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

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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; AIIIIBV compounds.

1. Introduction

The recent successful fabrication of the optoelectronic devices based on AIIIB V and AIIIBVI 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 AIII-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 ħω 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 Cij 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 [100], [110] and [111] directions respectively [16].
For elastic waves propagating along the [100] 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]:

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

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]:

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

For plane waves propagating along the [111] 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]:

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

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, $C_{12}$=120 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].**

| 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]   |
|          |                           | [001]$^b$             | 7740     | 7730 [17]   | 8360 [19]   |
| BSb      | [110]                    | [111]$^b$             | 4507     | 3900 [17]   | 4110 [19]   |
|          |                           | [110]$^b$             | 4981     | 4650 [17]   | 8570 [19]   |
|          |                           | [110]$^b$             | 7837     | 7870 [17]   | 4520 [19]   |
|          | [100]                    | [111]$^b$             | 5614     | 4170 [17]   | 4520 [19]   |
|          |                           | [100]$^b$             | 3737     |              |             |
|          | [110]                    | [111]$^b$             | 5862     |              |             |
|          |                           | [111]$^b$             | 3334     |              |             |
|          | [110]                    | [111]$^b$             | 3737     |              |             |
|          |                           | (111)$^b$             | 5943     |              |             |
|          |                           | (111)$^b$             | 3474     |              |             |

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

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

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]:

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

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 \( v_1 \) is inferior to the value (15816.03 m/s) of \( v_3 \), this isn’t true in the case of BAs material (we can see in our table 2 that \( v_1, v_3 \) 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. \( a = 4.777 \text{ Å} \), see input data in table 1 of the Ref. [11]) which we used in our work, so as to estimate the values of \( v_1, v_3 \) and \( v_{in} \) and if we substitute their numerical values of the elastic constants: \( C_{11} = 289 \text{ GPa}, C_{12} = 70 \text{ GPa} \) and \( C_{44} = 160 \text{ GPa} \) and the numerical value of the density \( (\text{g} = 5.224 \text{ g/cm}^3) \) in Eqs. 4 and 5, we obtain the results \( (v_1 = 7902.71 \text{ m/s, } v_3 = 5129.27 \text{ m/s, and } v_{in} = 5626.04 \text{ m/s respectively}) \) 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 \( (v_1) \), transverse \( (v_3) \) and average \( (v_{in}) \) 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 \( v_{in} \) is inferior to the value (5470 m/s) of \( v_1 \), this isn’t true for BSb material (because in this type of materials, we have always: \( v_1, v_{in} > v_3 \)); second one, the authors of Ref. [20] used also the same formulas which we used here, with a value of the lattice constant \( (a = 5.12 \text{ Å}, \text{see input data in table 2 of the Ref. [20]}) \), so as to estimate the values of \( v_1, v_3 \) and \( v_{in} \) and if we substitute their numerical values of the elastic constants: \( C_{11} = 169.4 \text{ GPa}, C_{12} = 17.6 \text{ GPa} \) and \( C_{44} = 254 \text{ GPa} \) and the numerical value of the density \( (\text{g} = 6.561 \text{ g/cm}^3) \) in Eqs. 4 and 5, we obtain the results \( (v_1 = 6502.18 \text{ m/s, } v_3 = 4890.06 \text{ m/s, and } v_{in} = 5249.23 \text{ m/s respectively}) \) which also are in general in agreement with other theoretical data of the literature.

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 \( v_{in} \) (in km/s) and the lattice parameter \( a \) (in Å) by means of the simple following equation [23]:

\[
\Theta_D \approx \frac{(595.467) v_{in}}{a}
\]  

(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.

\[
\Theta_D^3 = \frac{3.15}{8\pi} \left( \frac{h}{k} \right)^3 \left( \frac{n}{g} \right)^{3/2} \left( \frac{C_{11} - C_{12}}{C_{11} + C_{12} + 2C_{44}} \right)^{1/2} \left( C_{44} \right)^{1/2}
\]  

(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 BA 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 \( \Theta_D \) are in good agreement with other theoretical results. For BSb compound, our obtained value of \( \Theta_D \) (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]

\[
T_m = 553 + \frac{591}{Mbar} C_{11} \pm 300K
\]  

(8)

The calculated melting point \( T_m \) 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 \( \Theta_D \) is roughly proportional to the melting point \( T_m \), these two quantities are related by the following expression [29]

\[
\Theta_D \approx 2000 \sqrt{T_m / M} \text{K}
\]  

(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 $\overline{M}a^3$ for some group-IV, III-V and II-VI semiconductors can be given by the following relation ($\overline{M}a^3$) in amu.cm.K$^3$; $K$ in W/cm.K) [17].

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

(10)

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

Using the values of $\theta_D$ 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 $\alpha_L$ and the melting temperature $T_m$ for tetrahedral structure are related by the following formula [31]

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

(11)

Where: $A$ is constant, and $d$ is the equilibrium bond length. The value of the constant $A =$0.021[31]. For semiconductor $\Lambda^{16}$-B$^3$, the values of $B$ and $d_0$ are equal to: 10 (10$^{-4}$ K$^{-1}$) and 1.561 Å respectively [31].

The values of $\alpha_L$ for BX (X = As, Sb) compounds have been calculated, the results are estimated at 7.96 x 10$^{-4}$ K$^{-1}$ for BAs material and 8.98 x 10$^{-4}$ K$^{-1}$ for BSb material respectively. It is clear that our results are relatively higher than the values (4.0366 x10$^{-4}$ K$^{-1}$ and 4.7513 x10$^{-4}$ K$^{-1}$) obtained at 300 K by Wang [26].

| Material | Parameter | Our work | Other works |
|----------|-----------|----------|-------------|
|          | $\theta_D$ (K) | 657.37$^\circ$ | 329.19 [8] |
| BAs      | $T_m$ (K)  | 2264.30$^\pm$ | 2333.57$^\pm$ |
|          | $\alpha_L$ | 7.96 | 4.0366 [26] |
| BSb      | $T_m$ (K)  | 1758.05$^\pm$ | 1641.734$\pm$ |
|          | $\alpha_L$ | 8.98 | 4.7513 [26] |

### 2.3. The Grüneisen parameter

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

$$C_{12} - C_{44} = -27n^2k^2T/\nu_Z \Rightarrow \gamma = \left[\frac{\nu_z}{(C_{12} - C_{44})V_z} / 27nkT\right]^{0.5}$$

(12)

Where $n$ is the number of atoms in the unit cell, $k$ is the Boltzmann constant ($k = 1.3806488 \times 10^{-23}$ 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 $V_Z$ ($V_Z = a^3$ where $a$ is lattice parameter) in ($\overline{A}^3$) by means of the following formula:

$$\gamma = 3343.27x10^{-5} \left[\frac{C_{44} - C_{12}}{V_Z}\right]^{0.5}$$

(13)

The Grüneisen parameter $\gamma$ is also given as function of the longitudinal ($v_L$) and the transverse ($v_T$) sound velocities by using the following expression [13]:

$$\gamma = \frac{[9(v_L^2 - (d/2)v_T^2)]}{[2v_L^2 + 2v_T^2]}$$

(14)

Using Eqs. (13) and (14), the numerical values of $\gamma$ 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 $\gamma$ 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 $\gamma$ for BAs and BSB compounds.

3. Conclusion

Employing the empirical 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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