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Research paper

Sound velocities and thermal properties of BeX (X=S, Se and Te) alkaline-earth chalcogenides

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Abstract

The sound velocities and some thermal properties of BeX (X=S, Se and Te) beryllium-chalcogenides large band gaps semiconductors have been estimated by employing some usual theoretical and emperical formulas. The lattice parameters and the elastic stiffness constants used here are taken from the literature. The longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity and the Grüneisen parameter are successfully predicted and analyzed in comparison with the available experimental and theoretical data. In general, our obtained results of these quantities agree well with the experimental and other theoretical data of the literature.

Keywords: *Elastic Wave Velocity; Thermal Properties; Beryllium-Chalcogenides Large Band Gaps Semiconductors.*

1. Introduction

Recently, II-VI and III-V semiconductors were largely and successfully used in the fabrication of the optoelectronic devices. These semiconductor materials are characterized by different degrees of covalent, ionic, and metallic bonding, and the majority of them crystallize in zincblende and wurtzite structures [1].
The Beryllium-monochalcogenides BeX (X=S, Se and Te) binary semiconductors belong to II-VI group of the periodic table. In normal conditions, they are crystallizing in cubic zincblende crystallographic structure. Most of the materials that are used in microelectronic industry have the cubic zincblende structure. The BeX (X=S, Se and Te) semiconductors are in extensive study in the recent years due to their useful physical, electro-optical and other properties [2]. In addition, these semiconductors have an indirect band gap along Γ–X symmetry. They have large band gaps (2.7 - 5.5 eV) and a high bulk modulus [2].
Using first principle full potential-linearized augmented plane wave method (FP-LAPW) within density functional theory, the ground state properties, the structural phase transformation, elastic constants and the electronic properties of beryllium-chalcogenides (BeS, BeSe, and BeTe) have been investigated by El Haj Hassan and Akbarzadeh [3].
Bouamama et al. [4] used an Ab initio calculation in the virtual-crystal approximation to predict the structural and the elastic properties of BeS_xSe_{1-x} alloys under high pressure. They found that the elastic constants increase monotony with increasing on the sulfide fraction (x). They found also that the lattice parameter, the phase transition pressure and the elastic constants (and their derivatives with respect to the pressure) of BeS_xSe_{1-x} alloys follow a quadratic law in the sulfide fraction (x).
Using FP-LAPW method with the generalized gradient approximation (GGA) and the modified Becke Johnson (TB-mBJ) potential for exchange correlation, Rai et al. [2] have investigated the electronic, optical, elastic and some thermal properties of BeX (X=S, Se and Te) materials. They found that the modified Becke Johnson (TB-mBJ) potential improves the band gap as compared to the generalized gradient approximation and in close agreement with the experimental results. The sound velocity and the Debye temperature of BeX (X=S, Se and Te) binary semiconductors are also predicted by means of different approximations [2], [5-10].
Dabhi et al. [7] have established a systematic theoretical study of structural, mechanical, electronic, vibrational and thermodynamical properties of three Beryllium-monochalcogenides BeX (X=S, Se and Te) binary semiconductors in zinc blende, NiAs and rock salt phases by performing ab initio calculations based on density-functional theory. They found that the phonon dispersion curves of these materials in cubic zincblende phase depict their dynamical stability in this phase at ambient condition. They found also that the variation of lattice-specific heat with temperature of these compounds obeys the classical Dulong–Petit's law at high temperature, while at low-temperature it obeys the Debye's T^3 law
Ji et al. [11] have investigated the effect of high pressure on the phase's transition and several other properties of BeS material. They found that for both B3 and B8 phases, the longitudinal wave (v_l) changes faster than the transverse waves (v_t). They found also that the longitudinal wave velocity (v_l) for B3 structure increases with pressure, while the transverse (v_t) and average (v_m) wave velocities have no obvious change with increasing pressure.
Recently, McCammon et al. [12] used the nuclear inelastic scattering (NIS) to determine sound velocities of five compositions of (Mg,Fe)(Si,Al)O3 bridgmanite at pressures between 0 and 89 GPa and at room temperature.
In the present work, we have made an attempt to predict the longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity, and Grüneisen parameter γ of BeX (X=S, Se and Te) semiconductors based on the experimental lattice parameters and elastic constants taken from the literature. Our results are discussed in detail,

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analyzed and then compared with other theoretical and experimental data of the literature.

2. Theory, calculations and results

2. 1. Sound velocities

To study the directional dependence of elastic wave velocities, the solving of the Christoffel equation which relates the sound-wave velocity and the elastic constants C_{ij} was usually used. For cubic crystals, the three independent elastic constants, C_{11}, C_{12}, and C_{44} may be determined with the help of the sound velocities propagate in the [l00], [l10] and [l11] directions respectively [13]. And vise-versa, if the three elastic constants C_{11}, C_{12} and C_{44} are know, it is possible to determine the directional dependence of the elastic wave velocities. The different formulas used here to obtain the directional dependence of the sound velocities are cited in our previous work [13] and in other Refs [14], [15].
The numerical values the elastic constants C_{ij} and crystal density of different Beryllium- semiconductors BeX (X=S, Se and Te) are taken from the Ref [14], and they are reported in table. 1.

Table 1: The Elastic Constants C_{ij} and Crystal Density g of Bex (X=S, Se and Te) Materials Cited by Adachi [14]

Parameter	BeS	BeSe	BeTe
C_{11}	123	110	88.7
C_{12}	73	66.6	55.4
C_{44}	56.9	50.3	38.6
g (g/cm^3)	2.37	4.311	5.12

The numerical values obtained of the sound velocities for major directions in the Beryllium-monochalcogenides binary semiconductors BeX (X=S, Se and Te) are reported in table. 2. To the best of our knowledge, there are no data available in the literature on the sound velocities for major directions in BeX (X=S, Se and Te) materials. The data reported in table. 2, shows that the sound velocities are directly proportional to the elastic constants C_{ij} of the compounds; and they are inversely proportional to their molar mass or their crystal density.

Table 2: Sound Velocities V In (m/s) for Major Directions in BeX (X=S, Se and Te) Materials. [a] Longitudinal Waves, [b] Transverse Waves.

Propagation (Direction)	Plane of Polarization	BeS	BeSe	BeTe
[100]	[100][a]	7204	5051	4162
	(100)[b]	4900	3416	2746
[110]	[100][a]	8084	5670	4649
	[001][b]	3248	2244	1803
	$[1\,\bar{1}\,0]$[b]	4900	3416	2746
[111]	[111][a]	8357	5862	4800
	[100][a]	3878	2692	2164

For polycrystalline materials, the average quantities are usually used. The average sound velocity (v_m) is determined from the longitudinal (v_l) and transverse (v_t) wave velocities by using the following formula [13]

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

The longitudinal and transverse wave velocities can be calculated by using the following expressions [13]:

$$v_l = \sqrt{(3B + 4G)/3g}\,, \text{ and } v_t = \sqrt{G/g} \quad (2)$$

Where: B is the bulk modulus, G is the isotropic shear modulus, and g is the crystal density.
The calculated values of the longitudinal (v_l), transverse (v_t) and average (v_m) elastic wave velocities of BeX (X=S, Se and Te) semiconductors are presented in table 3 and compared with the available theoretical data [5], [6]. It is seen that, the different values of the average sound velocities obtained in this work are in general in good accordance with the data available in the literature. For example, for BeSe material, our result is localized between the two values of the Ref. [5] and the Ref. [6]. For BeS material, Ji et al. [11] have investigated the effect of high pressure on the longitudinal (v_l), transverse (v_t) and average (v_m) wave velocities. Despite, Ji et al. [11] did not give the exact numerical values (the results are given in curves and not in tables) which allow making an exact comparison; our results are in very good agreement with these of Ji et al. [11]. To the best of our knowledge, there are no data available in the literature on the longitudinal and transverse sound velocities BeTe material.

Table 3: Computed Values of the Sound Velocities V_l, V_t, and V_m In (m/s) Along with Those Computed Through other Methods [5] and [6].

	BeS		BeSe		BeTe	
	Our work	Other works	Our work	Other works	Our work	Other works
v_l	7800		5469	6023.5 [6]	4490	
v_t	4155		2886	3720.3 [6]	2320	
v_m	4642	3620 [5]	3226	2400 [5] 4103.5 [6]	2597	1830 [5]

2.2. Debye temperature, melting temperature, the thermal conductivity and the grüneisen parameter

Usually, the Debye temperature of solid is obtained from the elastic constants or from the measurement of the specific heat capacity. For several crystals, the Debye temperature can be estimated from the elastic constants (elastic wave velocity) by [16]:

$$\theta_D = \frac{h}{k}\left[\left(6\pi^2 n \frac{N\rho}{M}\right)\right]^{1/3} v_m \quad (3)$$

Here: $h = h/2\pi$, h is the Planck's constant, k is the Boltzmann constant, N is the Avogadro number, ρ is the crystal density, M is the molecular weight, n is the number of atoms per molecule, and v_m is the average sound velocity.
For materials with cubic zincblende structure, the Debye temperature θ_D can be obtained from the average sound velocity v_m (given in km/s) and the lattice parameter a (given in Å) by means of the following equation [13], [17]:

$$\theta_D \approx (595.467) v_m / a \quad (4)$$

Another formula proposed by Blackman's [18], it relate the Debye temperature θ_D to the elastic constants C_{ij} in the cubic system, it is given by the following expression [13]

$$\theta_D^3 = \frac{3.15}{8\pi}\left(\frac{h}{k}\right)^3 \left(\frac{n}{g^{3/2} v_a}\right) (C_{11} - C_{12})^{1/2} (C_{11} + C_{12} + 2C_{44})^{1/2} (C_{44})^{1/2} \quad (5)$$

Where: h is the Planck's constant, k is the Boltzmann constant, n is the number of atoms in unit cell of volume v_a, and g is the density.
Using the values: 4.865, 5.137 and 5.617 Å [14] of the lattice parameter a for BeS, BeSe and BeTe respectively, our calculated values of the Debye temperature are listed in table 4, and compared with the available theoretical data [5-10], [19], [20]. They are also presented in Figure 1. Our obtained values of θ_D are also in general in good agreement with the majority of other theoretical results [5-10], [19], [20]. For BeS compound, our obtained value (628 K) of θ_D is equal exactly the theoretical value of Ref. [5], it is deviates from the theoretical value 643.18 K (calculated at 300 K and 0 GPa) of Ref. [20] by only about 2.36 %.
For BeTe compound, our obtained value of θ_D (275 K) is in good agreement with the theoretical value (289 K) of Ref. [5]; the deviation being only about 4.84 %. It was reported in the literature [14] that in II-VI and III-V materials, the high Debye temperature

reflects high elastic stiffness constants C_{ij}, low atomic mass, and short interatomic bond-length (short lattice paramater). This important observation is consistent well the present case since the bond-length of BeS (d = 2.107 Å) is smaller than that of BeSe (d= 2.224 Å), which is also smaller than that of BeTe (d= 2.432 Å).

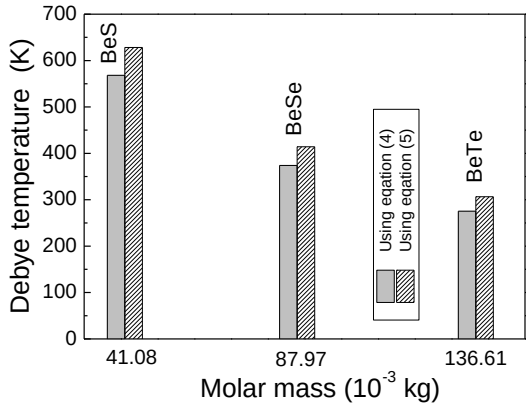


Fig. 1: Debye Temperature of Bex (X=S, Se and Te) Semiconductors as Function of the Molar Mass of the Compound.

The melting temperature of several crystals can be estimated as function of the elastic constant C_{11} by [11], [17]:

$$Tm = 553 + (591/Mbar)C_{11} \pm 300K \quad (6)$$

The calculated melting point T_m of BeS, BeSe and BeTe materials are about 1280 ± 300 K, 1203 ± 300 K, and 1077 ± 300 K respectively; they are also listed in table 4, and compared with the available results of the literature [10], [19], [21], [22]. Our calculated values of the calculated melting point T_m are relatively lower from the theoretical and experimental data of Benosman et al. [21] and of Van Vechten [22]. They are also very lower from the theoretical data of Kumar et al. [10]. Another experimental work [23] mentioned that BeTe compound dissociates appreciably by vaporization at temperatures above 1000 °C, and the upper limit of the melting point of BeTe material is 1300 °C (~1570 K) , which is agree very well with the result of Van Vechten [22].

The results reported in table. 4, shows also that the Debye temperature, the melting temperature, and the thermal conductivity are inversely proportional to the molar mass and the crystal density of the considered compounds.

Thermal conductivity of material is the property that indicates its ability to conduct heat. However, in order to known if the material is a potential application for thermal barrier coating, the investigation of its thermal conductivity becomes necessary [24]. So, the thermal conductivity is one of important thermal parameter of materials, it is directly related to the nature of bonding in solid. The total thermal conductivity of crystal is a resultant of two components; first one is the lattice (phonons or lattice vibrations) thermal conductivity, and the second one is the electronic thermal conductivity. The lattice thermal conductivity is the most dominant in the case of the insulators materials, such as the ceramics (complex oxides); whereas the electronic thermal conductivity is the most dominant for the conductors' materials, such as the metals (Aluminum…etc). The knowledge of the numerical thermal conductivity K is fundamental parameter for thermo-electronic devices [14]. At T = 300 K, the thermal conductivity K (in W/K.cm) versus scaling parameter $\bar{M}a\theta_D^3$ ($\bar{M}a\theta_D^3$ in amu.cm.K^3) for group-IV, III-V and II-VI semiconductors can be given by the following relation [14]:

$$K = 1.17 \times 10^{-3} (\bar{M}a\theta_D^3)^{1.15} \quad (7)$$

Where $\bar{M}$ is the average mass of an atom in the crystal, M is the molecular mass per formula unit, a is the lattice constant and θ_D is the Debye temperature.

The lattice thermal conductivity (K in W/K.cm) of III-V and II-VI semiconductors may be also evaluated using the ionic charge by the following relation [25]:

$$K = S(Z_1Z_2)^V / d^5 \quad (8)$$

Where: Z_1 and Z_2 are the ionic charge of the first and the second atoms, respectively, d is the nearest-neighbor distance given in Å, S and V are constants, which depends up on crystal structure; for cubic zincblende structured solids , S and V have values of 2 and 1.5, respectively [25].

Using the Debye temperature obtained from Blackman's [18] formula of Eq. (5), and the lattice parameters cited by Adachi [14], our calculated values of the thermal conductivity K for BeX (X=S, Se and Te) materials are listed also in Table 4. From the results of thermal conductivity listed in Table 4, it is observed that our calculated values of the thermal conductivity of BeX (X=S, Se and Te) materials obtained from the formula of Eq. (7) are all superior to these obtained from the formula of Eq. (8). I think that, this is quite natural, because the first one presents the sum of the lattice thermal conductivity and the electronic thermal conductivity; whereas the second one presents only the lattice thermal conductivity component. These results show also that the lattice thermal conductivity component is the more dominant than that of the electronic component in these materials.

It is observed that our calculated value (0.26 W/K.cm) of the thermal conductivity of BeTe material is very nearly to the value (0.27 W/K.cm) of β-ZnS material predicted by Adachi [14].

However, to the best of our knowledge, no theoretical or experimental data of the thermal conductivity of BeX (X=S, Se and Te) materials have appeared anywhere in literature. So, future experimental works or other theoretical calculations will contribute for the validating of our calculated results of this quantity.

Table 4: Our Values of the Debye Temperature and the Melting Point of BeS, BeSe and BeTe Materials Along with the Available Those Computed Through other Methods [5-10], [19-22], and [23]. [a] Using Eq. (4), [b] Using Eq. (5). [c] Using Eq. (7), [d] Using Eq. (8). * Experimental Data.

	Parameter	Our work	Other works
BeS	θ_D (K)	568 [a] 628 [b]	628 [5] 723 [7] 748 [8] 951 [9] from 612 to 1110 [10] 838.08 [19] 643.18 [20] at 300 K
	T_m(K)	1280 ± 300	from 2328.42 to 2657.33 [10] 3255 [19] 1658.17[21]
	K (W/K.cm)	0.66 [c] 0.39 [d]	
BeSe	θ_D (K)	374 [a] 414 [b]	399 [5] 407.93 [6] 456 [7] 459 [8] 850 [9] from 498.42 to 850 [10] 502.47[19]
	T_m(K)	1203 ± 300	from 2089.98 to 2424.83 [10] 2300.64 [19]
	K (W/K.cm)	0.40 [c] 0.29 [d]	
BeTe	θ_D (K)	275 [a] 307 [b]	289 [5] 332 [7] 333 [8] 766 [9] from 380.48 to 766 [10] 334.09 [19]
	T_m(K)	1077 ± 300	from 1842.6 to 1925 [10] 1452 [22] <1570 [22, 23] *
	K (W/K.cm)	0.26 [c] 0.19 [d]	

The Grüneisen parameter γ is a thermophysical quantity, which describes the anharmonic effects in the vibrating lattice. At low-temperature, it was dominated by lower-frequency transverse modes [6]. The temperature-dependent of the Grüneisen parameter and other thermal properties are usually obtained from the quasi-harmonic Debye model approximation. For several materials, the Grüneisen parameter γ is related to the longitudinal and the transverse sound velocities by the following expression [13], [17]:

$$\gamma = \left(9(v_l^2 - (4/3)vt^2\right) / \left(2(v_l^2 + 2vt^2\right) \quad (9)$$

Using the longitudinal (v_l) and the transverse (v_t) sound velocities obtained from Eq. (2), the numerical values of the Grüneisen parameter γ for BeS, BeSe and BeTe materials have been calculated and to be found: 1.79, 1.82 and 1.89 respectively. Our calculated value (1.82) of γ for BeSe material is in excellent agreement compared to the theoretical value (1.79) reported by Kong and Jiang [6], the deviation between the two values being only about 1.6 %. Our calculated value (1.79) of the Grüneisen parameter γ for BeS compound is relatively higher than the theoretical value 1.703 (calculated at 300 K and zero-pressure) reported by Chang et al. [20]. To the best of our knowledge, there is no data available in the literature on γ for BeTe compound.

3. Conclusion

Using the elastic constants, the crystal density and the lattice parameters of Adachi [14]; the sound velocities and some thermal properties of BeX (X=S, Se and Te) materials have been predicted and analyzed. The longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity, and the Grüneisen parameter are calculated and compared with available data of the literature.

It is observed that the material having higher Debye temperature associated with higher thermal conductivity, higher melting temperature and smaller Grüneisen parameter.

The Debye temperature of BeX (X=S, Se and Te) semiconductors is calculated from two empirical formulas, the results obtained are in good agreement with the previous data of the literature.

Our obtained results of the longitudinal, transverse and average elastic wave velocities and Grüneisen parameter of the aggregate are also in general in agreement with the majority of previous experimental and theoretical data of the literature.

Our calculated values of the melting temperature are relatively lower from the previous data of the literature.

To the best of our knowledge, our calculated values of the thermal conductivity are new, so future experimental and other theoretical results are needed for the validating of our finding data.

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