EasyChair Preprint

№ 15834

Thermal and Elastic Properties of Compounds TlInX2 (X-S,Se,Te)

Coshgun Bairamov, Naile Sardarova, Sara Sadikova,
Ragib Damiorv and Kifayat Kulieva

February 14, 2025

Thermal and elastic properties of compounds $TlInX_2$ $(X-S,Se,Te)$

C.D.Bairamov, N.S. Sardarova, S.R.Sadikova, R.Y.Damirov* and K.A.Kulieva.

Sumgait State University, Sumgait, Azerbaijan

**Baku State University*

ragibdamirov@bsu.edu.az

Abstract*. The thermal exspansion coefficients of $TlInS_2, TlInSe_2, and\ TlInTe_2$ were measured in the range 77-350K. The data for both single-crystal and polycrystalline imean-square dynamic atomic displacements. In goinq from $TlInS_2, TlInSe_2, and\ TlInTe_2$, the Debye temperature increases and the root-mean-square atomic displacement decreases, which can be attributed to the increase in bond ionic.*

Keywords: *solid solution, layered structure, tetraqonal layerchain structure, scattering mechanism, Debye temperatures, modulus of rigidity.*

It is well known that crystals with layer and chain structures tend to undergo various phase transitions, as exemplified by $TlMX_2$, $(\mathrm{M}-\mathrm{In,Ga;X}-\mathrm{S,Se,Te})$ [1 – 4].

In this work, thermal expansion measurements on TlInS2, TlInSe2 and TlInTe2 in the temperature range from 77 to 350K are used to analyze the infiunce of bonding confiquration on thermal exspansion and phase transitions. The measurements were performed with the equipment described previously [2].

The figure shows the temperature dependences of the thermal expansion coefficient α for $TlInS_2, TlInSe_2, and\ TlInTe_2$. The curves for $, TlInSe_2, and\ TlInTe_2$, the compounds closely similar in crystal structure and chemical bonding, differ insignificantly: α first rises sharply with temperature and then, above 200K, varies little. Both curves show no anomalies.

The α(T) curve for single-crystal $TlInS_2$ shows two anomalies, associated with the ferroelectric and commensurate- incommensurate phase transitions [1 – 4]. The curve for polycrystalline TlInS2 exhibits only one anomaly, extending over a wide temperature range.
Similar anomalies were found earlier in the temperature-dependent heat capacity data for single-crystal and polycrystaline Sn2PrS6[5].

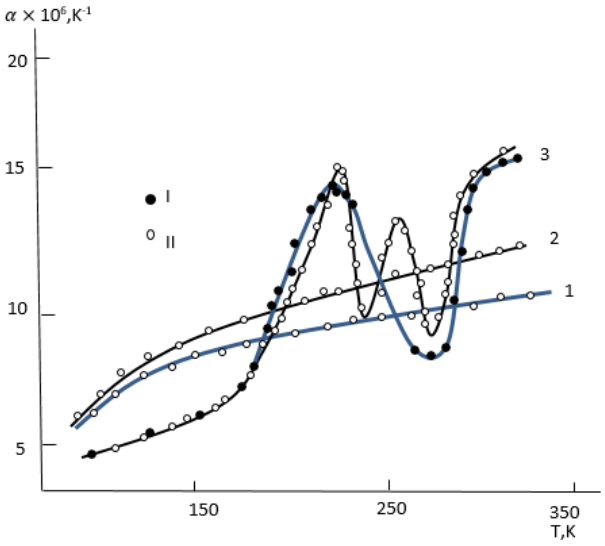
The distinction between the α(T) dependences for single-crystal and polycrystalline $TlInS_2$ is atttributable to “random-field” and “random-temperature” effects[5], which leads to a nonzero order parameter, irrespective of crystal symmetry, and give rise to an electric field strongly affecting commensurate and incommensurate phases.

The anomalies in the α(T) data for $TlInS_2$ are related to distinctive features of its quasi-tetraqonal layerchain structure: in contrast to the chain structure of $TlInSe_2, and\ TlInTe_2$, the anion sheets and cation chains in the structure of $TlInS_2$ are weakly bonded to each other, which facilitates phase transitions.
The α(T) data for $TlInS_2, TlInSe_2, and\ TlInTe_2$ were used to calculate the Debye temperatures θ and rootmean-square dynamic atomic displacements by the empirical formulas [6,7]

$$\theta = \frac{19.37}{\sqrt{\bar{A}\,V^{2/3}\alpha}},$$

$$\sqrt{\overline{U^2}}=4.3\mathrm{x}10^{-14}(\mathrm{D}(\theta/T)/(\theta/T)+1/4)(\bar{A}\theta)^{-1},$$

Where $\bar{A}$ is the root-mean- square atomic weight, V is the atomic volume, and D(θ/T) is the Debye function [7].



Temperature dependences of α for (1) $TlInSe_2$, (2) $TlInSe_2$ and (3) polycrystalline (solid circles) and single-crystal (open circles) $TlInSe_2$.

THERMAL EXPANSION OF $TlInX_2$ $(X - S, Se, Te)$

Calculated Debye temperatures and rms atomic displacements

T,K	θ,K	$\sqrt{\overline{U^2}}$,$\dot{A}$	θ,K	$\sqrt{\overline{U^2}}$, $\dot{A}$	θ,K	$\sqrt{\overline{U^2}}$, $\dot{A}$
	$TlInS_2$		$TlInSe_2$		$TlInTe_2$	
80	335	0.066	380	0.074	476	0.056
90	324	0.070	314	0.082	431	0.061
100	312	0.075	277	0.097	371	0.070
120	290	0.085	264	0.107	337	0.090
140	266	0.098	260	0.114	333	0.088
160	240	0.113	254	0.123	328	0.092
180	206	0.139	252	0.131	324	0.097
200	182	0.166	250	0.139	319	0.103
220	178	0.177	248	0.143	314	0.108
240	220	0.150	247	0.149	307	0.116
260	201	0.173	247	0.156	302	0.123
280	174	0.201	246	0.164	297	0.129
300	172	0.207	245	0.175	289	0.136
350	170	0.230	243	0.181	280	1.153

The results of our calculations are given in the table. Above 160 K, θ increases and $\sqrt{\overline{U^2}}$ decreases in to going from $TlInSe_2$ *to* $TlInTe_2$, which is explainable by the increase in bond ionic.

İn conclusion, the thermal expansion of $TlInX_2$ $(X - S, Se, Te)$ was measured. The temperature dependences of α for both single- crystal and polycrystalline $TlInSe_2$ were found to

exhibit features attributable to ferroelectric and commensurate- studied, θ decreases and $\sqrt{\overline{U^2}}$ increases with increasing temperature.

The elasticity parameters of the triple compounds $TlInS_2, TlInSe_2, and\ TlInTe_2$ are calculated based on the one-dimensional values of their isothermal compression: The difference between heat capacities at constant pressure and constant volume – $C_P - C_V = \frac{\beta^2 VT}{\gamma_T}$ (Here, β=3α, where β is the volumetric expansion coefficient); Young's modulus –

$\sqrt{\mathrm{E}} = \frac{\theta \mathrm{m}^{\frac{1}{3}} \rho^{\frac{1}{6}}}{1{,}6818 \cdot 10^3}$ (Here ρ-is density, m- mass); modulus of rigidity - $\mu = \frac{\mathrm{E}}{3(1-2\sigma)}$ and Poisson's coefficient – $\sigma = 1 - \frac{E}{3k}$ are calculated. The calculation results have shown that during the transition from sulfides to tellurides, the value of Young's modulus decreases, Poisson's coefficient, modulus of rigidity, and the difference between heat capacities at constant pressure and constant volume increase. This further demonstrates that the interatomic chemical bonding strength in compound $TlInS_2$ is smaller compared to that in the $TlInSe_2, and\ TlInTe_2$ crystals.

REFERENCES

1. Volkov. A. A., Goncharov, Yu. T., Kozlov, G.V.., et al.., Structural Phase Transitions in $TlInS_2$ Crystals, Fiz. Tverd. Tela (Leningrad), 1983, vol. 25, no. 12, pp. 3583-3585.
2. Allakhverdiev, K.R., Babaev. S.S., Bakhyshev, N.A., et al., Anormalous Temperature Variation of the Near-Edge Electronic Spectrum of $TlInS_2$,Fiz Tekh. Poluprovodn. (Leningrad), 1984, vol. 18, no. 7, pp. 1307-1309.
3. Gadzhiev, V.A., Kurbanov, M.M., Zeinnalov, N.M., et al., Electroabsorption and Thermal Expansion of β- $TlInS_2$, Izv. Akad. Nauk SSSR, Neorg. Mater., 1990, vol. 26, no. 9, pp. 1325-1327.
4. Aldzhanov, M.A., Guseinov, N.G., and Mamedov, Z.N, Heat Capacity of $TlInS_2$- $TlInSe_2$ Crystals, Fiz. Tverd. Tela Leningrad), 1988, vol.30,no.2,p.580.
5. Rizak, I.M., Rizak, V.M., Vysochanskii, Yu.M., et al., Influence of Defects on the Heat Capacity Anormalies Related to Structural Phase Transitions of Sn_2PrS_6 Type Crystals, Ukr.Fiz. Zh. (Russ. Ed.), 1992, vol.37,no.8, pp. 1262-1268.
6. Sirota, N.N., Fizika i Fiziko- khimicheskii analiz (Physics and Physicochemical Analysis), Moscow: Sudpromgiz, 1957, issue 1.
7. Frantsevich, N.N., Voprosy poroshkovoi metallurgii i prochnosti materialov (Problems in Powder Metallurgy and Materials Strength), Kiev: Akad. Nauk Ukr. SSR, 1956, issue 3.