

ENERGY OF CRYSTAL LATTICE THERMAL OSCILLATIONS IN TlGaS₂ SEMICONDUCTOR COMPOUND

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This article presents the results of a study of the temperature dependences of the coefficients of thermal expansion and isothermal compressibility of the ternary compound TlGaS₂. In the studied temperature range (80-400 K), no anomalies were found in the temperature dependences of these properties. The thermal expansion coefficient of the TlGaS₂ semiconductor compound is calculated based on empirical formulas including Debye temperature and Debye functions, and the average energy of the crystal lattice is calculated and its temperature dependence is tabulated. It was shown that the energy of the crystal lattice depends on the degree of anharmonicity of the oscillations.

Keywords: Semiconductor; Thermal expansion; Thermal oscillation; Crystal lattice; Debye temperature; Young's modulus; Anharmonicity

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INTRODUCTION

The class of thallium chalcogenide compounds of $TlB^{III}C_2^{VI}$ ($B = In, Ga, C = S, Se, Te$) exhibits a layered-chain structure, is classified as 2D crystals and is characterised by anisotropic physical properties [1]. These compounds are characterized by weak van der Waals bonding between layers and covalent bonding within each layer. The charge carriers in $TlB^{III}C_2^{VI}$ single crystals can move within the layers, while their motion between the layers is restricted by van der Waals interaction. Crystals of this family are of not only scientific but also significant practical interest, since they are optically active, have high photosensitivity in a wide spectral range and, as a result, are promising for use in optoelectronics.

The ternary compound $TlGaS_2$ belongs to a large group of layered crystals of the $TlB^{III}C_2^{VI}$ type exhibiting both semiconductor and ferroelectric properties, and crystallizes into a monoclinic structure in the space group C_{2h}^h ($C 2/c$) with unit cell parameters $a = 10.299 \text{ \AA}$, $b = 10.284 \text{ \AA}$, $c = 15.175 \text{ \AA}$, $\beta = 99.603^\circ$ [2, 3]. $TlGaS_2$ is a p -type wide bandgap layered semiconductor with melting point $T_{melt} = 1165 \text{ K}$, possesses a wide range of practically important physical characteristics such as high photo- and X-ray sensitivity. On the temperature dependences of various physical parameters of this compound, sharp peaks are observed. Sharp increases in the values of thermal parameters are often due to the temperature dependence of the Gruneisen parameter in these substances. The role of optical phonons in phonon-phonon scattering increases in these cases [4].

To assess the nature of chemical bonding and the dynamics of thermal oscillations in layered semiconductors, it is important to investigate the temperature dependences of thermal parameters. In complex semiconductor compounds, these dependencies are due to the degree of anharmonicity of crystal lattice vibrations, transverse and longitudinal acoustic phonons, as well as optical phonons.

Analysis of literature data shows that $TlGaS_2$ is a perspective semiconductor material in terms of practical applications [5, 6, 7, 8]. To elucidate the temperature range of applicability of a given material, it is necessary to know the thermal and thermodynamic properties in addition to the electrical properties. The coefficients of thermal expansion and isothermal compressibility are such parameters. These parameters are significant and informative characteristics of solids that are related to the thermodynamic and structural characteristics of the material. The objective of the present work is to investigate the temperature dependences of thermal expansion and isothermal compressibility coefficients of $TlGaS_2$, basing on experimental investigations of thermal properties of crystals to determine the Debye function, the energy of zero-point vibrations in the lattice, the values of average lattice energy and the Debye temperature.

EXPERIMENTAL METHOD

The samples were synthesized from the elements taken in stoichiometric ratios by their direct fusion in quartz ampoules evacuated to 10^{-3} Pa at 1180 ± 5 K for 5–7 h. High purity chemical elements were used as initial components: Tl (Tl00), Ga (Ga 5N), S (HP 165). During the synthesis process, the ampoules were shaken frequently to ensure better mixing of the components. The samples based on $TlGaS_2$ were annealed in vacuum at 750 K for 120 h in order to homogenize. Homogenizing annealing of the resulting single-phase samples was carried out in a spectrally pure argon environment. The annealed alloys were cooled to room temperature in a switched-off furnace mode. Completeness of synthesis and homogeneity of the obtained samples, as well as their individuality, were controlled by DTA and XRD methods. The single crystals of materials investigated by us were grown applying a modified Bridgman method – a method of slow cooling at a constant temperature gradient along the ingot. The structural and morphological properties of $TlGaS_2$ thin films were investigated by XRD, SEM and AFM techniques.

The angular positions of the diffraction spectrum lines of the synthesized $TlGaS_2$ samples were recorded on a Bruker D8 ADVANCE X-ray diffractometer in 40 kV, 40 mA mode with $CuK\alpha$ -radiation ($\lambda = 1.5406$ Å) on a 450K TTC type temperature chamber. Samples for measurements were prepared by grinding crystals and their subsequent pressing in a special holder. Diffraction reflections were recorded in the range 2θ 0–90°, indexed by the TOPAS program, and crystallographic parameters refined by using EVA program. To study the morphology and microcomposition of the sample surface, a scanning electron microscope of Japanese brand JEOL JSM6610-LV was used.

Cleavage along the basal plane (001) $TlGaS_2$ was carried out immediately before the experiments. Electron diffraction patterns and micrographs were taken on freshly cleaved surfaces. AFM surface micrographs were obtained for 3–5 samples, from which the clearest images reflecting the general trend were selected.

Measurements of the coefficient of thermal expansion (α_L) and isothermal compressibility ($T\chi$) were carried out using the dilatometric setup described in [9, 10]. For these measurements, cylindrical samples with a length of 0.03 m and a diameter of 0.005 m were made from synthesized ingots. The measurements were carried out in a direction perpendicular to the layers. The relative measurement error was 0.5%.

RESULTS AND DISCUSSION

The X-ray pattern of $TlGaS_2$ recorded at offset angle 2θ in the range of 0–90°, is depicted in Figure 1a). Analysis of the intensities of X-ray reflections shows the presence of a predominant direction in the crystal, as well as that the investigated sample consists of a single phase. It is evident that the diffraction peaks in the control pattern of the sample appeared at $2\theta = 24.35^\circ, 36.15^\circ$ and 48.45° . These peaks are associated with the (400), (–422) and (215) planes, respectively. Diffraction patterns recorded from different areas of single crystals corresponded to the monoclinic syngony. The unit cell parameter calculated by the least squares method for the reflections is $a = 10.299$ Å, $b = 10.284$ Å, $c = 15.175$ Å, $\beta = 99.603^\circ$, agreeing satisfactorily with the results of [11, 12].

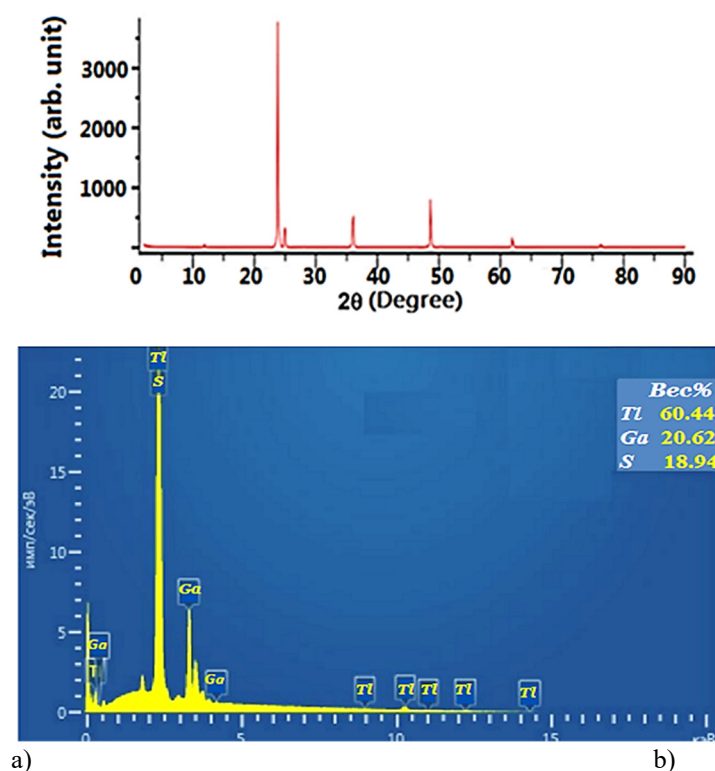


Figure 1. a) X-ray diffraction pattern of the $TlGaS_2$ crystal; b) microanalysis of the crystal surface

Quantitative X-ray microanalysis determined the phase composition and distribution of chemical elements on the surface of the investigated sample (Fig. 1b). Analysis of the obtained results shows the homogeneity of the surface, but with a change in stoichiometry within the homogeneity region $TlGaS_2$ towards the excess of thallium.

The results of microprobe X-ray spectral analysis showed that the content of elements in the grown single crystals corresponds to the formula - $[Tl] : [Ga] : [S] = 1 : 1 : 2$.

A two-dimensional image of $TlGaS_2$ single crystals obtained by magnifying a relatively homogeneous surface area $5 \cdot 10^3 \times 5 \cdot 10^3 nm$ in an atomic force microscope is presented in Fig. 2. a). Fig. 2.b). shows a volumetric description of a part with a relatively uniform relief on the surface of this single crystal. As is clear from the figure, the surface of $TlGaS_2$ single crystal is quite homogeneous and smooth.

Although the $TlGaS_2$ single crystal is a layered crystal, certain irregularities are observed on the natural fracture surface. Analysis of the histogram of the atomic force microscope image shows that the natural surface of the $TlGaS_2$ single crystal is varied in a uniform arrangement of $25 nm$. The average grain size is $55 nm$. The observed certain roughness in the boundary layer is most likely associated with the presence of weak van der Waals forces between the layers. In the process of separation, groups of atoms, rather than individual atoms, remain on the crystal surface [13].

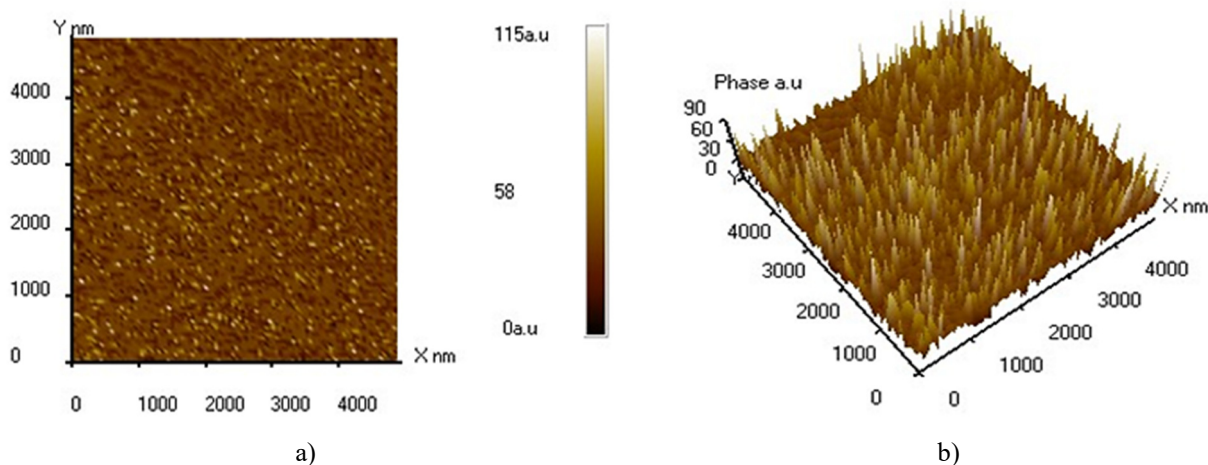


Figure 2. 2D (a) and 3D (b) images of $TlGaS_2$ single crystal surface

The measurement results of the coefficient of linear thermal expansion (CLTE) are presented in Fig. 3. Analysis of the obtained results demonstrates that α_L in the temperature range $80 - 220 K$ increases sharply from $3.8 \cdot 10^{-6}$ to $9.9 \cdot 10^{-6} K^{-1}$, and above ($260 - 300 K$) the growth of α_L slows down and depends weakly on temperature, and with further temperature increase remains almost constant. This behavior of α_L is probably related to the change in the degree of anharmonicity of thermal vibrations of atoms in single crystals of the ternary compound $TlGaS_2$.

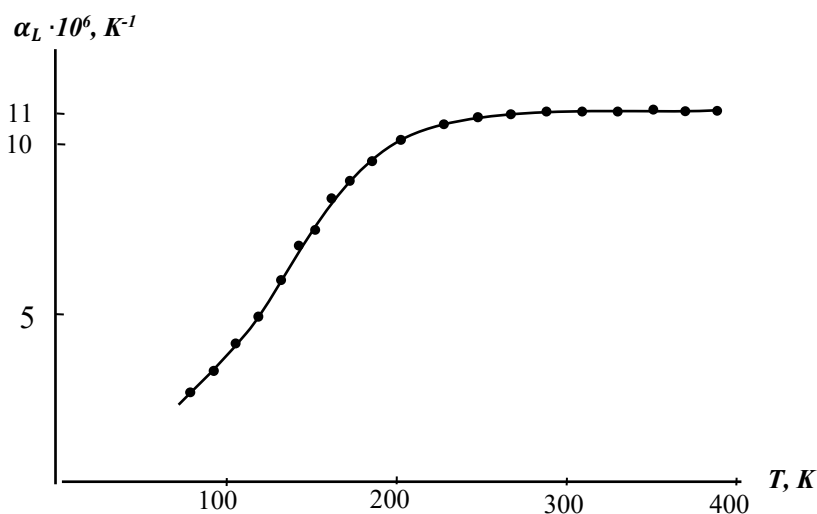


Figure 3. Temperature dependence of the coefficient of thermal expansion of $TlGaS_2$

The CLTE of solids is due to the anharmonicity of the resulting interaction potential of atoms in the crystal lattice. The CLTE is known to be directly proportional to the anharmonicity coefficient [14,15]. Therefore, a sharp increase in

CLTE in the temperature range 80 – 220K and a slight change in its relatively high temperatures is caused by a change in the coefficient of anharmonicity of thermal atomic vibrations in the crystal lattice. Since at low temperatures, the degree of temperature dependence of the vibration coefficient in the TlGaS₂ lattice is greater than that at relatively high temperatures. The Gruneisen constant, which is a measure of the anharmonicity of atomic vibrations, decreases with increasing temperature, and starting at a temperature of ~280 K, it practically remains constant [16].

The isothermal compressibility measurement results of TlGaS₂ in the temperature range of 80 – 400 K are presented in Fig. 4. It is evident from the figure that in the entire investigated temperature range, the isothermal compressibility coefficient χ_T increases slightly from $6.4 \cdot 10^{-12} \frac{m^2}{N}$ to $6.9 \cdot 10^{-12} \frac{m^2}{N}$ as the temperature increases.

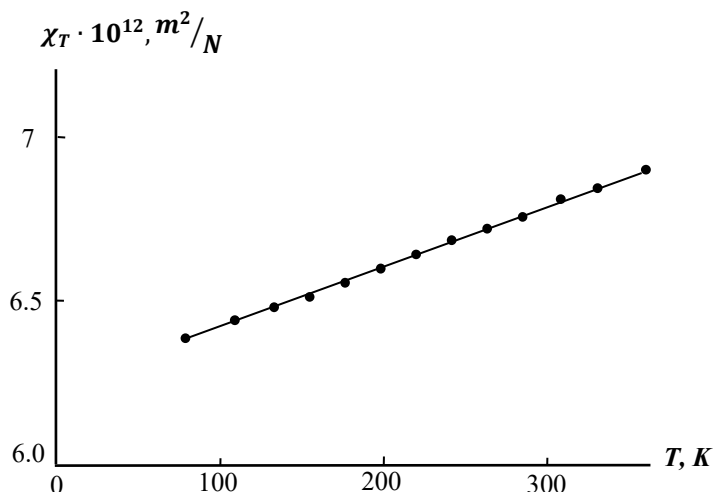


Figure 4. Temperature dependence of the isothermal compressibility coefficient of TlGaS₂

A comparison of CLTE and isothermal compressibility shows that changes in CLTE are considerably larger in magnitude than changes in the isothermal compressibility coefficient. In the temperature range 80-400 K, the increase in the isothermal compression coefficient is 8%, and in this range an increase in CLTE of more than 3 times is observed. This significant change of CLTE in the investigated temperature range in comparison with isothermal compressibility is associated with the fact that thermal expansion also changes the amplitude of vibrations of atoms in the crystal lattice, which in turn leads to isothermal compressibility.

It is apparent from Figures 3 and 4 that no anomalies are noticed in the temperature dependences of the coefficient of linear thermal expansion and isothermal compressibility in the analyzed temperature range. This confirms that no phase transformations are present in the indicated temperature range.

As is known, a number of physical properties of crystalline bodies depend greatly on the value of the interaction energy between the atoms and molecules that make up it. As the temperature increases, the vibrational motion of the atoms that make up the crystal lattice also increases, and this, in turn, leads to an increase in the energy of the lattice as a whole. Based on the existing theoretical models, the average energy of the crystal can be calculated with the help of thermodynamic parameters [17].

$$W = \frac{9}{8} N k_0 \theta + 3 k_0 N T D \left(\frac{\theta}{T} \right). \quad (1)$$

Here, $W_0 = \frac{9}{8} N k_0 \theta$ - is the energy of the zero-point oscillations of the lattice, θ - Debye temperature, N - is the Avogadro number, k_0 - is the Boltzmann constant, T - is the absolute temperature, and $D(\theta/T)$ - is the Debye function. The value of the Debye temperature is determined from the expression

$$\theta = \frac{h \nu_{max}}{k_0}. \quad (2)$$

Here h - Planck's constant, ν_{max} - is the maximum frequency of thermal oscillations of atoms. The value of this frequency

$$\nu_{max} = \frac{1}{2\pi} \sqrt{\frac{\beta}{m}}, \quad (3)$$

is determined from the expression. Here β - is the coefficient of the harmonic oscillation limits, m - is the mass of the atom. The value of β can be determined using values of Young's modulus (E) and lattice parameter a_0 [18]. In this case

$$E \frac{\Delta\alpha}{a_0} = \frac{F}{a_0^2}, \tag{4}$$

$$F = -\beta\Delta\alpha, \tag{5}$$

equations are used.

In the existing literature, the values of E , β and ν_{max} have been reported for solids that crystallize in the cubic structure. As a result of the calculations, a value of approximately 10^{13} Hz was obtained for the ν_{max} value, as shown in Einstein's theory. It is interesting from both theoretical and practical point of view how useful these expressions are for complex semiconductor compounds.

In this study, using the values of the Debye characteristic temperature (θ_D) and Young's modulus (E) calculated based on the experimental values of the thermal expansion coefficient for the TlGaS₂ semiconductor compound, the energy of the zero-point oscillations of the crystal lattice and the values of the average energy of the lattice as a whole were determined. The Debye characteristic temperature and Young's modulus values were calculated using existing empirical formulas [19, 20].

$$\theta_D = \frac{19.37}{\sqrt{AV^{2/3}\alpha}}, \tag{6}$$

and

$$\theta_D = \frac{1.6818 \cdot 10^3 \sqrt{E}}{M^{1/3} \rho^{1/6}}. \tag{7}$$

Here, the value of Young's modulus is given in units of 10 kg/cm^2 . M - molecular weight, ρ - density, \bar{A} - root mean square atomic mass, V - molar volume, α - coefficient of linear thermal expansion.

It should be noted that the values of θ_D and E calculated from these expressions depend on the temperature according to the change of the value of α .

Since the Debye approximation is used in the reported formula (1), the maximum value of E was taken to find the value of θ . In this case, the calculated zero-point energy for the crystal lattice can be taken as constant. Thus, the average energy of the lattice and its temperature dependence were determined by adding the temperature and the Debye function to this energy each time.

The values of α , $D(\frac{\theta}{T})$, W for the TlGaS₂ compound given in the Table 1. The value of the $D(\frac{\theta}{T})$ - Debye function corresponding to different temperatures is taken from the literature [20].

Table 1. Thermodynamic parameters and values of Debye function of TlGaS₂

T, K	$\alpha, 10^{-6}$ 1/K	$D(\frac{\theta}{T})$	W_0 , J/mol	W , J/mol	θ_D , K
80	3.85	0.521	1972.71	3009.37	325
90	4.29	0.549	1972.71	3206.24	319
100	4.75	0.590	1972.71	3442.98	302
120	5.24	0.651	1972.71	3916.46	276
140	6.42	0.680	1972.71	4345.07	267
160	6.92	0.725	1972.71	4863.42	258
180	7.28	0.765	1972.71	5404.18	243
200	8.21	0.770	1972.71	5810.36	228
220	9.57	0.812	1972.71	6424.41	225
240	9.76	0.835	1972.71	6966.65	222
260	9.89	0.840	1972.71	7415.22	218
280	10.83	0.848	1972.71	7896.68	215
300	10.86	0.854	1972.71	8352.21	212

As can be seen from the table, with the increase in temperature, both the Debye function, but also the average energy of the lattice increases. These increases can be attributed to the anharmonic oscillation of atoms in the crystal lattice.

To confirm this idea, the ratio of the coefficient (γ) characterizing the degree of anharmonicity of oscillations to the square of the coefficient characterizing the degree of harmonicity (β^2) for the TlGaS₂ compound was calculated and presented in the table (Table 2). For this purpose, the formula given in the literature was used [21].

$$\alpha = \frac{\gamma k_0}{a\beta^2}$$

Here, α is the thermal linear expansion coefficient, k_0 is the Boltzmann constant, and a is the lattice parameter.

Table 2. Temperature dependence of the degree of anharmonicity of TlGaS₂

T, K	80	90	100	120	140	160	180	200	220	240	260	280	300
$\frac{\gamma}{\beta^2}, 10^7 N^{-1}$	28.73	31.18	34.53	38.09	46.67	50.31	52.92	62.95	66.57	70.95	72.17	76.73	78.95

As can be seen from the table, the ratio $\frac{\gamma}{\beta^2}$ increases with the increase in temperature. This suggests that the value of the coefficient of thermal expansion is a function $D\left(\frac{\theta}{T}\right)$ and the values of the average energy of the lattice depend on the degree of anharmonic oscillation of atoms.

CONCLUSION

The morphology of natural fracture surfaces of layered TlGaS₂ single crystals grown by the Bridgman method has been investigated. Analysis of the data obtained on a scanning probe microscope has revealed that the root mean square roughness of the film surface is 25 nm, and the average grain size is 55 nm. Temperature dependences of the coefficient of linear thermal expansion and isothermal compressibility exhibit no anomalies, showing that there is no phase transition in the investigated temperature range (80 – 400 K). By calculations based on the experimental values of CLTE, the characteristic Debye temperature decreases with increasing temperature, whereas the value of the average lattice energy and the Debye function increase. It has been shown that these increases are determined by the anharmonicity of vibrations of the atoms of the crystal lattice.

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REFERENCES

- [1] M. Isik, A. Karatay, and N.M. Gasanly, "Structural and optical characteristics of thermally evaporated TlGaSe₂ thin films," *Optical Materials*, **124**, 112018 (2022). <https://doi.org/10.1016/j.optmat.2022.112018>
- [2] W. Henkel, H.D. Hochheimer, C. Carlone, A. Werner, S. Ves, and H.G. Schnering, "High-pressure Raman study of the ternary chalcogenides TlGaS₂, TlGaSe₂, TlInS₂ and TlInSe₂," *Phys. Rev. B*, **26**(6), 3211–3221 (1982). <https://doi.org/10.1103/PhysRevB.26.3211>
- [3] G.E. Delgado, A.J. Mora, F.V. Perez, and J. Gonzalez, "Crystal structure of the ternary semiconductor compound thallium gallium sulfide, TlGaS₂," *Physica B: Condens. Matter*, **391**(2), 385–388 (2007). <https://doi.org/10.1016/j.physb.2006.10.030>
- [4] D.I.Huseynov, M.I.Murguzov, Sh.S.Ismailov Thermal conductivity of Er_xSn_{1-x}Se ($x \leq 0.025$) solid solutions," *Inorganic Materials*, **44**, 467–469 (2008). <https://doi.org/10.1134/S0020168508050063>
- [5] X. Xin, F. Liu, X.-Q. Yan, W. Hui, X. Zhao, X. Gao, Z.-B. Liu, and J.-G.Tian, "Two-photon absorption and non-resonant electronic nonlinearities of layered semiconductor TlGaS₂," *Opt Express*, **26**(26), 33895–33905 (2018). <https://doi.org/10.1364/OE.26.033895>
- [6] Y. Fu, D. He, J. He, X. Han, J. Bai, Y. Wang, and H. Zhao, "Photocarrier dynamics in TlGaS₂ nanoflakes and van der waals heterostructures with hexagonal boron nitride and WS₂ nanoflakes: implications for optoelectronic applications," *ACS Applied Nano Materials*, **3**, 8702–8707 (2020). <https://doi.org/10.1021/acsanm.0c01448>
- [7] B.A. Ünlü, A. Karatay, E.A. Yildiz, T. Dinçbay, H. Ünver, N. Gasanly, and A. Elmali, "Defect assisted nonlinear absorption and optical limiting in amorphous TlGaS_{2(1-x)}Se_{2x} ($0 \leq x \leq 1$) thin films," *Journal of Luminescence*, **241**, 118540 (2022). <https://doi.org/10.1016/j.jlumin.2021.118540>
- [8] S.Delice, M.Isik, N.M. asanly, Thermoluminescence properties and trapping parameters of TlGaS₂ single crystals // *Journal of Luminescence*, 2022, 244, 118714, <https://doi.org/10.1016/j.jlumin.2021.118714>
- [9] A. Say, D. Adamenko, O. Gomonnai, I. Roman, I. Martynyuk-Lototska, and R. Vlokh, "Anisotropy of thermal expansion of TlGaSe₂ crystals," *Phase Transitions*, **92**(9), 824–830 (2019). <https://doi.org/10.1080/01411594.2019.1642475>
- [10] I. Martynyuk-Lototska, O. Mys, A. Say, et al., "Anisotropy of acoustic and thermal expansion properties of TlInSe₂ crystals," *Phase Transitions*, **92**(1), 23–35 (2019). <https://doi.org/10.1080/01411594.2018.1545227>
- [11] B. Gurkan, and S. Berber, "Structural and electronic properties of layered semiconductor chalcogenide crystals: TlGaSe₂, TlGaS₂ and TlInS₂," *J. Indian Chem. Soc.* **96**, 1123–1130 (2019). <https://doi.org/10.5281/zenodo.5643212>
- [12] M. Isik, A. Karatay, A.N. Ech-Chergui, and N.M. Gasanly, "Study of the structural and optical properties of thallium gallium disulfide (TlGaS₂) thin films grown via thermal evaporation," *Physica Scripta*, **97**(7), 075808 (2022). <https://doi.org/10.1088/1402-4896/ac74f0>
- [13] Z. Cicek, S. Yakut, D. Deger, D. Bozoglu, S. Mustafaeva, P. Ismailova, A.A. Hasanov, and K. Ulutas, "Thickness dependence of dielectric properties of TlGaS₂ thin films," *Materials Science in Semiconductor Processing*, **166**, 107733 (2023). <https://doi.org/10.1016/j.mssp.2023.107733>
- [14] Y.S. Touloukian, R.K. Kirby, R.E. Taylor, and T.Y.R. Lee, *Thermal Expansion: Nonmetallic Solids (Thermophysical properties of matter*, vol. 13, (IFI/Plenum, New York, 1977).
- [15] M.S. Barabashko, A.I. Krivchikov, R. Basnukaeva, O.A. Korolyuk, and A. Jeżowski, "Proportional correlation between heat capacity and thermal expansion of atomic, molecular crystals and carbon nanostructures," *Condensed Matter Physics*, **26**(3), 33602 (2023). <https://doi.org/10.5488/CMP.26.33602>
- [16] C. Kittel, *Introduction to Solid State Physics*, 8th ed. (John Wiley & Sons: New York, USA, 2005).
- [17] B.M. Askerov, and S.R. Figarova, *Thermodynamics, Gibbs Method and Statistical Physics of Electron Gases*, (Springer-Verlag, Berlin, Heidelberg, 2010).

- [18] M.T. Cao-Rial, C. Moreno, and P. Quintela, "Determination of Young modulus by using Rayleigh waves," *Applied Mathematical Modelling*, **77**, Part 1, 439-455 (2020). <https://doi.org/10.1016/j.apm.2019.07.051>
- [19] O.L. Anderson, "A simplified method for calculating the Debye temperature from elastic constants," *Journal of Physics and Chemistry of Solids*, **24**(7), 909-917 (1963). [https://doi.org/10.1016/0022-3697\(63\)90067-2](https://doi.org/10.1016/0022-3697(63)90067-2)
- [20] D.C. Wallace, *Thermodynamics of crystals*, (Dover Publications, Wiley, New York, 1998).
- [21] O. Madelung, *Introduction to Solid-State Theory*, (Springer Science & Business Media, 1996).

ЕНЕРГІЯ ТЕПЛОВИХ КОЛИВАНЬ КРИСТАЛІЧНОЇ ГРАТКИ В НАПІВПРОВІДНИКОВІЙ СПОЛУЦІ TlGaS₂
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У статті наведено результати дослідження температурної залежності коефіцієнтів теплового розширення та ізотермічної стисливості потрійної сполуки TlGaS₂. У досліджуваному діапазоні температур (80-400 К) аномалій температурних залежності цих властивостей не виявлено. Коефіцієнт теплового розширення напівпровідникової сполуки TlGaS₂ розраховано на основі емпіричних формул, включаючи температуру Дебая та функції Дебая, а також розраховано середню енергію кристалічної решітки та її температурну залежність які наведені в таблиці. Показано, що енергія кристалічної решітки залежить від ступеня ангармонійності коливань.

Ключові слова: напівпровідник; теплове розширення; теплові коливання; кристалічна решітка; температура Дебая; модуль Юнга; ангармонічність