481	73.6	6158	198.0	0.483	67.0	5831
220	224.0	0.481	75.6	6263	214.5	0.481	72.4	6111	194.8	0.484	65.9	5783
240	218.8	0.482	73.9	6190	209.4	0.482	70.6	6037	188.3	0.484	63.6	5686
280	217.1	0.483	73.3	6166	206.1	0.483	69.6	5989	182.0	0.484	61.5	5590
310	215.4	0.484	72.7	6142	204.5	0.484	69.1	5966	178.9	0.485	60.4	5542
350	213.7	0.485	72.1	6118	202.8	0.485	68.5	5941	175.8	0.485	59.4	5494

The temperature dependence of the bandgap of the applied solid solutions ($E_g(T)$) is studied. For this, the empirical formula shown in [18, 19] is used:

$$E_g(T) = E_g(0) - \frac{\gamma\theta}{2} \sqrt{1 + \frac{\pi^2}{6} \left(\left(\frac{2T}{\theta} \right)^2 + \left(\frac{2T}{\theta} \right)^4 - 1 \right)}. \quad (3)$$

Here γ — constant is $\gamma = 3.7 \cdot 10^{-4}$. θ — temperature is found from the relation $\theta = \frac{3}{4}\theta_D$ — Debay temperature (Table 2). The result of the calculation is given in Figure 6 (solid line). As can be seen, with the increase in the amount of TlGdS_2 in TlInS_2 , the value of $E_g(T)$ decreases. In all compositions, the value of $E_g(T)$ increases with the decrease in temperature.

In order to verify the accuracy of the obtained results, the value of $E_g(T)$ is also calculated for the $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ solid solutions at different temperatures using the value $\frac{\partial E_g}{\partial T} = -6 \cdot 10^{-4} \sum \nu / K$, which is found based on the experimental values of photoconductivity. The calculation is carried out using the following empirical formula.

$$E_g(T) = E_g(0) - \frac{\partial E_g}{\partial T} \cdot \frac{T^2}{(T + \theta_D)}. \quad (4)$$

The obtained results are shown in Figure 6 (with the Δ -symbol). As can be seen from the figure, the values calculated for $E_g(T)$ by formulas (3) and (4) coincide with each other and lie on a straight line. This change in the band gap with composition and temperature can be explained by the increase in defects and the weakening of the chemical bond between atoms due to the increase in the amount of TlGdS_2 in solid solutions.

The values of the specific heat capacity at constant volume (C_V) of the solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ are calculated using the experimental values of the specific heat capacity at constant pressure (C_p) [20].

$$C_V = C_p - \frac{9\alpha^2 VT}{\mu T}. \quad (5)$$

The results of the calculation are given in Table 4. As can be seen from the table, the band gap of the investigated solid solutions at different temperatures, the temperature dependence of the electrical conductivity, and the values calculated using (3) and (4) are in good agreement. With increasing temperature, the value of C_V varies for different compositions (Table 4).

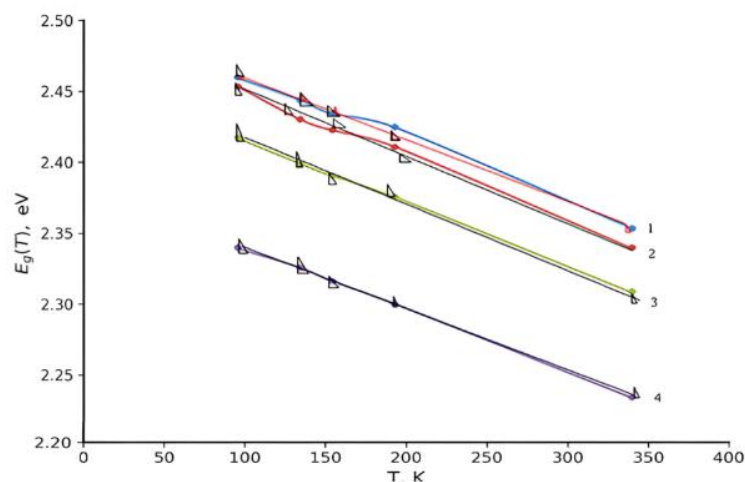


Figure 6. Temperature dependence of the bandgap of $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ solid solutions (1 — $x = 0$; 2 — $x = 0.02$; 3 — $x = 0.05$; 4 — $x = 0.10$)

Table 4

Zone and thermal parameters of $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ solid solutions

Example	E_{g0} , eV $\lg \sigma = f(10^3/T)$	T , K	$E_g(T)$, eV (Eq. 3)	$E_g(T)$ (Eq. 4)	C_p $c/kq \cdot K$	C_v $c/kq \cdot K$
$x = 0.02$	2.510	100	2.467	2.486	219.5	217.4
		140	2.445	2.473	244.3	238.8
		160	2.438	2.465	252.1	244.2
		200	2.427	2.448	264.9	251.8
		350	2.360	2.378	279.8	251.2
$x = 0.05$	2.482	100	2.433	2.455	228.7	228.3
		140	2.416	2.442	253.2	252.4
		160	2.408	2.434	260.6	259.6
		200	2.394	2.417	272.6	270.9
		350	2.331	2.346	285.1	281.1
$x = 0.10$	2.413	100	2.360	2.425	246.4	243.9
		140	2.347	2.411	268.3	263.1
		160	2.338	2.403	274.5	267.7
		200	2.323	2.370	286.1	275.5

Conclusion

Using X-ray diffraction and chemical analysis, the solid-solution region in the $\text{TlInS}_2 - \text{TlGdS}_2$ system based on TlInS_2 is established to extend up to 10 mol% of TlGdS_2 at room temperature. The solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$, like TlInS_2 itself, crystallize in the monoclinic system. The observed anomalous behavior of electrical conductivity and the Hall coefficient in the solid solutions is associated with impurity-related hopping conductivity. The band gap decreases with increasing TlGdS_2 content in the solid solutions. A phase transition is detected in the temperature dependence of the thermal expansion coefficient and isothermal compressibility of TlInS_2 . It is shown that, in all the studied solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$, no phase transformation occurs within the temperature range 77–400 K. With increasing TlGdS_2 content in TlInS_2 , the values of the thermal expansion coefficient and isothermal compressibility increase at all investigated temperatures. For TlInS_2 and its solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$, the Debye temperatures, mean-square dynamic displacements in the crystal lattice, the difference between specific heat capacities at constant pressure and constant volume, Young's modulus, shear modulus, Poisson's ratio, and the propagation velocity of longitudinal ultrasonic waves are calculated. The calculation results indicate that with increasing TlGdS_2 content in TlInS_2 , the chemical bonding between atoms in the solid solutions $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ changes significantly, leading to a pronounced modification in the degree of anharmonicity of thermal vibrations. It is shown that there is good agreement between the experimental and calculated values of $E_g(T)$.

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 $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ қатты ерітінділеріндегі температуралық эффектілер

$\text{TlInS}_2 - \text{TlGdS}_2$ жүйесінің қорытпалары синтезделіп, олардың монокристалдары Бриджмен әдісімен өсірілді. Рентгенқұрылымдық зерттеулер TlGdS_2 қосылысының TlInS_2 құрамындағы ерігіштік аймағын анықтады. TlInS_2 және $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ ($0 \leq x \leq 0.10$) қатты ерітінділерінің сызықтық жылулық ұлғаю коэффициенті (α_L) мен изотермиялық сығылғыштығы (χ_T) 80–400 К температура аралығында зерттелді. α_L және χ_T тәжірибелік мәндері негізінде Дебай температурасы, атомдардың орташа квадраттық ығысуы, Юнг модулі, ығысу модулі, Пуассон коэффициенті және $C_p - C_v$ айырмасы есептелді. Тыйым салынған аймақ ені электрөткізгіштіктің температуралық тәуелділігі бойынша анықталып, жылулық және оптикалық әдістермен алынған мәндермен салыстырылды. Электрөткізгіштіктің аномальды тәртібі тыйым салынған аймақтағы локальданған күйлер мен стехиометриялық вакансияларға байланысты секірмелі өткізгіштікпен түсіндірілді. TlInS_2 қосылысынан айырмашылығы, зерттелген қатты ерітінділерде 80–400 К аралығында фазалық ауысулар байқалмады. TlGdS_2 мөлшерінің артуы жылулық ұлғаю мен сығылғыштық коэффициенттерінің өсуіне әкеліп, атомаралық байланыстардың әлсіреуін және жылулық тербелістер ангармониясының күшеюін көрсетті. Алынған нәтижелер қабатты халькогенидті жартылай өткізгіштердегі кристалдық құрылым, химиялық байланыс және физикалық қасиеттер арасындағы өзара байланысты анықтайды.

Кілт сөздер: қатты ерітінділер, сызықтық жылулық ұлғаю, изотермиялық сығылғыштық, ығысу модулі, ангармониялық, тыйым салынған аймақ ені, фотөткізгіштік, монокристалдар, Бриджмен әдісі, рентгенқұрылымдық талдау

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Температурные эффекты в твердых растворах $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$

Сплавы системы $\text{TlInS}_2 - \text{TlGdS}_2$ были синтезированы, а их монокристаллы выращены методом Бриджмена. Рентгеноструктурные исследования позволили установить область растворимости TlGdS_2 в TlInS_2 . Коэффициент линейного теплового расширения (α_L) и изотермическая сжимаемость (χ_T) TlInS_2 и твердых растворов $(\text{TlInS}_2)_{1-x}(\text{TlGdS}_2)_x$ ($0 \leq x \leq 0.10$) исследованы в интервале температур 80–400 К. На основе экспериментальных значений α_L и χ_T определены температура Дебая, среднеквадратичное смещение атомов, модуль Юнга, модуль сдвига, коэффициент Пуассона и разность теплоемкостей $C_p - C_v$. Ширина запрещенной зоны рассчитана по температурной зависимости электропроводности и сопоставлена со значениями, полученными тепловыми и оптическими методами. Аномальное поведение электропроводности объясняется прыжковой проводимостью, связанной со стехиометрическими вакансиями и локализованными состояниями в запрещенной зоне. В отличие от TlInS_2 , в исследованных твердых растворах в диапазоне 80–400 К фазовые переходы не обнаружены. Увеличение концентрации TlGdS_2 приводит к росту коэффициентов теплового расширения и сжимаемости, что свидетельствует об ослаблении межатомных связей и усилении ангармоничности тепловых колебаний. Полученные результаты выявляют взаимосвязь между кристаллической структурой, химической связью и физическими свойствами слоистых халькогенидных полупроводников.

Ключевые слова: твердые растворы, линейное тепловое расширение, изотермическая сжимаемость, модуль сдвига, ангармоничность, ширина запрещенной зоны, фотопроводимость, монокристаллы, метод Бриджмена, рентгеноструктурный анализ

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