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DEBYE TEMPERATURE OF $TlInSe_2$ UNDER PRESSURE FROM FIRST-PRINCIPLES

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Abstract. The effects of pressure on the Debye temperature of $TlInSe_2$ were investigated by the local-density approximation (LDA) with a Perdew-Zunger exchange-correlation function using density-functional theory. And results indicate that pressure can improve the hardness of $TlInSe_2$ compound. The calculated Debye temperature 81 K at 0 GPa for this crystal is shown to be in excellent agreement with the available known values at 0 GPa pressure. The Debye temperature Θ_D calculated from elastic modulus increases along with the pressure. Acoustic wave velocity under different pressures were also successfully estimated from the calculations and determined that acoustic wave velocity goes up with the increasing pressure.

Keywords: *First principle, Debye temperature, acoustic wave velocity, local-density approximation.*

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1. Introduction

There are several reasons for investigation the ternary compound $TlInSe_2$ which crystallize into a tetragonal quasi one-dimensional chain structure Fig.1 (a) (Müller *et al.*, 1973). One of them is related to very interesting thermoelectric properties (Guseinov *et al.*, 1969; Mamedov *et al.*, 2006) of $TlInSe_2$. For this crystal Seebeck coefficient reaches giant values of 106 μV/K at temperatures below 413 K (Mamedov *et al.*, 2006) Debay temperature was calculated.

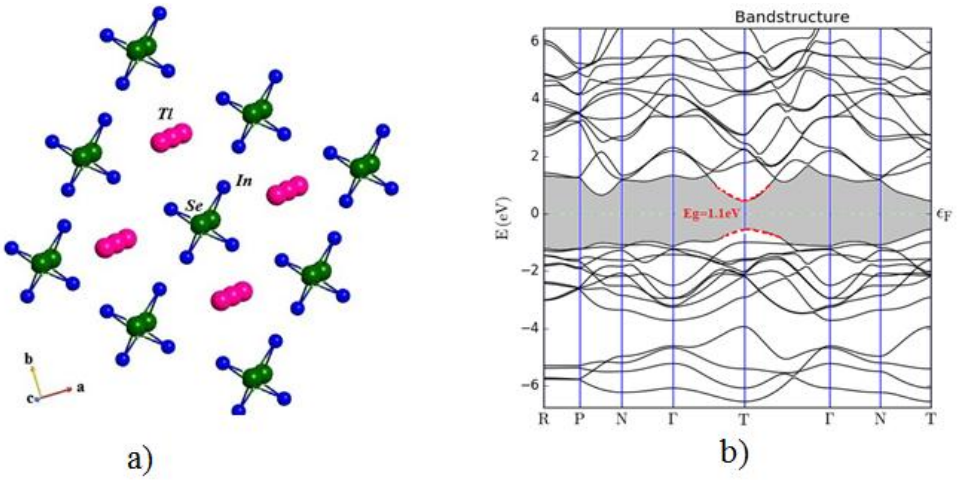

Fig. 1. a) Crystal structure of $TlInSe_2$, b) Electronic band structure of $TlInSe_2$

The physical properties of $TlInSe_2$ crystal have been widely investigated. The first electronic structure calculations of $TlInSe_2$ based on pseudopotential model reported in the literature (Gashimzade & Orudzhev, 1980) revealed an indirect energy gap for $TlInSe_2$. Calculations using non-local ionic pseudopotentials, where screening and exchange-correlation effects were treated within Hubbard-Sham model with selected parameters of the charge distribution around each particular ion, showed that $TlInSe_2$ is a direct gap semiconductor (both the valence band maximum and conduction band minimum are located at the T point on the surface of the Brillouin zone) (Orudzhev *et al.*, 2003). Our previous theoretical study by DFT method (Ismayilova *et al.*, 2017) also confirmed this result Fig.1 (b) (Orudzhev *et al.*, 2003).

In our previous study (Orudzhev *et al.*, 2017) were investigated band structure and effective masses of $TlInSe_2$ under pressure in the range of 0 to 21 GPa. Determined that, with increase of the pressure, the band gap decreases and at 8 GPa, the fundamental absorption edge changes from direct to indirect gap and increase of pressure leads to overlapping of bands and reaching zero of the band gap at metallization pressure P = 14 GPa.

In theoretical investigation (Mamedov *et al.*, 2009) report the data on thermal capacity at constant volume (CV), Debye temperature, and bulk modulus, was calculated based on calculations (Shin & Hahimoto, 1972) of the phonon band structure of TlSe ($Tl^{1+}Tl^{3+}Se_2$). But in the literature date there is not any work devoted to the debye temperature under pressure for this crystal. For this reason in this work from first principle calculation we calculated debye temperature under pressure up to 30 GPa.

2. Method of calculation

The computations have been performed using the DFT (Hohenberg & Kohn, 1964) within the local-density approximation (LDA) (Kohn & Sham, 1965) with the Perdew-Zunger parametrization (Perdew & Zunger, 1981). Correlation energy of a homogeneous electron gas calculated by Ceperley-Alder (Ceperley & Alder, 1980).The Tl - $6\boldsymbol{s}^2 6\boldsymbol{p}^1$, In - $5\boldsymbol{s}^2 5\boldsymbol{p}^1$ and Se - $3\boldsymbol{s}^2 3\boldsymbol{p}^4$ electrons have been treated as a valence electrons. The electron-ion interactions were taken into account through norm-conserving Fritz Haber Institute pseudopotentials (Martin & Matthias, 1999). The single-particle Kohn-Sham wave functions (Kohn & Sham, 1965) were expanded in a linear combination of numerical real-space atomic orbitals as a basis set with a kinetic energy cutoff of 300 Ry. Double zeta polarized basis sets were used in our calculations. The reciprocal space integration was performed by sampling the Brillouin zone with the 9×9×9 Monkhorst-Pack sets (Monkhorst & Pack, 1976).

The Debye temperature QD was calculated from elastic constants by using the average sound velocity (v_m) according to the following equation (Anderson, 1963):

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} v_m$$

where h is the Planck's constant; k_B is the Boltzmann's constant; n is the total number of atoms per formula; N_A is the Avogadro number; ρ is the density; M is the molecular weight. The average wave velocity (v_m) in the polycrystalline material can be approximately calculated by using the following equation (Xiao *et al.*, 2010):

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3}$$

where v_t and v_l stand for the shear and longitudinal sound velocities, respectively, which can be obtained by using the values of Hill's bulk modulus B and shear modulus G according to the approach of Voigte Reusse Hill.

3. Results and discussion

Debye temperature as a fundamental parameter for the materials thermodynamic properties is closely correlated with many physical properties of solids, such as specific heat, stability of lattices, melting points. For making a further comprehension of the thermodynamic behaviors and lattice stability under pressure, it is necessary to calculate the Debye temperature values under pressure and know its variation rule. This information is significant for the design and development of related materials. By using the VRH method, the shear sound velocity v_t, longitudinal sound velocity v_l, average wave velocity v_m (Fig.2) and Debye temperatures with pressure range from 0 to 30 GPa is calculated. Nonlinear pressure dependencies of these parameters are shown in Fig. 3.

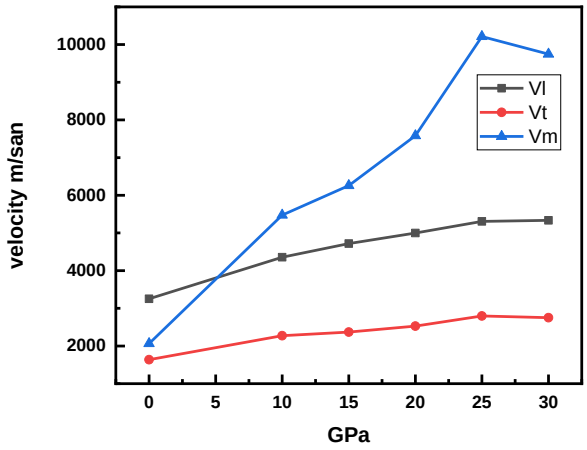

Fig. 2. Variations of shear sound velocity v_t, longitudinal sound velocity v_l, average wave velocity v_m of $TlInSe_2$ with pressure

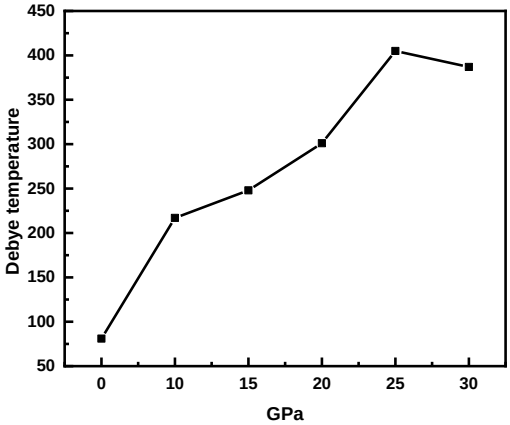

Fig. 3. Variations of Debye temperature of $TlInSe_2$ with pressure

The calculated Debye temperature of $TlInSe_2$ at 0 K and 0 GPa is 81 K, which is close to the result 96 K derived from elasticity measurements [9]. Our results are in line with others, confirming the present calculation is correct and available. But there is not any experimental result in laterite for comparison. So, the present results could be served as a prediction for future experiment. Besides, it can be found that the Debye temperature increases with pressure going up for $TlInSe_2$ compound. As we already know, the Debye temperature can be used to characterize the strength of covalent bonds in solids. The higher the Debye temperature is more stable the covalent bonds. Hence, with rising pressure, the covalent bonds become stronger, which is coherent with the analysis of electronic structure.

4. Conclusion

In this paper, we have performed first-principles calculations on tetragonal $TlInSe_2$, including Debye temperature and the acoustic wave velocity under pressure. The calculation of Debye temperature under pressure is further obtained by elastic constants is useful not only for the potential application of $TlInSe_2$ on thermoelectric and thermal resistance materials but also for the development of thermoelectric materials in future. It was found that with increasing pressure, the Debye temperature increases, and the acoustic wave velocity also increases. This in turn allows us to conclude that an increase in the Debye temperature leads to the stability of covalent bonds. Finally, investigated the acoustic wave velocities show that the velocity of longitudinal waves is about two times higher than the velocity of transverse waves.

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