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Research Paper

Sound velocities and thermal properties of BX (X=As, Sb) compounds

Salah Daoud

Laboratoire Matériaux et Systèmes Electroniques (LMSE), Université de Bordj Bou Arreridj, 34000, Algérie
E-mail: salah_daoud07@yahoo.fr

Abstract

The sound velocities and thermal properties of Boron-Arsenide (BAs) and Boron- Antimonide (BSb) materials have been predicted with the help of the empirical elastic constants which are taken from our previous work which is accepted to publication in International Journal of Scientific World. The longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity, the linear thermal expansion coefficient and finally the Grüneisen parameter are predicted and analyzed in comparison with the available theoretical data of the literature. Our obtained results are in general in very good agreement with the previous experimental and theoretical data of the literature.

***Keywords**: Sound velocity; Thermal Properties; AIIIBV compounds.*

1. Introduction

The recent successful fabrication of the optoelectronic devices based on $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductor materials has renewed interest in their physical properties. These materials are characterized by different degrees of covalent, ionic, and metallic bonding, and they crystallize in different crystal structures such as wurtzite and zincblende [1].
The boron based pnictides BX (X = P, As and Sb) are semiconductors with zincblende structure at ambient conditions, they show strong covalent character and exhibits an unusual behavior due to small core and absence of “p” electrons in boron atom compared to other ordinary A^{III}-B^{V} (GaAs, GaP,…, etc) compounds [2]. Unfortunately, as far as we know, the zincblende (B3) structure of the BSb compound was synthesized for the first time in 1967 [3]. Recently, the zincblende structure of boron antimonide thin films is also successful syntheses from B/Sb multilayer films which deposited onto silicon substrate [4, 5], and several physical properties of this compound were obtained; the optical band gap is about 0.59 eV [5], and a plasmon energy $\hbar\omega_p$ varied from 15.62 eV to 15.67 eV [4, 5].
Furthermore many experimental [6, 7] and theoretical works [8-15] have been study structural, elastic, electronic and some other physical properties of boron based pnictides BX (X = P, As and Sb).
In the present work, we report an empirical calculation of the longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity, the linear thermal expansion coefficient and the Grüneisen parameter of two boron based pnictides BX (X = As and Sb). Our results are analyzed and compared with experimental and other theoretical data of the literature.

2. Theory, results and calculations

2. 1. Sound velocities

Usually, to obtain the elastic constants C_{ij} of crystal solids, the elastic sound velocities and the crystal densities are 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 [16].

For elastic waves propagating along the [l00] direction, the longitudinal waves (pure mode with particle displacements u_1 in direction of propagation, u_2 and u_3 = 0), and transverse waves (pure mode with particle displacements u_1 = 0, u_2 and u_3 perpendicular to the direction of propagation) have respectively the following formulas [16-18]:

$$v_1 = \sqrt{C_{11}/g} \quad \text{and} \quad v_2 = v_3 = \sqrt{C_{44}/g} \tag{1}$$

For elastic waves propagating along the [110] direction, the two elastic transverse waves within a polarization along the [001] and [110] directions have two different formulas to calculate their numerical velocities. The elastic waves have the following velocities along the [110] direction [16-18]:

$$v_1 = \sqrt{\left(C_{11} + C_{12} + 2C_{44}\right)/2g}\ ; \quad v_2 = \sqrt{\left(C_{11} - C_{12}\right)/2g} \quad \text{and} \quad v_3 = \sqrt{C_{44}/g} \tag{2}$$

For plane waves propagating along the [l11] direction, the longitudinal waves (pure mode with particle displacements $u_1 = u_2$, $u_3 = 0$), and transverse waves (pure mode with particle displacements $u_1 = u_2 = u_3$) have values given the following expressions respectively [16-18]:

$$v_1 = \sqrt{\left(C_{11} + 2C_{12} + 4C_{44}\right)/3g} \quad \text{and} \quad v_2 = v_3 = \sqrt{\left(C_{11} - C_{12} + C_{44}\right)/3g} \tag{3}$$

The predicted values of the sound velocities for major directions in the (B3) BAs and BSb materials at T=300 K are reported in table. 1, and compared with the available theoretical data [17, 19]. For (B3) BAs material, our numerical values of the sound velocities lie in the range 7444 m/s - 7837 m/s for the longitudinal waves and are less than 5000 m/s for transverse waves. It can be seen that, our results of the sound velocities are in excellent agreement in comparison with those of the Ref. [17]. This later reference used the theoretical values of the elastic constants: C_{11}=279 GPa, C_{12}= l20 GPa and C_{44}=113 GPa and the same numerical value of the density which is used in our work (g= 5.224 g/cm^3).

For (B3) BSb material, our numerical values of the sound velocities lie in the range 5614 m/s - 5943 m/s for the longitudinal waves and are less than 3740 m/s for transverse waves. Unfortunately, to the best of our knowledge, there are no data available in the literature on the sound velocities for major directions in the (B3) BSb.

Table 1: Sound Velocities In (m/s) for Major Directions in the Bas and BSb Materials in Comparison with Other Theoretical Data [17], [19].
^{A} Longitudinal Acoustic Waves, ^{B} Transverse Acoustic Waves.

Material	Propagation (Direction)	Plane of Polarization	Our work	Other works	
BAs	[100]	$[100]^a$	7444	7310 [17]	7700 [19]
		$(100)^b$	4981	4650 [17]	5240 [19]
	[110]	$[100]^a$	7740	7730 [17]	8360 [19]
		$[001]^b$	4507	3900 [17]	
		$[1\bar{1}0]^b$	4981	4650 [17]	4110 [19]
	[111]	$[111]^a$	7837	7870 [17]	8570 [19]
		$(111)^b$	4670	4170 [17]	4520 [19]
BSb	[100]	$[100]^a$	5614		
		$(100)^b$	3737		
	[110]	$[100]^a$	5862		
	[110]	$[001]^b$	3334		
		$[1\bar{1}0]^b$	3737		
	[111]	$[111]^a$	5943		
		$(111)^b$	3474		

For polycristallin solids, the average sound velocity v_m is usually given by the following formula: [18]

$$v_m = \left[\left(2v_t^{-3} + v_l^{-3}\right)/3\right]^{-1/3} \tag{4}$$

Where: v_l and v_t are the longitudinal and transverse elastic wave velocities respectively. They are calculated by using the following expressions [8, 20]:

$$v_l = \sqrt{(3B + 4G)/3g}\ \text{, and } v_t = \sqrt{G/g} \tag{5}$$

Where: B is the bulk modulus, G is named the isotropic shear modulus (for polycrystalline aggregate is termed the Hill shear modulus, which is related to the Voigt shear modulus and to the Reuss shear modulus), and g is the crystal density. The calculated values of the longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities of BX (X = As, Sb) materials are presented in table 2 and compared with the available theoretical data [8], [11], [13-15], [17], [20-22]. It is seen that, our calculated values of the different types of sound velocities are in good accordance with the data available in the literature. For example, for BAs material, the deviation between our value of v_l and that of Ustundag et al. [14] is only about 1.37 %.

It is to be noted that the values 8188 m/s, 15816.03 m/s and 10884.2 m/s respectively of the longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities for BAs material obtained by Sarwan et al. [11] seem to be inaccurate; this is for two reasons. First one, we observe that the value (8188 m/s) of v_l is inferior to the value (15816.03 m/s) of v_t, this isn't true in the case of BAs material (we can see in our table 2 that $v_l > v_t$ for all authors of the literature); second one because the authors of Ref. [11] used the same formulas which we used here, and also the same experimental value of the lattice constant a (i.e. a = 4.777 Å, see input data in table 1 of the Ref. [11]) which we used in our work, so as to estimate the values of v_l, v_t, and v_m, and if we substitute their numerical values of the elastic constants: C_{11}=289 GPa, C_{12}= 70 GPa and C_{44}=160 GPa and the numerical value of the density (g= 5.224 g/cm^3) in Eqs. 4 and 5, we obtain the results (v_l = 7902.71 m/s, v_t = 5129.27 m/s, and v_m = 5626.04 m/s respectively) which are in good agreement with our values and other data of the literature.

It is also to be noted that the values 7150 m/s, 5470 m/s and 1250 m/s respectively of the longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities for BSb material obtained previously by Varshney et al. [20] seem to be also inaccurate; this is also for two reasons. First one, we observe that the value (1250 m/s) of v_m is inferior to the value (5470 m/s) of v_t, this isn't true for BSb material (because in this type of materials, we have always: $v_l > v_m > v_t$); second one, the authors of Ref. [20] used also the same formulas which we used here, with a value of the lattice constant (a = 5.12 Å, see input data in table 2 of the Ref. [20]), so as to estimate the values of of v_l, v_t, and v_m, and if we substitute their numerical values of the elastic constants: C_{11}=169.4 GPa, C_{12}= 17.6 GPa and C_{44}=254 GPa and the numerical value of the density (g= 6.561 g/cm^3) in Eqs. 4 and 5, we obtain the results (v_l = 6502.18 m/s, v_t = 4890.06 m/s, and v_m = 5249.23 m/s respectively) which also are in general in agreement with other theoretical data of the literature.

Table 2: The Computed Values of the Sound Velocities V_l, V_t, and V_m in (m/s) Of BAs And BSb Materials Along with Those Computed Through Other Methods [8], [11], [13], [14], [15], [17], [20], [21], and [22].

Material	Parameter	Our work	Other works				
BAs	v_l	7673	8350 [8]	8188 [11]	7779.69 [14]	7373 [15]	7310[17]
	v_t	4786	4500 [8]	15816.03 [11]	5114.69 [14]	5039 [15]	3900[17]
	v_m	5273	6023 [8]	10884.2 [11]	5601.24 [14]	5490 [15]	
BSb	v_l	5804	6550.4[13]	6072.134[14]	7150 [20]	6170.5 [21]	7068.6[22]
	v_t	3570	4237.6[13]	3932.59[14]	5470 [20]	3911.22 [21]	4323.68 [22]
	v_m	3940	4649.9[13]	4314.58[14]	1250 [20]	4302.35 [21]	4777.60 [22]

2. 2. Debye temperature, melting temperature, thermal conductivity and the linear thermal expansion

At low temperature, the Debye temperature can be obtained from the sound velocities. For material with cubic-zincblende phase, the Debye temperature can be obtained from the average sound velocity v_m (in km/s) and the lattice parameter a (in Å) by means of the simple following equation [23]:

$$\theta_D \approx (595.467) v_m / a \tag{6}$$

Blackman [24] has also proposed a semi-empirical formula to relate the Debye temperature to the elastic constants in the cubic system, which is given in the following.

$$\theta_D^3 = \frac{3.15}{8\pi}\left(\frac{h}{k}\right)^3 \left(\frac{n}{g^{3/2} v_a}\right) (C_{11} - C_{12})^{1/2} (C_{11} + C_{12} + 2C_{44})^{1/2} (C_{44})^{1/2} \tag{7}$$

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. Our calculated values of the Debye temperature of BAs and BSb compounds are listed in table 3, and compared with the available experimental [17] and theoretical [8], [11], [13-15], [20-23], [25-28] data. Our obtained values of θ_D are in good agreement with other theoretical results. For BSb compound, our obtained value of θ_D (491.88 K) is in excellent agreement with the theoretical value 495 K cited in the Ref. [28]; the deviation being only about 0.63 %.

The melting point of a substance depends naturally with the pressure and with the temperature. The melting temperature of several materials can be estimated with the help of the elastic constant C_{11} by the following empirical expression [23]

$$Tm = 553 + 591/Mbar\ C_{11} \pm 300K \tag{8}$$

The calculated melting point Tm of BA and BSb materials are about 2264.30± 300 K and 1758.05 ± 300 K respectively; they are also listed in table 3, and compared with the available experimental [17] and theoretical [15, 25] data. For BA compound, our obtained value of T_m is in excellent agreement with the experimental value 2300K cited in the Ref. [17]; the deviation is only about 1.55 %.

For many solids the Debye temperature θ_D is roughly proportional to the melting point T_m, these two quantities are related by the following expression [29]

$$\theta_D \approx 200/V^{1/3}\ \ Tm/M^{\ 1/2} \tag{9}$$

Where: V is the molar volume in cm^3/mole, M the molar mass in grams/mole (in our case we take $\overline{M}$ which is the average molar mass), and T_m the melting point in Kelvin.

Using our calculated values of the melting point T_m of BA and BSb materials which are: 2264.30 K and 1758.05 K respectively; the calculated values of the Debye temperature of BAs and BSb compounds are: 720.66 K and 474.22 K respectively. These two values are also in excellent agreement with the available experimental and theoretical data, and with our results obtained via the application of the formulas of Eq. (6) and Eq. (7) respectively.

The thermal conductivity K is an import property in condensed matter physics. By simple definition the thermal conductivity of solid, is the property of a solid's ability to conduct heat. At T = 300 K, the thermal conductivity K versus scaling parameter $\overline{M}a\theta_D^3$ for some group-IV, III-V and II-VI semiconductors can be given by the following relation ($\overline{M}a\theta_D^3$ in amu.cm.K^3 ; K in W/cm.K) [17].

$$K = 1.17 \times 10^{-3} (\overline{M}a\theta_D^3)^{1.15} \tag{10}$$

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

Using the values of θ_D obtained from the formula of Eq. (6), the calculated values of the thermal conductivity K are consistent with the reported data, 1.77 W/cm.K (1.53 W/cm.K [30]), and 0.90 W/cm.K (4.65 W/cm.K [28], 0.96 W/cm.K [30]) for BAs and BSb, respectively.

Our results obtained of K are in general in agreement with the results obtained in the previous work of the Ref. [30].

The linear thermal expansion coefficient α_L and the melting temperature T_m for tetrahedral structure are related by the following formula [31]

$$\alpha_L = (A / T_m) - B[d - d_0]^3 \tag{11}$$

Where: A is constant, and d is the equilibrium bond length. The value of the constant A =0.021[31]. For semiconductor A^{III}-B^{V}, the values of B and d_0 are equal to: 10 (10^{-6} K^{-1}Å^{-3}) and 1.561Å respectively [31].

The values of α_L for BX (X = As, Sb) compounds have been calculated, the results are estimated at 7.96 x $10^{-6}K^{-1}$ for BAs material and 8.98 x $10^{-6}K^{-1}$ for BSb material respectively. It is clear that our results are relatively higher than the values (4.0366 x10^{-6} K^{-1} and 4.7513 x10^{-6} K^{-1}) obtained at 300 K by Wang [26].

Table 3: The Computed Values of the Debye Temperature, the Melting Point and the Linear Thermal Expansion Coefficient α_L In (10^{-6} K^{-1}) of BX (X = As, Sb) Compounds Along with the Available Experimental Values [17] and Those Computed Through other Methods [8], [11], [13-15], [20-23], [25- 27] and [28]. [a] Using Eq. (6), [b] Using Eq. (7).

Material	Parameter	Our work	Other works
BAs	θ_D (K)	657.37 [a] 707.12 [b]	329.19 [8] 511.53 [11] 698.16 [15] 800[17] at 300K from 580.99 to 758.52 [25] 759.93[26] 956[27]
	T_m(K)	2264.30 ± 300	2333.57 ± 300[15] 2300 [17] at 300K from 2086.44 to 2505.9 [25]
	α_L	7.96	4.0366 [26] at 300K
BSb	θ_D (K)	456.07 [a] 491.88 [b]	484.8[13] 486.858[14] 228.35[20] 505.90 [21] 628.49 [26] 495[28]
	T_m(K)	1758.05 ± 300	1641.734±300 [14] 1696±300 [21]
	α_L	8.98	4.7513[26] at 300K

2. 3. The Grüneisen parameter

For cubic parameter-free crystals, the elastic constants C_{12} and C_{44}, the Grüneisen parameter γ and the temperature T are related by [32]

$$(C_{12} - C_{44}) = -27n\gamma^2 kT \ / Vz \quad \Rightarrow \quad \gamma = \left[\left[-(C_{12} - C_{44})Vz \right] / \ 27nkT \right]^{0.5} \tag{12}$$

Where n is the number of atoms in the unit cell, k is the Boltzmann constant (k = 1.3806488 × 10^{-23} m^2 kg s^{-2} K^{-1}), and V_Z is the unit-cell volume. If we make the appropriate simplifications for the zinc-blende phase, the Grüneisen parameter can be approximately estimated from the elastic constants (C_{12} and C_{44}) in (GPa) and the volume of a conventional unit cell Vz (Vz= a^3 where a is lattice parameter) in (Å^3) by means of the following formula:

$$\gamma \approx 3343.27 x10^{-5} \left[(C_{44} - C_{12})Vz \right]^{0.5} \tag{13}$$

The Grüneisen parameter γ is also given as function of the longitudinal (v_l) and the transverse (v_t) sound velocities by using the following expression [13]:

$$\gamma = \left[9(v_l^2 - (4/3)v_t^2) \right] / \left[2(v_l^2 + 2v_t^2) \right] \tag{14}$$

Using Eqs. (13) And (14), the numerical values of γ for BAs and BSb materials have been calculated and found to be 2.52 and 1.22 for BAs material and 2.15 and 1.27 for BSb material respectively. As can be noted, that our calculated values of γ for BAs material are relatively different than the theoretical value of 1.921 reported by Varshney et al. [8]. Unfortunately as far as we know, there is no another data available in the literature on γ for BAs and BSb compounds.

3. Conclusion

Employing the emperical elastic constants which are taken from our previous work which is accepted to publication in International Journal of Scientific World. The sound velocities and thermal properties of BAs and BSb materials have been predicted. The longitudinal, transverse and average elastic wave velocities, the Debye temperature, the melting temperature, the thermal conductivity, the linear thermal expansion coefficient and finally the Grüneisen parameter are predicted and analyzed in comparison with the available theoretical data of the literature. Our obtained results are in good agreement with the previous experimental and theoretical data of the literature. Except, for some thermal quantities such as the linear thermal expansion coefficient and the melting temperature of BSb material are relatively higher than the previous theoretical data of the literature.

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