THERMAL EXPANSION OF $TlInTe_2$, $InGaTe_2$, AND $TlIn_2GaTe_4$ COMPOUNDS

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In the presented article, the temperature dependence of the thermal expansion coefficient of $TlInTe_2$, $InGaTe_2$, and $TlIn_2GaTe_4$ compounds has been investigated, and the obtained results are illustrated based on the corresponding graphs. It has been determined that the differences in the thermal expansion coefficients of these compounds within the same temperature range arise from the complexity of their vibrational spectra. This, in turn, is attributed to the differences in the masses of the constituent atoms and the nature of the chemical bonding between them.

Experimental results have shown that an increase in the statistical weight of halogens in $TlInX_2$ and $TlIn_2GaX_4$ (X = Se, Te) compounds leads to a decrease in the thermal expansion coefficient.

Keywords: thermal expansion coefficient, heat capacity, phase transition, thermal vibrations.
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EXPERIMENTAL SECTION AND DISCUSSION OF RESULTS

With the advancement of science and technology, the demand for complex semiconductor materials with broad functional capabilities is increasing. These materials enable the resolution of new physical and technological problems. From this perspective, one of the leading directions in physics is the investigation of semiconductors containing heavy elements and defect structures that exhibit high thermoelectric efficiency and strain sensitivity.

To determine the nature of the fundamental processes occurring in semiconductor materials, it is essential to study their crystal structure, electrophysical, and thermophysical properties. In the absence of sufficient information in this area, it becomes impossible to develop new devices based on complex semiconductor materials formed on the $A^{III}B^{IV}$-type structural framework.

It is well known that various methods exist for measuring thermal expansion and determiningthermal expansion coefficients of solids. The measurement of thermal expansion is based on dilatometric and

X-ray methods. In dilatometric techniques, changes in the length of the sample are measured as the temperature varies. In this case, the linear thermal expansion coefficient is calculated using the formula

$$\delta = \frac{1}{l_0} \cdot \frac{l - l_0}{\Delta T}$$

where δ -$\Delta T = T_2 - T_1$ the average value of the thermal expansion coefficient within the temperature interval; T_1-the initial temperature; T_2-the final temperature; l and l_0 are the lengths of the sample at temperatures T_2 and T_1.

In X-ray methods, the temperature dependence of the crystal lattice parameters is investigated. In this case, the thermal expansion coefficient is calculated based on the crystal lattice parameters:

$$\delta = \frac{1}{a} \frac{\Delta a}{\Delta T}$$

The measurements were carried out under a vacuum of 0.1 Pa and within the temperature range of (80–400)K using the dilatometric method [1,6]. The samples were prepared in cylindrical form with a height of 30 mm and a diameter of 5 mm. The relative measurement error was 1.5%.

$TlInTe_2$ Compound. $TlInTe_2$ is one of the representatives of ternary compounds. As shown in studies [2,3,4], the crystal structure of the $TlInTe_2$ compound has been determined based on physicochemical analysis and X-ray phase analysis. Articles [4,5,6] present the results of investigations of the electrophysical properties of this compound.

The measurements were mainly carried out in the direction perpendicular to the layers. The obtained results are presented in Figure 1. As can be seen from the graph, at low temperatures the thermal expansion coefficient increases with rising temperature, while at high temperatures it remains practically constant.

No anomalies were observed in the variation of the thermal expansion coefficient within the investigated temperature range. This indicates the absence of any phase transition in the given system.

The temperature-dependent variation of the thermal expansion coefficient in the $TlInTe_2$ crystal is associated with changes in the heat capacity and the anharmonicity parameter of the interatomic bonding.

$InGaTe_2$ Compound. For $InGaTe_2$, the experimental results obtained in the (80–400) K temperature range are presented in Figure 1.

$TlIn_2GaTe_4$ Compound.The lattice parameters of the $TlIn_2GaTe_4$ compound differ significantly from their initial values. It has been established that this process is associated with the formation of a new phase resulting from the rearrangement of atoms. The experimental results obtained for the thermal expansion coefficient in the (80–400) K temperature interval are presented in Figure 1. As can be seen, no anomalies are observed in δ(T) its temperature dependence.

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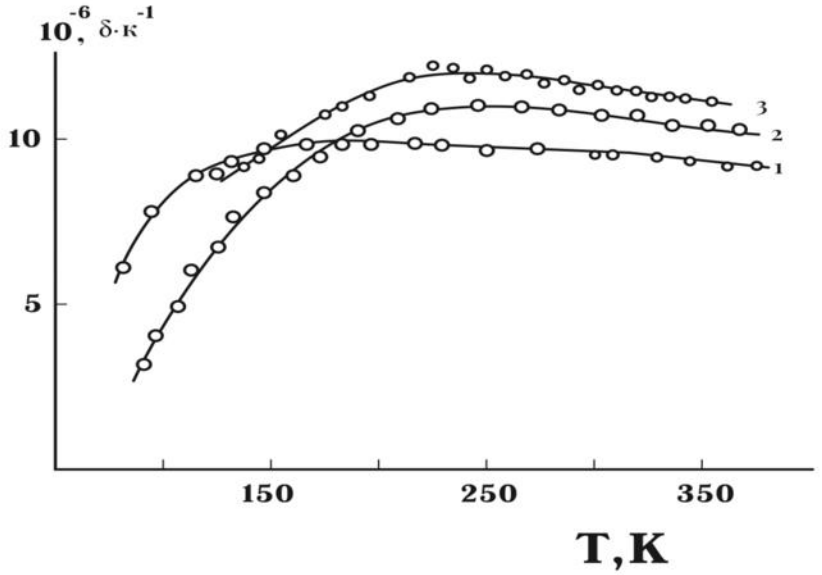

Fig. 1. Temperature dependence of the thermal expansion coefficient:1 — $TlInTe_2$, 2 — $TlIn_2GaTe_4$, 3 — $InGaTe_2$

It is known [5] that the overall value of the thermal expansion coefficient is determined by the combined contributions of electronic, lattice, magnetic, and other components. Typically, the influence of electrons on thermal expansion becomes noticeable only at very low temperatures $T < 0.1\theta$, θ -is the Debye temperature. Thus, in the (150–180) K temperature interval, the "contribution" of the lattice in the $TlIn_2GaTe_4$ compound leads to a noticeable increase in the thermal expansion coefficient. Due to the sharp change in the anharmonicity of thermal vibrations, the value of δ increases significantly in the (80–290) K temperature interval. The thermal expansion coefficient varies from $6.7 \cdot 10^{-6}$ K^{-1} to $20.5 \cdot 10^{-6}$ K^{-1}. This indicates that, within the specified temperature range, the chemical bonding in the $TlIn_2GaTe_4$ compound is mainly dependent on the interatomic distance.

The differences in the thermal expansion coefficients of the studied compounds within the same temperature interval are related to the complexity of their vibrational spectra, which arises from differences in atomic masses and the nature of the chemical bonding.

Experimental results show that in $TlInX_2$ and $TlIn_2GaX_4$ compounds (X = Se, Te), an increase in the statistical weight of halogens leads to a decrease in the thermal expansion coefficient.

CONCLUSION

Based on the conducted research, the following conclusions can be drawn:

1. In the presented article, the temperature dependences of the thermal expansion coefficient of $TlInTe_2$, $TlIn_2$ $GaTe_4$, compounds within the (80–400) K temperature range have been investigated.
2. For each compound, graphs illustrating the temperature dependence of the thermal expansion coefficient have been constructed.
3. The obtained results have been theoretically substantiated.

[1] *I.V. Bodnar, A.A. Feschenko.* Thermal Expansion and Thermal Conductivity of Solid Solutions. Physics and Technique of Semiconductors, 2021, Vol. 2, p. 99–102.

[2] *V.V. Kozinets.* Thermophysical Properties of Solids. Ukraine, Kharkiv University, 2011, 72 p.

[3] *A.M. Ahmedova, G.H. Ismayilova.* Thermoelectric Properties of System Solid Solution. Azerbaijan Journal of Physics (AJP), Vol. 20, № 4, 2014, p. 29–30.

[4] *Kh.O. Sadig, N.M. Suleymanova.* On the Nature of Formation of Ternary Compounds of the Type Tl $A^{III}X_2^{VI}$(A = Ln, In, Ga). Scientific Works. Fundamental Sciences Journal, Baku, 2008, № 2, p. 3–6.

[5] *E.M. Godjaev, Kh.O. Sadygova.* Electrical Properties of Monocrystals. Proceedings of the Russian Academy of Sciences, Inorganic Materials, 1992, Vol. 28.

[6] *E.M. Godjaev.* Dilatometer for Measuring the Thermal Expansion Coefficient of Solids in a Wide Temperature Range. Moscow, Measuring Technique, 1985, № 2, pp. 44–45.

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