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Research paper

Some physical properties of K_2TlAsX_6 (X = Cl, Br) and $CsPbBr_3$ semiconducting compounds

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Abstract

Some physical properties of K_2TlAsX_6 (X = Cl, Br) double perovskite compounds have been predicted using the theoretical unit cell parameters and elastic constants computed by Munir et al. (Materials Science and Engineering B 298 (2023) 116830). At equilibrium the Debye temperatures of $K_2TlAsCl_6$ and $K_2TlAsBr_6$ materials were found to be 193.5 K and 159.6 K, respectively.
Furthermore, the mass density, the longitudinal, transverse and mean acoustic wave speeds, the acoustic impedance and the Debye temperature of Cesium Lead Bromide ($CsPbBr_3$) inorganic perovskite compound under high stress up to 15 GPa have been predicted using the theoretical unit cell parameters and elastic constants computed by Junaid Zaidi et al. (Materials Research Express, Vol. 9, No. 12, (2022) 125501). To the best of our knowledge, there is no any data in the literature that can be compared to the findings we've achieved on the Debye temperature of K_2TlAsX_6 (X = Cl, Br) and $CsPbBr_3$ materials.

Keywords: *K_2TlAsX_6 (X = Cl, Br) Double Perovskites; $CsPbBr_3$ Compound; Mechanical Properties; Debye Temperature.*

1. Introduction

In the past decade, a wide range of semiconductors were known; however, attention was focused on the simplest the III-V and II-VI compounds [1]. Debye temperature θ_D of material is an essential parameter in solid state physic [2-6], this because it is correlated with many physical properties of solids; such as specific heat, elastic moduli, melting point, and lattice energy [7]. At low temperature, the vibrational excitations arise solely from acoustic vibrations, with consequence the Debye temperature calculated from elastic constants is the same as that determined from the measurements of the specific heat [8].
In the recent time Double perovskite compounds have attracted an increasing amount of attention due to their fascinating properties and possible applications [9]. Using the full potential linearized augmented plane wave (FP-LAPW) method, Munir et al. [10] have investigated the equilibrium structural parameters, elastic constants and electronic and optical properties of potassium-based double perovskites K_2TlAsX_6 (X = Cl, Br), and found the possibility of the application of these materials in optoelectronic and renewable energy
Junaid Zaidi et al. [11] have evaluated the modulation in the electronic properties, elastic constants, and optical behavior of $CsPbBr_3$ semiconducting material under the effect of stress up to 15 GPa, while very recently, Zemzemi [12] has studied theoretically the thermoelectric properties of a particular material family of metal halide cubic perovskites $CsBX_3$ (B = Ge, Sn, Pb and X = Cl, Br, I).
In the present work we tried to predict some physical properties of K_2TlAsX_6 (X = Cl, Br) double perovskite compounds and $CsPbBr_3$ semiconducting compounds using the theoretical unit cell parameters and the elastic constants computed by Munir et al. [10], and those of Junaid Zaidi et al. [11], respectively.
Theory and discussion of the results
In object to determine the elastic wave velocities, the Debye temperature and the acoustic impedance of $K_2TlAsCl_6$ and $K_2TlAsBr_6$ materials, we used the unit cell parameters and the elastic constants reported by Munir et al. [10], while for the Cesium Lead Bromide ($CsPbBr_3$) compound, we used the unit cell parameters and the elastic constants reported by Junaid Zaidi et al. [11]. First we recalculate the bulk modulus B, shear modulus G, Pugh ratio (B/G), Young modulus E and the Poisson's ratio σ, then the Debye temperature θ_D.
In cubic polycrystalline crystals, the bulk modulus B could be calculated from the elastic constants C_{ij} as follows: $B = (C_{11} + 2C_{12})/3$ [3, 13], while the shear modulus G was usually calculated using the Voigt-Reuss-Hill approach, which is expressed as follows: $G = (G_V + G_R)/2$ [3, 13], where G_V is the Voigt shear modulus, while G_R is the Reuss shear modulus. The Lamé's first parameter λ is expressed as follows: $\lambda = \sigma E/[(1+\sigma)(1-2\sigma)]$ [14]. At equilibrium, our obtained values of the bulk modulus B, shear moduli G_V, G_R, and G, Pugh ratio (B/G), Young modulus E, Poisson's ratio σ, and Lamé's first parameter λ for K_2TlAsX_6 (X = Cl, Br) semiconducting materials are tabulated in Table 1, along the results reported in Ref. [10].

Table 1: Bulk Modulus B, Shear Moduli G_V, G_R, and G, Pugh Ratio (B/G), Young Modulus E, Poisson's Ratio σ, And Lamé's First Parameter λ for K_2TlAsX_6 (X = Cl, Br) Semiconducting Materials, * from Ref [10]

Material	B (GPa)	GV (GPa)	GR (GPa)	G (GPa)	B/G	E (GPa)	σ	λ (GPa)
$K_2TlAsCl_6$	23.96, 24.00*	12.47	7.37	9.92, 7.87 *	2.42, 3.04*	26.15, 21.28*	0.32, 0.35*	17.34
$K_2TlAsBr_6$	20.30, 20.31*	10.67	8.34	9.50, 9.46 *	2.14, 2.14*	24.66, 24.56*	0.30, 0.29*	13.96

Our obtained values of the shear modulus G, Young Modulus E and Poisson's ratio σ are the same to those of Ref [10] for $K_2TlAsBr_6$ compound, but for $K_2TlAsCl_6$ material, they are different compared to those obtained in Ref [10]. For covalent materials, in general, the values of the Poisson's ratio σ are minimal (typically σ = 0.1), and there is little difference between G and B (G = 1.1B). A typical value of σ for ionic materials is 0.25 and G = 0.6B, while for metallic bonded materials σ is typically 0.33 and G = 0.4B [15].

There are different expressions usually used to calculate the Debye temperature θ_D of crystal from the acoustic wave speed [3, 13]. The expression used here is the same like that used in the work [3] for CaO compound (for more details on the calculation of the acoustic wave speed and the Debye temperature θ_D polycrystalline materials, please see for example the references [3, 13]). The mass density ρ of material is related to the atomic arrangement and corresponding electron density. The gravimetric density ρ can be calculated as follows: $\rho = ZM/N_AV$ [16, 17], where Z is the number of molecules per unit cell, M is the molecular weight, N_A is the Avogadro constant, and V is the unit cell volume. The acoustic impedance (Z) has been analyzed by the following equation: $Z = (\rho G)1/2$ [18], where G and ρ refer to the shear modulus and compound density, respectively. High values of these factors result in high acoustic impedance.

Our obtained values of the gravimetric density ρ, the acoustic wave speeds, the Debye temperature θ_D, and the acoustic impedance for K_2TlAsX_6 (X = Cl, Br) materials are tabulated in Table 2. The obtained Debye temperature for $K_2TlAsCl_6$ is higher than that of $K_2TlAsBr_6$ indicating that $K_2TlAsCl_6$ is harder than $K_2TlAsBr_6$ material. Unfortunately, to the best of our knowledge, there are no other theoretical or measured data available in the literature to compare with our results. Nevertheless, we hope that our results can support further experiments.

Table 2: Gravimetric Density, Acoustic Wave Speeds, Debye Temperature, and Acoustic Impedance for K_2TlAsX_6 (X = Cl, Br) Materials

Material	ρ (g/cm^3)	v_l (km/s)	v_t (km/s)	v_m (km/s)	θ_D (K)	Z (Rayl)
$K_2TlAsCl_6$	2.846	3.615	1.867	2.090	193.5	5.31×10^6
$K_2TlAsBr_6$	3.627	3.015	1.619	1.807	159.6	5.87×10^6

Longitudinal (v_l), transverse (v_t) and Mean (v_m) acoustic wave speeds of K_2TlAsX_6 (X = Cl, Br) materials discussed in the previous paragraph can be conveniently visualized through the schematic drawn in figure 1.

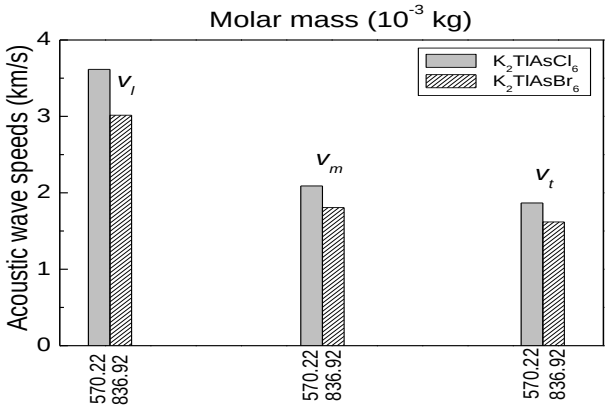

Fig. 1: Acoustic Wave Speeds Versus Molar Mass for K_2TlAsX_6 (X = Cl, Br) Materials at Equilibrium.

The melting point Tm of solids correlates with their elastic constants [19, 20]. We note that the melting point Tm of several solids having a cubic structure correlates with the bulk modulus B by this empirical formula: $T_m = 9.3B + 607$, where T_m is expressed in K, and B is expressed in GPa [17, 19]. Using the previous expression, the melting point T_m of $K_2TlAsCl_6$ and $K_2TlAsBr_6$ semiconducting materials were found to be 830 K and 796 K, respectively. To the best of our knowledge, there is no data in the literature that can be compared to the findings we've achieved on the Debye temperature and the melting point T_m of K_2TlAsX_6 (X = Cl, Br) compounds.

In general, the elastic compliance constants S_{ij} were used to investigate the three-dimensional (3D) mechanical moduli such as Young's modulus E, bulk modulus B, shear modulus G and Poisson's ratio σ [21, 22]. For cubic crystals, the elastic compliance constants Sij and the elastic stiffness constants C_{ij} are related by [23]:

$$S_{11} = (C_{11} + C_{12})/(C_{11} - C_{12})(C_{11} + 2C_{12}),\ S_{12} = -C_{12}/(C_{11} - C_{12})(C_{11} + 2C_{12}) = (-C_{12}/(C_{11} + C_{12}))S_{11},\ \text{and}\ S_{44} = 1/C_{44} \quad (1)$$

Our obtained values of the elastic compliance constants S_{ij} for K_2TlAsX_6 (X = Cl, Br) semiconducting materials are tabulated in Table 3.

Table 3: Elastic Compliance Constants Sij for K2TlAsX6 (X = Cl, Br) Semiconducting Materials

Material	S_{11} (GPa^{-1})	S_{12} (GPa^{-1})	S_{44} (GPa^{-1})
$K_2TlAsCl_6$	0. 0188	-0.0024	0.1980
$K_2TlAsBr_6$	0. 0247	-0.0041	0.1616

The Young's modulus and the Poisson's ratio within the crystallographic planes (100), (110) and (111) for K_2TlAsX_6 (X = Cl, Br) semiconducting materials, were be calculated using the expressions reported in Table 3.13 (page 54) of Ref. [23]. The obtained values of the Young's modulus and the Poisson's ratio for K_2TlAsX_6 (X = Cl, Br) semiconducting materials are tabulated in Table 4.

Table 4: Young's Modulus and Poisson's Ratio within the Crystallographic Planes (100), (110) and (111) for K_2TlAsX_6 (X = Cl, Br) Semiconducting Materials, m is The Direction for a Longitudinal Stress and n is The Direction for a Transverse Strain (Orthogonal to the Direction m)

Parameter	Plane	Direction	$K_2TlAsCl_6$	$K_2TlAsBr_6$
Young's modulus (GPa)	(100) plane	[001] direction	53.31	40.56
	(110) plane	[011] direction	17.34	19.74
		[001] direction	53.31	40.56
	(111) plane	[111] direction	14.16	16.86
			17.34	19.74
Poisson's ratio	(100) plane	m = [010], n = [001]	0.13	0.17
	(110) plane	m = [011], n = [0$\bar{1}$1]	0.72	0.59
		m = [001], n = [1$\bar{1}$0]	0.13	0.17
	(111) plane	m = [1$\bar{1}$1], n = [1$\bar{1}\bar{2}$]	0.40	0.36
			0.27	0.25

The study of the physical properties of materials under the impact of external pressure has been a popular topic in materials research in recent years [20]. We now turn our attention to the inorganic perovskite material Cesium Lead Bromide ($CsPbBr_3$) compound. To analyze the behavior of $CsPbBr_3$ compound under the influence of external pressure, we also examined the change in some physical properties when the pressure changes between 0 and 15 GPa. The Debye temperature θ_D, the acoustic impedance (Z) as well as the Cauchy pressure C_P of $CsPbBr_3$ compound under high stress has been predicted using the theoretical unit cell parameters and the elastic constants computed by Junaid Zaidi et al. [11], and the previous procedure. Under pressure, the Cauchy pressure C_P has been written $C_P = C_{12} - C_{44} - 2p$ [24, 25], where p is the pressure. Our obtained values of the mass density ρ, acoustic wave speeds (v_l, v_t, and v_m), Debye temperature θ_D, acoustic impedance Z, and the Cauchy pressure C_P up to 15 GPa for $CsPbBr_3$ material are tabulated in Table 5.

Table 5: Some Physical Properties Under Pressure Up to 15 GPa For $CsPbBr_3$ Semiconducting Compound, * From Ref [11]

Pressure(GPa)	ρ (g/cm^3)	v_l (km/s)	v_t (km/s)	v_m (km/s)	θ_D (K)	Z (Rayl)	C_P (GPa)
0	4.164	2.520	1.266	1.419	118	5.27×10^6	3.86*
5	5.015	3.149	1.378	1.556	137	6.91×10^6	1.89
10	5.598	3.634	1.489	1.685	154	8.33×10^6	0.38
15	6.182	3.849	1.522	1.725	163	9.41×10^6	- 3.64

Figure 2 illustrates the variation of the mass density ρ up to 15 GPa for $CsPbBr_3$ material. From this figure, we observe clearly that the mass density ρ of $CsPbBr_3$ material increase gradually with increasing in pressure from 0 to 15 GPa. Least-squares fit with polynomial form of our data on the mass density ρ versus pressure p for CsPbBr3 compound is given as follows: $\rho = 4.177 + 0.173\ p - 2.67\ x10\text{-}3\ p^2$, the mass density ρ is expressed in g/cm^3 and the pressure p is expressed in GPa.

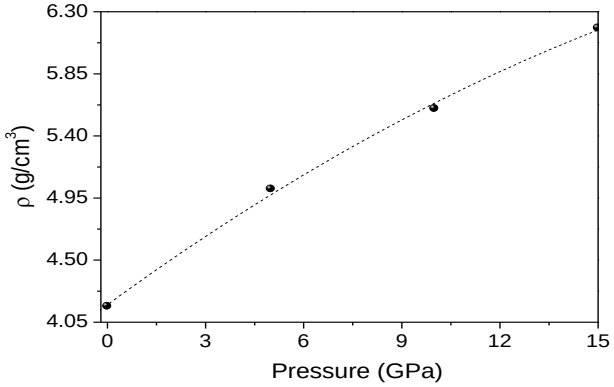

Fig. 2: Mass Density Versus Pressure for $CsPbBr_3$ Semiconducting Material Up to 15 GPa.

The acoustic wave speeds (v_l, v_t, and v_m) and the Debye temperature θ_D under pressure for $CsPbBr_3$ material are also traced in figure 3.

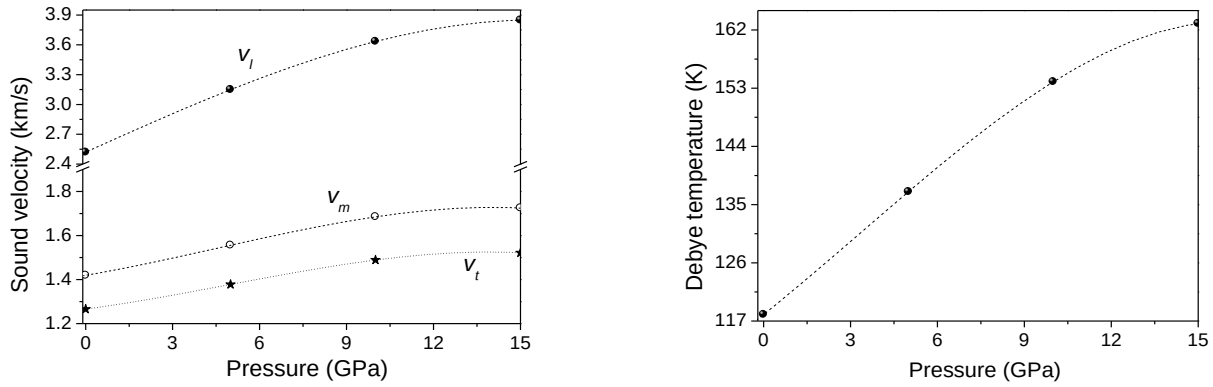

Fig. 3: Acoustic Wave Speeds (v_l, v_t, and v_m) and Debye Temperature Versus Pressure for $CsPbBr_3$ Semiconducting Material Up to 15 GPa.

From figure 3, we observe that the acoustic wave speeds and the Debye temperature θ_D of $CsPbBr_3$ material increase gradually with increasing in pressure from 0 to 15 GPa. The zero-pressure θ_D for $CsPbBr_3$ material is 118 K, which is much lower than many other types of semiconductors such as III-V and II-VI semiconducting compounds [2]. These behaviors agree with the findings in Ref. [4] for CaTe compound from 0 up to 27.8 GPa, in Ref. [26] for Cu_3N compound up to 30 GPa, in Ref. [27] for cubic zincblende boron nitride, in Ref.

[28] for cubic zincblende thallium-phosphide (TlP) from 0 up to 12 GPa, and in Ref. [29] for new iridium phosphide (Ir_2P) in cubic anti-fluorite structure from 0 up to 100 GPa. The same behaviors were also observed for both CuCl and CuBr semiconductors [30], for BeSe compound up to 50 GPa [31], for BSb material [32], for cubic Na_2He compound [25, 33], for Gabbro (igneous rock) material [34], for boron–bismuth (BBi) compound up to 30 GPa [35], for PdGa intermetallic compound up to 25 GPa [36], for hexagonal intermetallic compound Ti_3Al from 0 up to 80 GPa [37], and for wurtzite boron nitride [38]. Through the work of Wang et al. [39], we note also that the high pressures has little influence on θ_D values for M_2AlC (M = V, Nb and Ta) materials, while Gao et al. [40] found that the Debye temperature θ_D of $Cu_2ZnSiSe_4$ decrease slowly with increasing temperature from 0 to 500 K.

Our obtained values of the acoustic impedance Z and the Cauchy pressure C_P up to 15 GPa for CsPbBr3 material are also traced in figure 4. From figure 4, we observe that the acoustic impedance of $CsPbBr_3$ increases gradually with increasing in pressure from 0 to 15 GPa. Least-squares fit of our data on the acoustic impedance Z (expressed in 10^6 Rayl) versus pressure p (expressed in GPa) for $CsPbBr_3$ compound could be given as follows: $Z = 5.264 + 0.361\ p - 5.6\ x10\text{-}3\ p^2$.

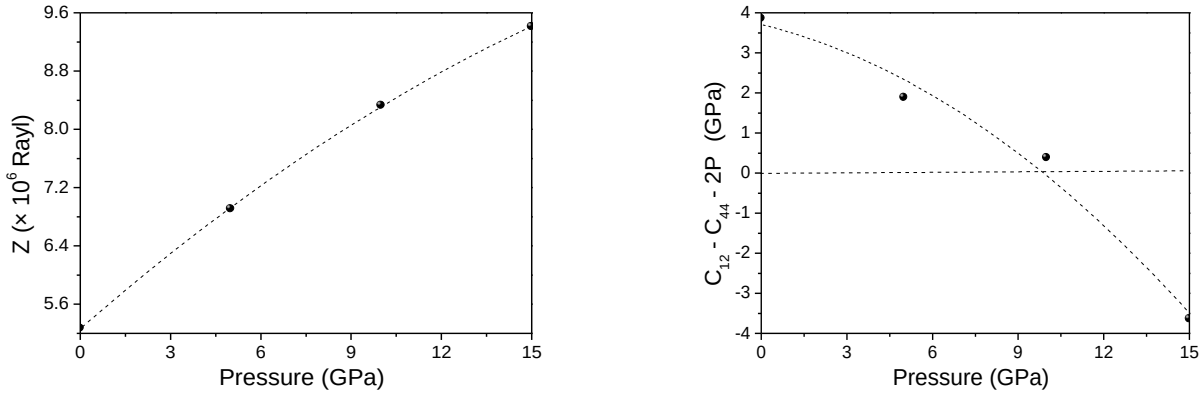

Fig. 4: Acoustic Impedance Z and Cauchy Pressure C_P Versus Pressure for $CsPbBr_3$ Semiconducting Material Up to 15 GPa.

As pressure is increased from 0 to 15 GPa, it is found that the values of the Cauchy pressure C_P of $CsPbBr_3$ semiconducting compound decreases monotonically and non-linearly. We note that a similar behavior was observed also for cubic Na_2He compound from 100 to 500 GPa [25], for both BP and BAs binary semiconducting materials [41] and for both MgO and SrO alkaline earth binary oxides [42]. The Cauchy pressure will be positive if the bonding is more metallic in character, while the more negative C_P indicates the more directional and nonmetallic character in the material [43]. Under hydrostatic pressure the low pressure phase (more stable phase) is destabilized and structural phase transition occurs [44, 45]. To the best of our knowledge, there are no experimental or theoretical data available in the literature on the pressure of phase transition P_T for $CsPbBr_3$ semiconducting compound.

2. Conclusion

Using the theoretical unit cell parameters and elastic constants published recently by Munir et al., firstly we recalculated several moduli of $K_2TlAsCl_6$ and $K_2TlAsBr_6$ materials already calculated by Munir et al., then we have determined some physical properties of $K_2TlAsCl_6$ and $K_2TlAsBr_6$ materials, their Debye temperatures are found to be 193.5 K and 159.6 K, respectively. Furthermore, the acoustic wave speeds, acoustic impedance, Debye temperature and Cauchy pressure of $CsPbBr_3$ compound under high stress up to 15 GPa have been predicted using the unit cell parameters and the elastic constants computed by Junaid Zaidi et al. Our results are analyzed and discussed. To the best of our knowledge, there is no data in the literature on the acoustic wave speeds, and on the Debye temperature of K_2TlAsX_6 (X = Cl, Br) and $CsPbBr_3$ compounds. Our results on θ_D could be useful as reference in the future.

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