

THEORETICAL PREDICTION OF MECHANICAL PROPERTIES OF $B_xAl_{1-x}Sb$ TERNARY SEMICONDUCTING ALLOYS

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Article Info	Abstract
Received: 03.02.2022 Accepted: 06.04.2022 Keywords: $B_xAl_{1-x}Sb$ ternary alloys, Elastic constant, Microhardness, Debye temperature	The present work aims to predict the elastic constants and other significant properties of ordered $B_xAl_{1-x}Sb$ ($0 \leq x \leq 1$) ternary semiconducting alloys. We report the initial results of the elastic stiffness constants, the bulk modulus, the aggregate shear modulus, the Cauchy ratio, the aggregate Young's modulus, the Born ratio, the isotropy factor, the fracture toughness and the longitudinal, transverse and average sound velocities. The Debye temperature and the melting point were also predicted using two different empirical expressions. Except the Cauchy ratio, which decreases with enhancing boron content x, all other physical quantities of $B_xAl_{1-x}Sb$ alloys increase gradually and monotonically with increasing of boron concentration x in the range 0-1. Our obtained data for BSb and AlSb binary semiconducting compounds are discussed and analyzed in comparison with experimental and other theoretical values of the literature. Generally, our data for BSb and AlSb are in good agreement with other results reported previously in literature. Indeed, our obtained value (335.82 K) of the Debye temperature for AlSb compound overestimates the result (328.6 K) reported by Salehi et al. by around 2.03%, while that (1520 K) of the melting point for BSb overestimates the result (1500 K) reported recently by Bioud et al. by around 1.34%. Furthermore, to the best of our knowledge, no theoretical or experimental data were reported in the literature on the elastic constants and other properties for $B_xAl_{1-x}Sb$ alloys to compare with them.

1. Introduction

In recent years, III–V binary compounds and their alloys constitute one of important class of functional materials. These materials have been extensively studied, because they served as substances in the fabrication of optoelectronic and electronic devices [1, 2].

At ambient pressure and room temperature, both aluminum antimonide (AlSb) and boron antimonide (BSb) crystallize in the zincblende (B3) structure [1].

Daoud *et al.* [3] have determined some interesting properties of $B_xAl_{1-x}Sb$ alloys using different empirical expressions, while Benchehima *et al.* [4] have studied the structural parameters, electronic band structures, densities of states and optical properties of the ordered $B_xAl_{1-x}Sb$ at different boron concentrations x using full potential linearized augmented plane wave (FP-LAPW) method. The latter is based on the DFT with both the local density approximation (LDA) and the generalized gradient approximation of Wu and Cohen (GGA-WC).

Using FP-LAPW basis sets in the DFT with the Modified Becke Johnson (m-BJ) exchange correlation potential, Tiwari *et al.* [5], have very recently studied the optoelectronic properties of zincblende BSb compound. They found that BSb material could be very useful for realizing solar cells with better energy conversion efficiency (13.76% for BSb semiconducting material compared to 7.87% for the silicium).

Experimentally, Das and co-authors [6] have measured a narrower indirect-gap of around 0.52 eV for BSb thin films deposited on glass, fused silica and silicon substrates by pulsed laser deposition technique. It should be noted that the value (0.52 eV) of E_g reported by Das *et al.* [6] for BSb material required another experimental confirmation. Thus because a very higher theoretical values: 1.278 (1.096), 0.997 and 1.24 eV were reported by Benchehima *et al.* [4], Tiwari and co-authors [5], and Ge *et al.* [7], respectively.

Using the quasi-harmonic Debye model, Bioud *et al.* [8] have studied the effect of the temperature and pressure on the thermodynamic properties of BSb compound. They also estimated the microhardness, the electronic polarizability, and the thermal conductivity.

Vassiliev *et al.* [9] have determined several thermodynamic properties of seventeen III–V semiconducting materials using a correlate method between the thermodynamic quantities and other physical parameters, while Daoud *et al.* [10] have studied the pressure effect on the structural parameters, elastic constants and electronic properties of cubic BSb compound.

For some element having cubic diamond structure and several III-V compounds having cubic zincblende phase, Powell [11] proposed a simple method for the prediction of the elastic constants C_{ij} from the lattice constant a . He established two analytical models, the first based

on the experimental lattice constants, while the second is based on the theoretical lattice constants obtained from the DFT. The approach of Powell [11] was based on reliable parameterization of the Tersoff potential for III-P and III-Sb materials, which were previously not available [11], [12]. In order to obtain reliable parameterization of the Tersoff potential, Powell *et al.* [12] developed a simple algorithm, which is called *granular radial search*.

In the present paper, we predict the elastic constants and related properties of $B_xAl_{1-x}Sb$ alloys using a theoretical approach proposed by Powell [11].

2. Theory

It should be noted that the lattice constant is a fundamental structural parameter, which is related with the bond-length parameter [13]. In cubic crystals, there are three (C_{11} , C_{12} , and C_{44}) independent elastic constants [14], while for isotropic solids there are only 2 independent elastic constants.

The theoretical approach of Powell [11] is new model of Keyes' relation, which relates the elastic properties of crystal to the lattice parameter, established essentially for some element having cubic diamond structure and III-V materials having cubic zincblende phase. The major advantage of this approach is the possibility of the prediction of the elastic and cohesive properties of a material with the same accuracy as an *ab initio* calculation, but with a substantially lower computational demand; while the major disadvantage of this approach is that the empirical potentials (EPs) are not universal, so often different parametrizations can be found that correctly predict only a specific type of structural, cohesive or vibrational property [11], [12].

In the model proposed by Powell [11], the reduced elastic constants C_{11}^* , C_{12}^* , and C_{44}^* are calculated using the following 2nd order polynomial expressions [11]:

$$C_{11}^* = 0.0504a^2 - 0.5211a + 3.0524 \quad (1a)$$

$$C_{12}^* = -0.1206a^2 + 1.3079a - 2.6653 \quad (1b)$$

$$C_{44}^* = -0.0054a^2 - 0.0562a + 1.3893 \quad (1c)$$

where a is the equilibrium lattice constant. The equilibrium lattice constant a and cohesive energy E_{coh} (expressed in eV/atom) are easily estimated from the energy vs bond length relationship at the energy minimum [12].

All the lattice constants (predicted from the DFT) used here in the equations (1a), (1b), and (1c) were taken from the work of Benchehima *et al.* [4].

The independent elastic constants C_{11} , C_{12} , and C_{44} are expressed as follow [11]:

$$C_{11} = C_{11}^* c_0, C_{12} = C_{12}^* c_0, \text{ and } C_{44} = C_{44}^* c_0 \quad (2)$$

where $c_0 = e^2/d^4$ is a normalizing factor, d is the bonding distance, and e is the electronic charge ($e = 1.60217646 \times 10^{-19}\text{C}$).

So in the present work, we firstly calculate the reduced elastic constants C_{11}^* , C_{12}^* , and C_{44}^* using the equations (1a), (1b), and (1c), respectively; then, secondly, we determine the elastic constants C_{11} , C_{12} , and C_{44} through the equation (2). For cubic crystals, the elastic constants (C_{11} and C_{12}) and the bulk modulus B are related by $B = (C_{11} + 2C_{12})/3$ [2].

3. Discussion of results

3. 1. Elastic constants and modules

After the prediction of the elastic constants C_{ij} of any crystal, it is possible to calculate several other macroscopic elastic modules (bulk modulus B , Young modulus E ,...etc). Usually, both the bulk modulus B and the Young modulus E increase with increasing pressure, and decreases with enhancing temperature at atmospheric pressure.

Figure 1 presents the variation of the elastic constants C_{ij} and the bulk modulus B of zincblende $B_x\text{Al}_{1-x}\text{Sb}$ material as a function of boron concentration x . As shown in Fig. 1, we observe that all the C_{ij} and B increase monotonically with increasing boron content x . The elastic constants C_{11} , C_{12} , C_{44} and B for AlSb material are equal to: 91.68, 43.16, 44.23, and 59.33 GPa, respectively; while these of BSb were found to be: 170.97, 87.67, 95.40, and 115.43 GPa, respectively.

Our results of C_{ij} and B are in agreement with the experimental and other theoretical values of the literature. For example, our obtained value (43.16 GPa) of C_{12} for AlSb underestimates the experimental one (43.41 GPa) reported by Adachi [2] by around 0.58%, while our value (115.43 GPa) of B for BSb overestimates the theoretical result (115.05 GPa) reported by Salehi and co-authors [1] by around 0.33%. We note that no measurements of C_{ij} and other elastic moduli for BSb have been reported to date; however, the thin film crystal of BSb has been grown [6].

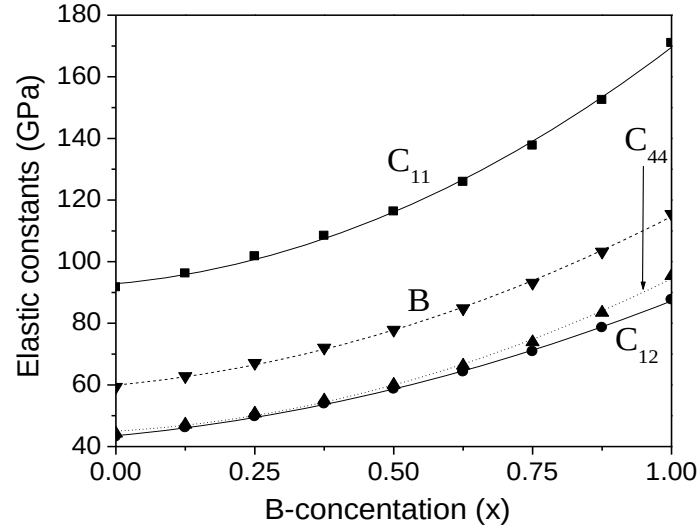


Figure 1. Elastic constants and bulk modulus of $B_xAl_{1-x}Sb$ versus boron concentration x

The mechanical stability of $B_xAl_{1-x}Sb$ alloys is checked in this study in terms of C_{ij} 's using the zero-pressure elastic stability criteria [15]:

$$C_{11} > 0; C_{44} > 0; (C_{11} + 2C_{12}) > 0; (C_{11} - C_{12}) > 0 \quad (3)$$

Based on our data, all criteria mentioned in Eq. (3) are satisfied for all boron concentrations ranging from 0 to 1, which indicates that $B_xAl_{1-x}Sb$ is mechanically stable for all boron contents in the range 0-1.

The best fits of our data regarding the elastic constants C_{ij} and the bulk modulus B for $B_xAl_{1-x}Sb$ as a function of x obey the following quadratic expressions:

$$C_{11} = 92.81 + 16.44x + 60.27x^2 \quad (4a)$$

$$C_{12} = 43.50 + 16.91x + 26.83x^2 \quad (4b)$$

$$C_{44} = 44.96 + 10.53x + 38.98x^2 \quad (4c)$$

$$B = 59.94 + 16.75x + 37.98x^2 \quad (4d)$$

Contrary to plastic deformation, in the elastic deformation, a linear proportionality between the stress and the strain was observed. The shear modulus G , Young's modulus E and Poisson's ratio σ play an important role in the mechanical properties of materials. The shear modulus was used to evaluate the resistance to deformation upon shear stress of the solid, while the Young modulus E was used to measure its stiffness [16]. In the aggregate material, the bulk

modulus B and the shear modulus G are firstly estimated via the Vogit-Reuss-Hill (VRS) approach [17], then the Young modulus E is derived from B and G as follow $E = [9BG/(3B+G)]$ [16]. The variations of G and E versus x for $B_xAl_{1-x}Sb$ alloys are plotted in Fig.2.

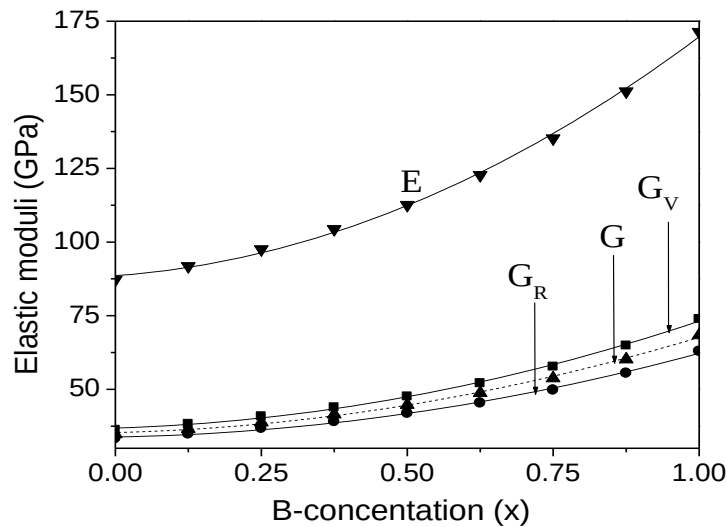


Figure 2. Variations of G and E for $B_xAl_{1-x}Sb$ alloys with x

Like as the elastic constants C_{ij} and the bulk modulus B , both G and E increase also monotonically with increasing B-concentration x , as it can be seen in Fig.2. The quadratic fits of our data regarding G and E as a function of x obey the following expressions, respectively: $G = 35.33 + 4.83x + 27.52x^2$, and $E = 88.58 + 14.15x + 66.92x^2$. The Young's modulus E of AlSb ($x = 0$) is equal to 88.58 GPa, this value is slightly lower than the theoretical result (91.92 GPa) reported by Salehi *et al.* [1]. Our value under-estimates the theoretical one reported by Salehi and co-authors [1] by around 3.7%.

In addition, our value of E for BSb was found 171.4 GPa. Although our value of E is lower than the theoretical result (210.06 GPa) reported by Salehi *et al.* [1], it is in general in agreement with the theoretical result (175.8 GPa) reported by Wang and Ye [18]. Our obtained result of E underestimates the theoretical value reported by Wang and Ye [18] by around 2.5%.

Another useful mechanical parameters are the Cauchy ratio Ca , the Born ratio Bo and the isotropy factor A . For crystals with diamond and cubic zincblende structures, the Cauchy ratio Ca , Born ratio Bo and the isotropy factor A are defined as [2]:

$$Ca = C_{12}/C_{44} \quad (5)$$

$$Bo = (C_{11} + C_{12})^2/[4C_{11}(C_{11} - C_{44})] \quad (6)$$

$$A = (C_{11} - C_{12})/(2C_{44}) \quad (7)$$

It should be noted that Bo and A are closely correlated with the bond ionicity in III-V and II-VI binary semiconducting compounds [2].

Fig.3 shows the dependence of Ca , Bo and A for $B_xAl_{1-x}Sb$ alloys as a function of x . The Cauchy ratio Ca begin with the value 0.976 at $x = 0$, it increases very slowly with increasing x up to 0.981 at $x = 0.25$, then decreases with increasing x up to 0.92 at $x = 1$. Beyond boron content $x > 0.25$, the effect of x on Ca becomes more pronounced. The present calculations regarding Bo yield values of approximately 1.04 for AlSb and 1.29 for BSb, respectively. As far as the boron content is increased in $B_xAl_{1-x}Sb$ ternary alloys, Bo enhanced also with increasing x , indicating that the change in the ionicity of the system of interest enhanced with increasing boron content x . The isotropy factor A of AlSb and BSb are found to be 0.549 and 0.437, respectively. As a matter of fact, anisotropic material must have $A=1$, whilst less or greater value of A than 1 points to anisotropic nature of the material. Hence, the degree of elastic anisotropy depends on the deviation of A from 1.

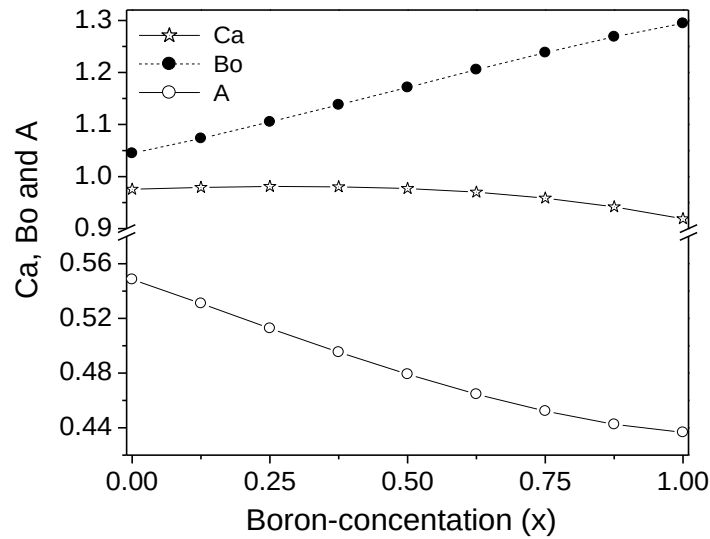


Figure 3. Variations of the Cauchy ratio Ca , Born ratio Bo and isotropy factor A for $B_xAl_{1-x}Sb$ as a function of x

Figure 3 shows also that the elastic isotropy in $B_xAl_{1-x}Sb$ alloys decreases with increasing x , reflecting the increase of the degree of the anisotropy with increasing x . The best fits of our data regarding Ca , Bo and A for $B_xAl_{1-x}Sb$ alloys as a function of x obey the following expressions:

$$Ca = 0.974 + 0.066x - 0.119x^2 \quad (8)$$

$$Bo = 1.042 + 0.264x - 0.008x^2 \quad (9)$$

$$A = 0.550 - 0.169x + 0.054x^2 \quad (10)$$

The bowing parameters are found to be equal -0.119 for Ca , -0.008 for Bo and 0.054 for the isotropy factor A , respectively. Our obtained values of Ca , Bo and A for AlSb are in very good agreement with the experimental results 1.00 , 1.05 and 0.543 , respectively [2]. The deviations between our values and these reported by Adachi [2] are only around 2.4 , 0.95 , and 1.1% , respectively.

Hardness H and fracture toughness K_{IC} of materials are two important mechanical parameters. H is defined as its ability to resist plastic deformation, while K_{IC} describes the resistance of a material against crack propagation [19]. Experimentally, the fracture toughness K_{IC} of material was usually estimated from the indentation load P and the trace length C of the crack measured from the center of the indentation. For ionic and covalent materials, the K_{IC} can be estimated from Niu's [20] empirical model, which is expressed as follow: $K_{IC} = V_0^{1/6}(B/G)^{1/2}G$, where V_0 is the volume of atom (expressed in m^3), B and G are the bulk modulus and the shear modulus, respectively (both B and G are expressed in MPa). The fracture toughness K_{IC} of AlSb and BSb are found to be 0.79 and 1.43 MPa.m^{1/2}, respectively. These two values are slightly higher than the value (0.44 MPa.m^{1/2}) of GaAs compound [20], and slightly lower than the theoretical values 2.82 and 3.12 MPa.m^{1/2} reported by Zhang and McMahon [19] for ZrC and HfC, respectively. The variations of K_{IC} versus the alloy composition x for $B_xAl_{1-x}Sb$ alloys is plotted in Fig. 4.

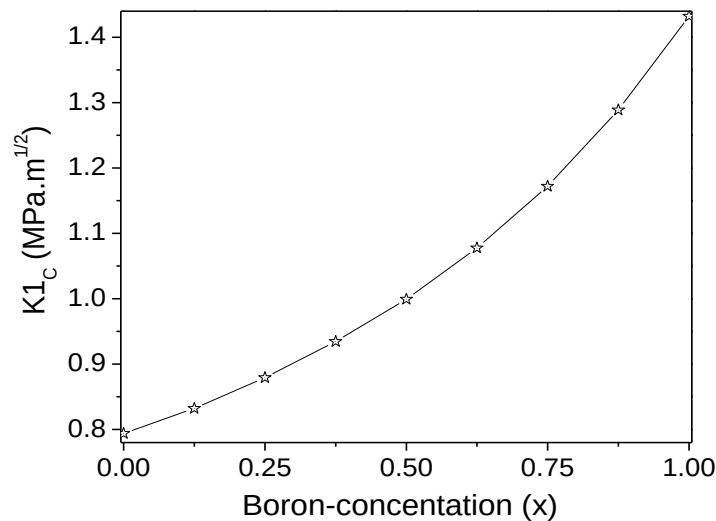


Figure 4. Dependence of K_{IC} with x for $B_xAl_{1-x}Sb$ ternary alloys

As can be seen in this figure, the fracture toughness K_{IC} increases monotonically with increasing x . The fit of our data on the K_{IC} as a function of x obeys the following expression:

$K_{IC} = 0.802 + 0.165x + 0.455x^2$. The quadratic term (0.455) in the previous equation is the bowing parameter of the fracture toughness.

3.2 Bulk sound velocity

Two types of waves were observed in anisotropic material, longitudinal waves and shear waves. If the mass density ρ and the stiffness elastic constant C_{ij} of a solid are known, usually one can calculate the bulk sound velocity. The average sound velocity is given by the following formula [1], [15]:

$$v_m = \left(\left(2/v_t^3 + 1/v_l^3 \right) / 3 \right)^{-1/3} \quad (11)$$

where v_t and v_l are the transverse and longitudinal sound velocity obtained by using the shear modulus G , the bulk modulus B and the mass density ρ [1], [15]:

$$v_t = (G/\rho)^{1/2}, \quad v_l = ((3B + 4G)/3\rho)^{1/2} \quad (12)$$

In general, the pure amorphous materials have lower density than the corresponding crystalline phases [21]. The variations of the longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities versus x for $B_xAl_{1-x}Sb$ alloys are plotted in Fig. 5. As can be seen in Fig. 5, all the sound velocities increase monotonically with increasing x . The quadratic fits of our data regarding the sound velocities for $B_xAl_{1-x}Sb$ ($0 \leq x \leq 1$) alloys as a function of x obey the following expressions:

$$v_l = 4.942 + 0.510x + 0.280x^2 \quad (13)$$

$$v_t = 2.837 + 0.207x + 0.251x^2 \quad (14)$$

$$v_m = 3.151 + 0.239x + 0.270x^2 \quad (15)$$

The longitudinal, transverse and average sound velocities of AlSb are equals to: 4940, 2833 and 3147 m/s, respectively, while these of BSb are equals to: 5736, 3300 and 3665 m/s, respectively. So, when the boron concentration x increases from 0 to 1, the corresponding enhancements in v_l , v_t and v_m are of about 16.11, 16.48, and 16.46%, respectively. Although our values of the sound velocities for BSb are slightly lower than the theoretical ones (6550.4, 4237.6 and 4649.9 m/s, respectively) reported in Ref. [1], these of AlSb are in general agree

with the values 5079.9, 3114 and 3437.5m/s, respectively reported by Salehi *et al.* [1].

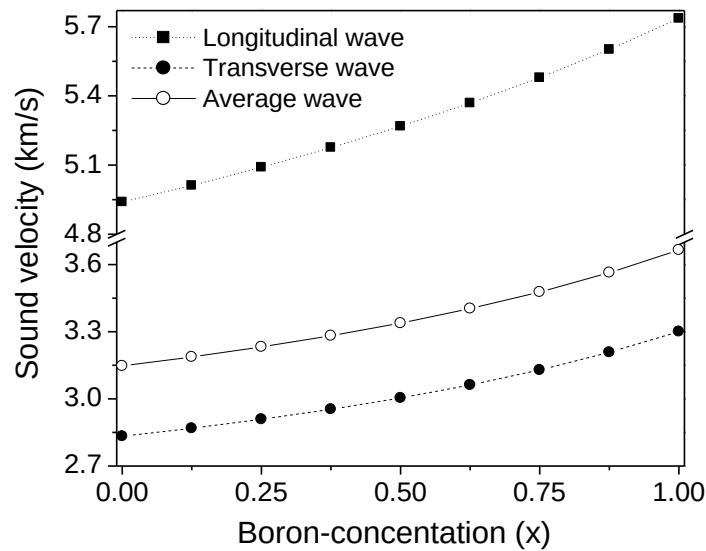


Figure 5. Boron content x induced variation in the sound velocities for the ordered $B_xAl_{1-x}Sb$ alloys

It is to be mentioned that the value of 1250 m/s of v_m for BSb obtained previously by Varshney *et al.* [22] seems to be incorrect. This is because the authors of Ref. [22] used the same formula which we used here (i.e. Eq. 11) so as to estimate the value of v_m , and if we substitute their values ($v_l = 7150$ m/s and $v_t = 5470$ m/s) in Eq. (11), we obtain the result ($v_m = 5854$ m/s) which is in general in agreement with the value 4649.9 m/s reported by Salehi *et al.* [1].

3.3. Thermal properties

Accurate knowledge of semiconductors, along with their thermal properties, is of particular importance in describing the effect of temperature on material properties. The Debye temperature θ_D is an important thermal property for the designing of materials [23]. It is fundamental parameter in the investigation of a large number of solid state problems involving lattice vibrations, especially the electrical resistivity, the scattering of thermal neutrons, and the thermal conductivity [14]. This quantity is usually obtained by fitting the observed specific heats C_v formula at the point of 0.5 Dulong-Petit value ($3Nk_B/2$), or from the ultrasonic measurement [2].

There have been several attempts to estimate the Debye temperature using simple expressions based on the atomic or molecular weight, lattice constant, plasmon energy, melting point, etc. The Debye temperature θ_D and the average sound velocity (v_m) are related by [15]:

$$\theta_D = (h/k_B)(3/4\pi V_a)^{1/3} v_m \quad (16)$$

where: h is the Planck constant; k_B is the Boltzmann constant, and V_a is the atomic volume.

The Debye temperature θ_D of AlSb and BSb compounds are found to be 306.71 and 420.12 K, respectively. Our value (306.71 K) of θ_D for AlSb is in very good agreement with the result (299.8K) reported by Verma *et al.* [14]. The deviation between these two values is only around 2.3%. Figure 6 shows the variation of θ_D as a function of boron concentration x . The Debye temperature θ_D increases with increasing boron content x .

For several materials, the Debye temperature θ_D can be obtained from the elastic constants using this expression [24]:

$$\theta_D = C_B (a G_B / M)^{1/2} \quad (17)$$

where $C_B = 3.89 \times 10^{11} n^{-1/6} h / k_B$, n is the number of atoms in the unit cell, h is Planck's constant, k_B is Boltzmann's constant, M is the atomic weight, a is the lattice parameter, and G_B is a function of the elastic constants C_{ij} [24]. Using Eq. (17), the dependence of θ_D with x for $B_x Al_{1-x} Sb$ is also plotted in Fig. 6. The 2nd order polynomial fit of our data regarding θ_D for $B_x Al_{1-x} Sb$ alloys as a function of x obeys this expression: $\theta_D = 335.82 + 49.46x + 70.32x^2$. The Debye temperature θ_D of AlSb material is equals to 335.82 K, while that of BSb compound is found to be 456.9 K. Although our value of θ_D for AlSb is slightly lower than the experimental one (370 K) measured at $T = 273$ K [2], and slightly higher than the low-temperature limit $\theta_D(0) = 292$ K reported by Adachi [2], it is in good agreement with the result (328.6K) reported by Salehi *et al.* [1]. Our value of θ_D for AlSb overestimates the result (328.6 K) of Salehi and co-authors [1] by around 2.03%. Our result of θ_D is also largely higher than the result (170.21 K) reported by Varshney *et al.* [22].

The melting phenomenon happens when the Gibbs free energy of the liquid becomes lower than that of the solid phase for the considered material. In recent years, there has been a tremendous amount of works on the melting point T_m correlation with the elastic constants C_{ij} in solids [25], [26]. However, in spite of all this, no unique empirical model is available which can explain fairly well the correlation of the melting point T_m with the elastic constants for all solids in general [26]. For materials with cubic structures, the melting point T_m and the elastic constants C_{ij} are related by [15]:

$$T_m = 560.4 + 7.805 C_{11} - 3.094 C_{12} - 1.086 C_{44} \quad (18)$$

where the elastic constants C_{ij} are expressed in GPa, and the melting point T_m is expressed in K.

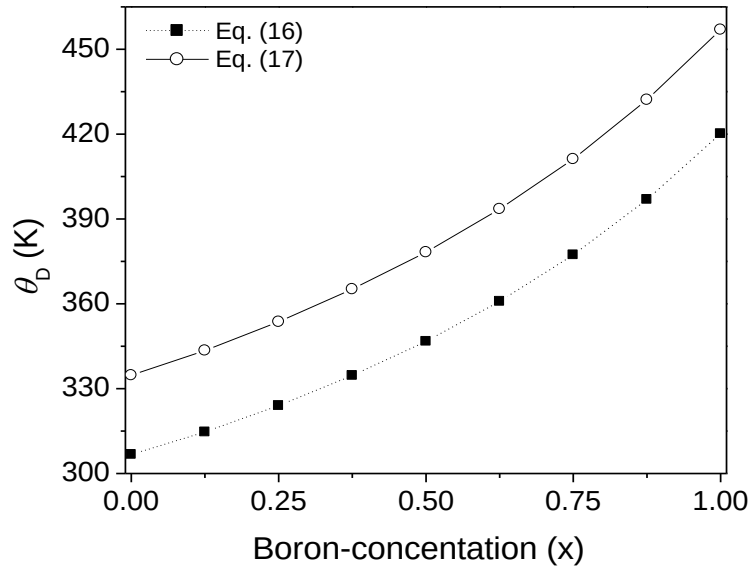


Figure 6. Dependence of θ_D with x for $B_xAl_{1-x}Sb$ ternary alloys

By substituting our calculated elastic constants into Eq. (18), T_m has been evaluated. The melting point T_m of AlSb is equals to 1094.4 K, while that of BSb is equals to 1520 K. Although our value of T_m for AlSb is slightly lower than the experimental one (1338 K) reported by Adachi [2], that of BSb compound is in very good agreement compared to the value (1500 K) reported by Bioud and co-authors [8]. The deviation between the two values is only around 1.34%. The variations of T_m with x for $B_xAl_{1-x}Sb$ are plotted in Fig. 7. The enhancing of T_m with increasing of x can explain the strong interatomic bonding in BSb compared to AlSb compound. The fit of our values on T_m for $B_xAl_{1-x}Sb$ alloys as a function of x obeys this expression: $T_m = 1101.36 + 64.60x + 345.08x^2$.

A second empirical expression correlates the elastic constant C_{11} (in Gpa) and the melting temperature T_m (in K) of cubic crystal; it is given as follow [27], [28]:

$$T_m = 553 + 5.91C_{11} \pm 300 \quad (19)$$

The variation of T_m with x for $B_xAl_{1-x}Sb$ alloys is also plotted in Fig. 7, along the results reported very recently by Daoud *et al.* [3]. The best fit of our values on T_m for $B_xAl_{1-x}Sb$ alloys as a function of x obeys this expression: $T_m = 1101.51 + 97.18x + 356.21x^2$.

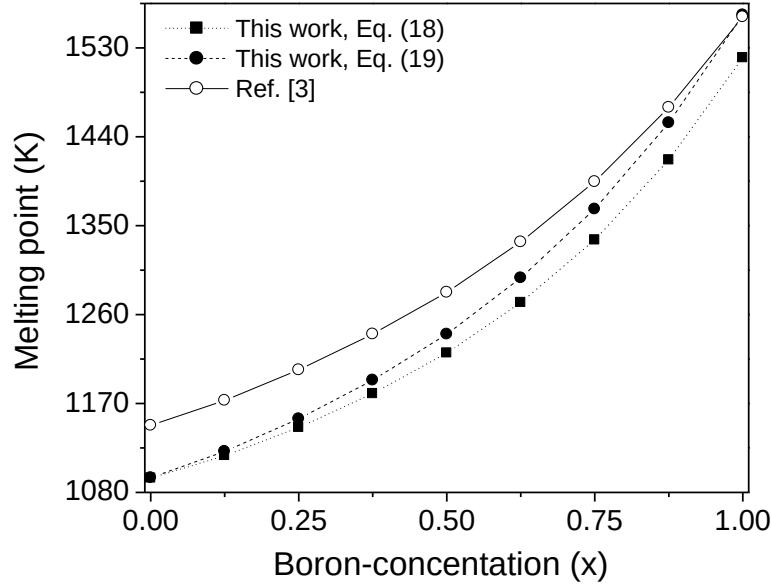


Figure 7. Dependence of T_m with boron concentration x for $B_xAl_{1-x}Sb$ alloys

The melting point of AlSb is equals to 1094.9 ± 300 K, while that of BSb is around 1563.4 ± 300 K, respectively. These two values are in good agreement with those obtained from Eq. (18). The deviation between our value (1563.4 K) of T_m for BSb and the value (1500 K) reported by Bioud *et al.*[8] is around 4.23%.

4. Conclusion

The Based on a theoretical approach and the lattice constants reported in the literature, the present work aims to calculate the elastic constants and some other properties of $B_xAl_{1-x}Sb$ alloys. Our study shows that the elastic constants and the directional anisotropy are closely related to chemical composition. Our investigation shows also a correlation between the elastic constants and the thermal properties. This correlation was also observed for most of the tetrahedral bonded semiconductors in the group III-V and II-VI families. The elastic constants, the fracture toughness, the Debye temperature, the sound velocities, and the melting point increase gradually and monotonically with increasing boron (B) concentration x .

The analysis of our data for AlSb and BSb binary compounds shows in good agreement with other values of the literature. For example the deviation between our obtained value of C_{12} for AlSb compound and the experimental one reported by Adachi [2] is only around 0.58%, while the deviation between our value of the Debye temperature θ_D of AlSb and the theoretical result reported by Salehi and co-authors is only around 2.03%.

Except the data existing in the literature for AlSb and BSb compounds, as far as we know, there is no data available in the literature on the elastic constants and other properties for $B_xAl_{1-x}Sb$ alloys. Thus, our findings are predictions and may shed some light on these alloys. Our findings still await experimental and other theoretical confirmation, they may also serve as a reference for future studies.

References

- [1] H. Salehi, H. Badehian, M. Farbod, Mater. Sci. Semicond. Process., **26** (2014) 477.
- [2] S. Adachi, *Properties of Group-IV, III-V and II-VI Semiconductors*, John Wiley & Sons Ltd: (2005).
- [3] S. Daoud, P. K. Saini, H. Rekab-Djabri, J. Nano- Electron. Phys., **12** (2020) 06008.
- [4] M. Benchehima, H. Abid, A.C. Chaouche, and A. Resfa, Eur. Phys. J. Appl. Phys., **77** (2017) 30101.
- [5] V. Tiwari, I. Mal, S. K. Agnihotri, D. P. Samajdar, Mater. Sci. Semicond. Process., **122** (2021) 105505.
- [6] S.N. Das, R. Bhunia, S. Hussain, R. Bhar, B.R. Chakraborty, A.K. Pal, Appl. Surf. Sci., **353** (2015) 439.
- [7] Y. Ge, W. Wan, X. Guo, Y. Liu, Opt. Express, **28** (2020) 238.
- [8] N. Bioud, X.W. Sun, S. Daoud, T. Song, Z.J. Liu, Mater. Res. Express., **5** (2018) 085904.
- [9] V.P. Vassiliev, B. Legendre, V.P. Zlomanov, Intermetallics, **19** (2011) 1891.
- [10] S. Daoud, N. Bioud, N. Lebga, L. Belagraa, R. Mezouar, Indian J. Phys., **87** (2013) 355.
- [11] D. Powell, *Elasticity, lattice dynamics and parameterisation techniques for the Tersoff potential applied to elemental and type III-V semiconductors*, Thesis of Doctor of Philosophy, University of Sheffield, South Yorkshire, England, (2006).
- [12] D. Powell, M.A Migliorato, A.G Cullis, Phys. Rev. B, **75** (2007) 115202.
- [13] S. Daoud, J. Nano- Electron. Phys., **11** (2019) 05004.
- [14] J.K.D. Verma, B.D. Nag, P.S. Nair, Z. Naturforsch. A, **19** (1964) 1561.
- [15] T. Özer, Can. J. Phys., **98** (2020) 357.
- [16] C. Wang, S. Liang, J. Cui, X. Wang, Y. Wei, Vacuum, **169** (2019) 108844.
- [17] H. Rekab-Djabri, M. M. Abdus Salam, S. Daoud, M. Drief, Y. Guermit, S. Louhibi-Fasla, J. Magnes. Alloy., **8** (2020) 1166.
- [18] S.Q. Wang, H.Q. Ye, Phys. Status Solidi B, **240** (2003) 45.
- [19] J. Zhang, J. M. McMahon, J. Mater. Sci., **56** (2021) 4266.
- [20] H. Niu, S. Niu, A.R. Oganov, J. Appl. Phys., **125** (2019) 065105.

- [21] S. Daoud, N. Bioud, N. Lebga, J. Optoelectron. Adv. Mater., **16** (2014) 207.
- [22] D. Varshney, G. Joshi, M. Varshney, S. Shriya, Physica B, **405** (2010) 1663.
- [23] A. Erkişi, Acta Phys. Pol. A, **140** (2021) 243.
- [24] P. K. Jha, M. Talati, Phys. Status Solidi B, **239** (2003) 291.
- [25] S. Daoud, N. Bouarissa, Theor. Chem. Accounts. **138** (2019) 49.
- [26] H. Rekab-Djabri, S. Daoud, M. M. Abdus Salam, S. Louhibi-Fasla, Acta Phys. Pol. A, **140** (2021) 34.
- [27] N. Bioud, X-W. Sun, S. Daoud, T. Song, R. Khenata, S. Bin Omran, Optik, **155** (2018) 17.
- [28] S. Daoud, N. Bouarissa, A. Benmakhlouf, O. Allaoui, Phys. Status Solidi B, **257** (2020) 1900537.