DEBYE TEMPERATURE AND SOME ELASTIC PROPERTIES OF SOLID SOLUTIONS $(TlGaSe_2)_{1-x}(TlInS_2)_x$ (x=0,1; 0,2)

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The adiabatic compressibility (χ_s), Young modulus (E) and velocity of sound (υ) are calculated by experimental data of thermal expansion coefficient (α) and isothermal compressibility (χ_T) of solid solutions $(TlGaSe_2)_{0,9}(TlInS_2)_{0,1}$ and $(TlGaSe_2)_{0,8}(TlInS_2)_{0,2}$. It is established that adiabatic compressibility increases with temperature increase and Young module and velocity of sound decreases.

Keywords: thermal expansion, isothermal compressibility, Young module, velocity of sound.
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INTRODUCTION

As it is known, the crystals with layer and chain structure have the series of interest physical properties. Such compounds are used in optic quantum generators and different sensitive sensors. The dilatometric and calorimetric investigations show that the phase transition takes place in these crystals [1-3].

Note that information about physical properties, in particular, thermalphysic and elastic characteristics of solid solutions on the base of $A^3B^3C_2^6$ (A - Tl; B – Ga, İn; C – S, Se, Te) compounds aren't enough. The temperature dependences of thermal expansion coefficient (α), isothermal (χ_T), and adiabatic (χ_S) compressibility of solid solutions $(TlGaSe_2)_{0,9}(TlInS_2)_{0,1}$ and $(TlGaSe_2)_{0,8}(TlInS_2)_{0,2}$ in wide temperature interval (90÷300K). The interconnection between isothermal and adiabatic compressibilities with Young modulus and velocity of sound in investigated solid solutions is established on the base of experimental data.

EXPERIMENTAL PART AND RESULT DISCUSSION

The solid solutions $(TlGaSe_2)_{0,9}(TlInS_2)_{0,1}$ and $(TlGaSe_2)_{0,8}(TlInS_2)_{0,2}$ are synthesized by two-temperature method in quartz ampoules evacuated up to 0,033Pa by melting of initial elements of high frequency [3]. The single-phase samples are checked by X-ray method and elementary cell parameters are defined. It is established that solid solutions $(TlGaSe_2)_{1-x}(TlInS_2)_x$ (x=0,1; 0,2) crystallize in monoclinic syngony.The thermal expansion and isothermal compressibility are measured by technique [4] in temperature interval 90÷300K. The samples for measurements are prepared from synthesized ingots of cylindrical form by length 0,3m and dilatometer 0,005m. The error at measurements is 0,5%.

Knowing the values of thermal expansion coefficient (α) and heat capacity at constant pressure (C_p), we caary out the calculations of coefficient difference of isothermal and adiabatic compressibilities (χ_T – χ_S) by thermodynamic formulae [3,5]:

$$\chi_T - \chi_s = \frac{9\alpha^2 VT}{C_p} \qquad (1)$$

where V is molar volume, T is temperature.

At C_p definition we use (C_p – C_v) values calculated from the thermodynamic ratios and by empirical formulae [6,7]:

$$C_p - C_V = \frac{9\alpha^2 VT}{\chi_T} \qquad (2)$$

$$C_P - C_V = 0{,}0214\frac{T}{T_{mel}}C_P \qquad (3)$$

C_p defined by such way, are given in table 1.

Using the experimental data by χ_T and calculated values ($\chi_T - \chi_S$), we obtain χ_S adiabatic compressibilities. χ_S values for both solid solutions at different temperatures are given in table 1 and 2. The phase transition takes place in temperature interval 105÷120K in χ_S temperature. Debye characteristic temperautres (θ_D) by emperical formulae [8] are cxalculated by us on α experimental data.

$$\theta_D = \frac{19{,}37}{\left(\bar{A}V^{2/3}\alpha\right)^{1/2}} \qquad (4)$$

Knowing the temperature dependence of Debye characteristic temperature we calculate Young modulus (E) on emperical formulae [9].

$$\theta_D = \frac{1{,}6810^8 \cdot 10^3\sqrt{E}}{M^{1/3}\rho^{1/6}} \qquad (5)$$

where M is molecular weight, ρ is density.

θ_D and E values calculated by such way, are given in tables 1 and 2.

Using the values of Young modulus we also calculate the velocity of sound (υ) in the given solid solution [10].

$$v = \sqrt{\frac{E}{\rho}} \qquad (6)$$

υ values are also given in1 and 2 tables.

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Table 1

Solid solution $(TlGaSe_2)_{0,9}(TlInS_2)_{0,1}$					
T,K	θ, K	$C_p, \frac{cal}{kg \cdot K}$	χ_s, $10^{-12} m^2/N$	E, $10^{10} N/m^2$	v, m/sec
90	421	92,41	6,32	9,8	3600
100	390	159,32	6,35	8,5	3435
120	379	167,42	6,37	7,9	3316
140	334	152,40	6,39	6,2	2932
160	309	152,88	6,41	5,3	2683
180	287	169,15	6,48	4,6	2518
200	280	203,95	6,51	4,3	2449
250	278	212,22	6,53	4,3	2449
300	275	224,95	6,55	4,2	2428

Table 2

Solid solution $(TlGaSe_2)_{0,8}(TlInS_2)_{0,2}$					
T,K	θ, K	$C_p, \frac{cal}{kg \cdot K}$	χ_s, $10^{-12} m^2/N$	E, $10^{10} N/m^2$	v, m/sec
90	425	100,85	6,26	6,7	3316
100	391	164,25	6,33	5,7	3049
120	382	173,30	6,34	5,4	2966
140	335	155,77	6,37	4,1	2588
160	310	153,69	6,40	3,5	2387
180	289	170,41	6,43	3,1	2252
200	281	204,76	6,49	2,9	2172
250	279	221,39	6,51	2,8	2167
300	277	228,88	6,53	2,8	2144

CONCLUSION

The experiments and calculations show that the temperature character dependence of α, χ_T and C_p is almost identical one, i.e. all thermal parameters increase, but Young modulus and velocity of sound decrease with temperature increase and increase of $TlInS_2$ content in composition. Such change can be connected with the fact that the weakening of interatomic chemical bonds in the lattice takes place with increase of $TlInS_2$ content in $(TlGaSe_2)_{1-x}(TlInS_2)_x$ composition and the crystal structure imperfection increases.

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