International Journal of Scientific World, *3 (1) (2015) 37-42*
www.sciencepubco.com/index.php/IJSW
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doi: 10.14419/ijsw.v3i1.4022
Research paper

Empirical study of elastic properties of BX (X = As, Sb) materials

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Abstract

The principal goal of this work is the prediction of elastic properties of Boron-Arsenide (BAs) and Boron- Antimonide (BSb) materials by means of some emperical formulas and with the help of two experimental physical quantities (the bond length and the bulk modulus which are taken from the literature for BAs material and the bond length only for BSb material). The homopolar and heteropolar energies, the bonding-antibonding energy gap, the covalency, the elastic constants, the Kleinman parameter, the Cauchy discrepancy in elastic constant, the Cauchy coefficient, the Born ratio, the cohesive energy and finally the Knoop microhardness are predicted and analyzed in comparison with the available theoretical data of the literature. Our obtained results are in general in agreement with other previous theoretical data.

Keywords: *Elastic Properties; Bond-Orbital Model; BAs and BSb Materials.*

1. Introduction

In view of their important properties for several technological applications, and especially in the linear and nonlinear optics, solar cells and light-emitting diodes; several binary compound materials with zinc-blende (ZB) and wurtzite (Wu)-type structure have attracted increasing research interest in the last few years [1].

Varshney et al. [2] have investigated the effect of the hydrostatic pressure on the mechanical properties, longitudinal and transverse sound velocity and Debye temperature of boron based pnictides BY (Y = N, P and As) in zincblende and NaCl phases by formulating an effective interionic interaction potential. By analyzing of the Poisson's ratio and the ratio $R_{S/B}$ they found that at low pressures, the boron monopnictides BY (Y = N, P and as) are brittle in nature in ZnS phase and ductile in nature at high pressures in both ZnS and NaCl phases.

Sarwan et al. [3] have studied the pressure induced phase transition from the zincblende to rocksalt structural phase and some other thermophysical properties of BP and BAs semiconductor compounds.

In object to study the electronic properties of BX (X= N, as and Sb) compounds, Bouhafs et al. [4] have performed an ab initio investigation using a plane-wave expansion within the local density and the pseudopotential approximations. They found that the electronic properties of these compounds have been features differ from those of other usual III-V materials (the direct band gap pressure coefficient is nearly independent of the anion substitutions). The Boron-Arsenide (BAs) material has been arousing increasing interest, both theoretically and experimentally, because of its potential inherent advantages [4-6].The anomalously deep-lying 2s and 2p levels have a marked effect on the ionicity of the BX (X= As, Sb) materials, they are strongly reduced (f_i = 0.044 for BAs, and f_i = 0.112 for BSb material) compared to other usual $A^{III}B^{V}$ semiconductors [6].

The BX (X= As, Sb) materials possess also some others important characteristics such as the inverse role between the cation and the anion in terms of charge transfer [5], [7]. The bulk modulus of BAs material has been determined experimentally by Greene et al. [8], it is measured at value 148 GPa.

In the present work, some physical quantities such as: the homopolar and heteropolar energies, the bonding-antibonding energy gap, the covalency, the elastic constants, the Kleinman parameter, the Cauchy discrepancy in elastic constant, the Cauchy coefficient, the Born ratio, the cohesive energy and the Knoop microhardness of BX (X= As, Sb) compounds are predicted, analyzed and compared with experimental and other theoretical data of the literature.

2. Theory, results and calculations

2. 1. Homopolar and heteropolar energies and the bonding-antibonding energy gap

One of the most popular ways of representing dependence in the physical properties of semiconductor materials is through the use of the bond length d. The bond length d named also Nearest-neighbors distance (NN), is in important factor and it plays a very important role in solid state physics; it was defined as the average distance between nearest-neighbor atoms. In the solids with cubic crystal, the bond lengths is equal to: $\sqrt{3}\, a_0/4$ (where: a is the lattice constant). For (B3) BAs compound, the experimental value of the bond length can be deduced from the experimental value of the lattice constant (a = 4.777 Å) [9]. So the bond length, $d = \sqrt{3}\, a/4 = \sqrt{3}\,(4.777)/4 = 2.069$ Å.

The experimental bond length (d) of BSb compound can be deduced from the d-spacing (d_{hkl}) obtained by the authors [10]. The d-spacing obtained by the authors [10] are about 0.21 nm which matched well for plane (112) of (B3) phase. In a cubic lattice, the perpendicular distance (d-spacing) between two adjacent planes of a set with the Miller indices (hkl) and the lattice constant an are related by the following formula:

$$d_{hkl} = a/\,(h^2+k^2+l^2)^{1/2} \Rightarrow a = d_{hkl}.(h^2+k^2+l^2)^{1/2} \qquad (1)$$

Using the d-spacing of the authors [10], which is equal to: 2.1 Å for the plane (112) of (B3) phase, we can obtain the value of the lattice constant (a = 5.144 Å), so the experimental bond length d of BSb material is: $d = \sqrt{3}\, a/4 \approx 2.227$ Å.

An empirical relation has been observed for some $A^{III}B^{V}$ semiconductors between the bulk modulus B (in GPa) and the nearest-neighbor distance d (in Å), it can be given by the following formula [11]:

$$B = 1761 d^{-3.5} \qquad (2)$$

Another empirical relation is observed for some group-IV, $A^{III}B^{V}$ and $A^{II}B^{VI}$ materials between the bulk modulus B (in 10^{11} dyn/cm^2) and the nearest-neighbor distance d (in Å), it can be given by the following expression [12].

$$B = (4.05/d)^{3.98} \qquad (3)$$

The results obtained of the bulk modulus for BSb material are given in Table 1, and compared with the previous theoretical data [5-7]. As can be seen that our calculated value (106.8 GPa) of the bulk modulus B is in excellent agreement with the previous calculation data, it's deviates from the theoretical value (108 GPa) of the Ref. [6] by only 1.11 %. As can be seen also that our value (108 GPa) of B obtained from the application of the Eq. (3) is also in excellent agreement with other available theoretical data [5-7], and with our previous value obtained from the relation of Eq. (2), the deviation between these two values being also about 1.11 %.

Table 1: Bulk Modulus B in (Gpa) Of BSb Material In Comparison With Other Theoretical Data [5-7]. [a] From the Relation of Equation (2), [b] from the Relation of Equation (3).

Parameter	Our work		Other works			
B	106.8 [a]	108 [b]	116[5]LDA	100[5]GGA	108[6]	103[7]

For some $A^{III}B^{V}$ materials, the homopolar energy (E_h) can be given as function of the bond length d by the following formula [13]:

$$E_h = 39.74\,(d)^{-2.48} \qquad (4)$$

On the other hand, the heteropolar energy (E_c), the bonding-antibonding energy gap ($E_{g(A\text{-}B)}$), the homopolar energy (E_h), and the ionicity (f_i) are related by the following relations [13]:

$$f_i = 1 - \left(E_h^2/\left|Eg_{(A-B)}\right|^2\right) \Rightarrow Eg_{(A-B)} = \sqrt{E_h^2/(1-f_i)} \Rightarrow Eg_{(A-B)} = E_h(1-f_i)^{-0.5} \qquad (5\text{-a})$$

$$\left|Eg_{(A-B)}\right|^2 = E_h^2 + E_c^2 \Rightarrow E_c = \sqrt{\left|Eg_{(A-B)}\right|^2 - E_h^2} \qquad (5\text{-b})$$

The numerical values of ionicity used here are taken also from the literature; they are equal to: 0.044 [6], [12] fro BAs material and 0.112 [6] for BSb material. The results obtained of: (E_h), (E_c) and ($E_{g(A\text{-}B)}$) are listed in Table 2 and compared with the available theoretical [13-16] data. It can be seen, that our calculated value of (E_h) for BAs compound is equal exactly to these of other theoretical calculations [13, 14, 16]; because, the same experiment value of the bond length d and also the same empirical formula is applied. Our value (E_h), (E_c) and ($E_{g(A\text{-}B)}$) for BAs material is in general in agreement with the previous theoretical results [13-16]. The deviations between our value of $E_{g(A\text{-}B)}$ and the value: (7.94 eV) of Kumar et al. [16] is about 15.6 %.

Unfortunately, to the best of our knowledge, there are no data available in the literature on the bonding-antibonding energy gap ($E_{g(A\text{-}B)}$), the heteropolar energy (E_c) and the homopolar energy (E_h) for Boron- Antimonide material.

Table 2: Homopolar Energy, Heteropolar Energy, and Bonding-Antibonding Energy $E_{g(A-B}$ of BAs and BSb Materials in Comparison with other Theoretical Values [13], [14], [15] and [16].

Material	Parameter	Our work	Other works			
BAs	E_h (eV)	6.55	6.55 [13]	6.55 [14]	8.33 [15]	6.55 [16]
	E_c (eV)	1.41	4.47 [13]	0.38 [14]	0.35 [15]	4.49 [16]
	$Eg_{(A-B)}$ (eV)	6.70	7.94 [16]			
BSb	E_h (eV)	5.46				
	E_c (eV)	1.93				
	$Eg_{(A-B)}$ (eV)	5.79				

2. 2. Covalency, elastic constants, shear modulus and the kleinman parameter

The Phillips ionicity f_i of semiconductor materials plays in important role in material science; it's related with the hybrid covalency α_c by the following expression [12]:

$$f_i = (1-\alpha_c^2) \ \Rightarrow \alpha_c^2 = (1-f_i) \ \Rightarrow \alpha_c = \sqrt{(1-f_i)} \tag{6}$$

The results of the covalency α_c obtained from the relation of Eq. (6) and the ionicity 0.044 [6, 12] for BAs material and 0.112 [6] for BSb material are equal to: 0.978 for BAs material and 0.942 for BSb material respectively. Our value the covalency α_c for BAs material is in very good agreement with the previous theoretical results [17, 18]. The deviations between our value of α_c for BAs material and the values: (0.993) of Kitamura et al. [17] and (0.992) of Shen [18] are only about 1.51 % and 1.41 % respectively.

For the investigation of the elastic deformation behavior of different isotropic materials, the elastic moduli are usually used. The elastic moduli of material are related to some other microscopic quantities named elastic constants C_{ij}. For cubic crystal, three elastic constants are distinguished (C_{11}, C_{12} and C_{44}). Based on a bond-orbital model (BOM), for some cubic $A^{III}B^{V}$ semiconductor compounds, it is possible to write the elastic constants: C_{ij}, as a function of the bulk modulus B and the covalency α_c by the following formulas [19]:

$$C_{11} = B(1+\alpha_c^2)\,;\ C_{12} = B(2-\alpha_c^2)/2 \ \text{ and } \ C_{44} = 9B\alpha_c^2/(6+4\alpha_c^2) \tag{7}$$

For some cubic group-IV, $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductor compounds, the single crystal shear modulus C_S and the elastic constants: C_{11} and C_{12} are related by the following expression [12]:

$$C_S = (C_{11} - C_{12})/2 \tag{8}$$

Using the experimental numerical value (148 GPa) [8] for BAs material and the empirical value (108 GPa) for BSb material of the bulk modulus; the results obtained of the elastic constants (C_{11}, C_{12} and C_{44}) and the single crystal shear modulus C_S are given in Table 2, and compared with other theoretical works [2], [3], [5], [12], [17], [20], [21], [22], [23] and [24].

Our values of the elastic constants and the single crystal shear modulus are in general in good agreement with the previous theoretical results. The deviation between our value of C_{11} for BAs material and that of Wang and Ye [20] is only about 0.63 %. Our value (77.25 GPa) of the elastic constant C_{12} is also in agreement with the result of Wang and Ye [20]. Our value of the Shear modulus C_S for BAs compound is in excellent agreement with other theoretical results [2, 3, 5, 20 and 21]; the deviation between our value of C_S and that of the Ref. [5] GGA is only about 0.11 %.

For the diamond and zincblende structures, the Kleinman parameter ξ and the elastic constants C_{11} and C_{12} are related by the following formula [25]

$$\xi = \left[B - C_s/3\right] / \left[B + 2C_s/3\right] \tag{9}$$

The results obtained of ξ are given also in Table 2, and compared with the theoretical works [17], [20], [21], [22] and [24]. Our values of ξ are in reasonably good agreement with most of the available theoretical data.

2. 3. Cauchy discrepancy parameter, cauchy coefficient, born ratio and the knoop microhardness

Varshney et al. [2] have investigated the discrepancy in elastic constant of boron based pnictides in zincblende phase by means of the Cauchy discrepancy parameter C^*, which is given by following formula [2]:

$$C^* = (C_{12} - C_{44})/(C_{12} + C_{44}) \tag{10}$$

Our values of C^* are equal to: -0.25 for BAs material and -0.20 for BSb material respectively. Contrary to the positive Cauchy discrepancy value (0.53) obtained by Varshney et al. [2] for BAs material; we observe that our values are negative for two BX (X= As, Sb) compounds. The reason of this discrepancy is due to the positive value of the quantity (C_{12} - C_{44}) obtained by Varshney et al. [2]. Unfortunately, to the best of our knowledge, there are no another data available in the literature on the Cauchy discrepancy parameter for BX (X= As, Sb) compounds to make comparison.

For cubic crystals, the Cauchy coefficient and Born ratio (C_a and B_o) are also related respectively to the elastic stiffness constants by the following relations [26]

$$C_a = C_{12} / C_{44} \quad \text{and} \quad B_O = \left[(C_{11} + C_{12})^2 \right] / \left[4C_{44} (C_{11} - C_{44}) \right] \tag{11}$$

The results obtained of the Cauchy coefficient and Born ratio are given in Table 2, and compared with other theoretical works [12]. Our values of C_a and B_o for BAs compound are in discrepancy with the previous results of the Ref. [12].

Table 2: Elastic Constants C_{ij}, Shear Modulus C_S In (Gpa), Internal Strain Parameter ξ, Cauchy Coefficient C_a and Born Ratio B_o of BX (X= As, Sb) Compounds in Comparison With Other Theoretical Data [2], [3], [5], [12], [20], [21], [22], [23], and [24].

Material	Parameter	Our work	Other works
BAs	C_{11}	289.56	410[2] 289[3] 295[5]LDA 275[5]GGA 279[12] 291[17] 291.4[20] 218[21] 274[22] 301.26 [23]
	C_{12}	77.25	166[2] 70[3] 78 [5]LDA 63[5]GGA 120[12] 73[17] 72.8 [20] 95[21] 70[22] 77.23[23]
	C_{44}	129.62	51[2] 160[3] 177[5]LDA 150[5]GGA 113[12] 158[17] 157.9 [20] 112[21] 123[22] 163.87[23]
	C_S	106.12	122[2] 109.5[3] 108.5[5]LDA 106[5]GGA 79.5[12] 109[17] 109.3 [20] 61.5[21] 102[22]
	ξ	0.52	0.40[17] 0.362[20] 0.57[21] 0.41[22]
	C_a	0.596	1.06[12]
	B_o	1.63	0.859[12]
BSb	C_{11}	203.90	223[5]LDA 207[5]GGA 205[20] 164[21] 184.22[24]
	C_{12}	60.05	62[5]LDA 47[5]GGA 62.5[20] 75[21] 54.78[24]
	C_{44}	90.36	140[5]LDA 105[5]GGA 112.1[20] 83 [21] 119.03[24]
	C_S	71.93	71.3[20] 44.5[21] 64.71[24]
	ξ	0.54	0.436[20] 059[21] 0.445[24]
	C_a	0.66	
	B_o	1.70	

Cohesive energy is one of the quantities which largely used to understand the nature of chemical bonding and predicting other several properties. Verma et al [27] have studied the cohesive energy trends in zinc-blende ($A^{III}B^{V}$ and $A^{II}B^{VI}$) structured compounds in terms of bond length (nearest-neighbour distance) using the following relation:

$$E_{coh} = C\left[(Z_1 Z_2)^{0.4} / d^{2.5}\right] \tag{12}$$

Where Z_1 and Z_2 are ionic charges of the cation and anion respectively, d is the nearest-neighbour distance in Å and C is constant. The value of constant C for zinc blende-type crystal structure is 710 [27].

The proposed relation Eq. (12) has been applied to evaluate the cohesive energy of B As and BSb compounds. The results obtained are about 277.69 kcal/mol for BAs material and 231.02 kcal/mol for BSb material respectively. Our results of the cohesive energy of BX (X= As, and Sb) compounds are in very good with other theoretical data of Verma et al [27] which are 287.7 kcal/mol for BAs material and 227.7 kcal/mol for BSb material respectively.

The hardness of the semiconductor material is a measure of the resistance offered by this material to the movement of dislocations. Hardness is an intrinsic property of the semiconductor material, because it is relatively independent of the applied load. For $A^{III}B^{V}$ group materials, the hardness and the bond length are related by the following expression [28]:

$$H(GPa) = 350[(N_e)^{2/3} e^{-1.191 f_i}]/d^{2.5} \tag{13}$$

Where Ne is the electron density expressed in the number of valence electrons per cubic angstrom, d is the bond length in angstroms, and f_i is the ionicity of the chemical bond in a crystal [28]. The result of the hardness obtained from the relation of Eq. (13) by using the experimental bond length d (2.069 Å) [9] and the ionicity (0.044) [6, 12] for BAs material and the experimental bond length d (2.227 Å) [10] and the ionicity (0.112) [6] for BSb materials are equal to: 23.82 GPa and 9.73 GPa respectively. Our values of the Hardness H are given in Table 3, and compared with the experimental value cited by Lide [29], and with other theoretical Data [16, 28, 30 and 31].

Our value of the Hardness for BAs material is relatively larger in comparison with the experimental value (19 GPa) of the Knoop hardness cited by Lide [29]. Our result of the hardness for BSb material is also relatively lower comparatively with the theoretical values (from 11.30 GPa to 16.51 GPa) of the micro-hardness obtained by Shaileshkumar [31]. The deviation between our value (9.73 GPa) and that (11.30 GPa) of the Ref. [31] is about 13.9 %.

The Knoop microhardness H as function of the bulk modulus B for some cubic group-IV, $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductor materials can be given by the following formula [12]:

$$H = 0.16\,B - 5.74 \tag{14}$$

The results of the Knoop microhardness H obtained from the relation of Eq. (14) are equal to: 17.94 GPa for BAs material and 11.54 GPa for BSb material respectively.

Table 3: Micro-Hardness H In (Gpa) Of BX (X= As, Sb) Compounds In Comparison With Experimental [29] And Other Theoretical Data [16], [28, 30] And [31]. ^{a} Using Eq. (13), ^{b} Using Eq. (14).

Material	Our work		Other works				
BAs	23.82 ^{a}	17.94 ^{b}	17.24 [16]	19.9 [28]	19 [29]	24.2 [30]	from 12.1 to 17.23[31]
BSb	9.73 ^{a}	11.54 ^{b}	from 11.3 to 16.51[31]				

Our value of the Knoop microhardness for BAs material is in agreement with the experimental value (19 GPa) cited by Lide [29]. The deviation between our value (17.94 GPa) and that (19 GPa) of Lide [29] is about 5.58 %. As can be seen also that our value (11.54 GPa) of H for BSb material is in good agreement with other theoretical data [31], the deviation between our value (11.54 GPa) and that (11.30 GPa) of Shaileshkumar [31] being only about 2.12 %.

3. Conclusion

Employing the experimental bond-length and the bulk modulus, and with the help of some emperical formulas and expressions, the homopolar and heteropolar energies, the bonding-antibonding energy gap, the covalency of BX (X= As, Sb) compounds are predicted. Moreover, the elastic constants, the shear modulus, the Kleinman parameter, the Cauchy discrepancy in elastic constant, the Cauchy coefficient, the Born ratio, the cohesive energy and the Knoop microhardness have been obtained by using the bond-orbital model (BOM). The majority of results obtained in this work are in good agreement with other previous theoretical data reported in the literature.

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