



Elastic constants and optical phonon frequencies of BX (X= P, As, and Sb) semiconductors: Semi-empirical prediction

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Abstract

Based on some simple empirical formulas established by Adachi in, Properties of group-IV, III-V and II-VI semiconductors, John Wiley & Sons, Chichester (2005), and the experimental lattice constants reported in the literature; the present work aims to predict the elastic constants and some other significant properties of cubic zinc-blende boron compounds (BP, BAs and BSb). The obtained values of C_{12} and C_{44} are in general good agreement with other data of the literature, while C_{11} and B are slightly lower. The zone-center longitudinal optical (LO) and transverse optical (TO) phonon frequencies are also obtained. The LO and TO phonon frequencies of BP compound were found at 866.6 and 834.5 cm^{-1} , respectively; these of BAs were found at 731.3 and 727.1 cm^{-1} , respectively; while for the BSb narrow-gap semiconducting compound were found at around 598.3 and 586.2 cm^{-1} , respectively. These two later values are in general slightly lower than the calculated values, and the observed Raman spectroscopy values reported in the literature.

Keywords: Boron Compounds; Lattice Parameter; Elastic Constants; Dynamical Properties; Thermal Properties.

1. Introduction

Among group III-V semiconducting materials, binary boron compounds, which have attracted great attention in recent years. These materials have many applications in electronic devices, optical devices that operate in the short wavelength range of the visible spectrum and in devices operating at high temperatures [1]. The majority of these materials crystallize in zincblende and wurtzite structures, and they are characterized by different degrees of covalent, ionic, and metallic bonding [2].

Boron with chemical symbol (B) and antimony with chemical symbol (Sb) are relatively two abundant elements in nature [3]. At room temperature, boron antimonite (BSb) material crystallizes in cubic zinc-blende phase; it is narrow-gap semiconducting material with an indirect gap of around 0.52 eV [3]. This band gap is smaller compared to that of silicon (i.e. smaller than 1.11 eV), which perhaps make this material as good candidate in the fabrication of the infrared detectors or the thermoelectric devices.

Boron and antimony have very different atomic masses; this characteristic specifies a wide gap between optical and acoustical phonon branches [3]. Yao et al. [4] have investigated the electronic and phononic properties of bulk boron-antimonide material using *ab initio* calculations. They conclude that BSb can be a good material candidate with low-cost and easily processed, for hot carrier absorbers (HCA) in high-efficiency solar cell.

Bouamama and coworkers [5] have used the density-functional perturbation theory (DFPT) in the framework first principles approach to investigate the high-pressure effects on the lattice dynamics and dielectric properties of the BN, BP, BAs, BSb and BBi binary compounds. They found that the calculated LO and TO phonon frequencies increase in quadratic form with pressure for all boron compounds. They also calculated the band structure of boron compounds along the high-symmetry directions in the Brillouin zone and found that all these materials have an indirect band gap. Lindsay and coworkers [6] have studied the thermal conductivity, the Debye temperature, and some other properties of III-V boron semiconducting compounds using first principles approach. They found that BSb material has a thermal conductivity near 465 $\text{Wm}^{-1}\text{K}^{-1}$, and a Debye temperature at around 495 K.

In our previous work [7-11], the elastic constants, the electronic and thermal properties, the piezoelectric coefficients, the sound velocities and several other physical properties of cubic zinc-blende BSb and BAs materials at equilibrium and under high pressure were studied using *ab-initio* calculations and some other semi-empirical approaches.

Recently, Bioud et al. [12] have investigated the temperature and pressure effect on the thermodynamic properties of BSb using the quasi-harmonic Debye model. They also predict several other parameters such as: the electronic polarizability, the microhardness, the structural phase transition under compression, the melting temperature, the plasmon energy, and the thermal conductivity at 300 K.

Very recently, Malica and Dal Corso [13] have investigated the room temperature phonon dispersions and the temperature dependence on the elastic constants and thermodynamic properties of BAs using an ab initio approach. They also investigated the effect of the temperature on the sound velocity of the longitudinal acoustic mode along the [111] direction.

In the present work, we predicted the elastic constants, thermal and thermodynamic properties, as well as the longitudinal and transverse optical phonon frequencies of BP, BAs and BSb semiconducting compounds using a semi-empirical approach.

2. Theory, calculations, results, and discussion

2.1. Crystal structure of BP, BAs and BSb binary compounds

The lattice spacing between the atoms of crystal is an important parameter; it affects several physical quantities, such as the elastic constants, the width of the gap in the semiconductors, the volumetric mass density, etc[8]. Most binary III-V semiconducting compounds can crystallize in either cubic zincblende (B3) or hexagonal wurtzite (B4) structures [14]. Some other materials (such as BN and AlN) can crystallize in both structures at ambient conditions. The cell geometry of B3 configuration was assigned as: $a = b = c$ (lattice constants), and $\alpha = \beta = \gamma = 90^\circ$ (lattice angles), while that of B4 phase was assigned as: $a = b \neq c$ (lattice constants), u (the internal parameter), $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$ (lattice angles). In both structures, the material is constituted from two different atoms per basis. At ambient conditions, the boron based materials (BP, BAs and BSb compounds) crystallize in cubic zincblende structure [3, 14], with the coordinates of the two basis atoms are (0, 0, 0) and (1/4, 1/4, 1/4), respectively. For our materials of interest, the experimental values of the lattice parameter are: (4.5383 Å) [14] for BP, (4.777 Å) [14] for BAs, and (~5.30 Å) [3] for BSb, respectively.

2.2. Elastic constants and their related properties

The present section focuses on investigating the elastic constants C_{ij} and their related parameters such as the Zener anisotropy parameter Z , the Knoop microhardness H , the elastic wave speed v , the Debye temperature θ_D and the melting point T_m of BP, BAs and BSb compounds. For certain cubic group-IV, III-V and II-VI semiconductor, the elastic constants C_{ij} and the lattice parameter a are related by the following expressions [14]:

$$\ln C_{11} = -4.59 \ln a + 10.33; \ln C_{12} = -2.54 \ln a + 6.07; \ln C_{44} = -5.20 \ln a + 10.59 \quad (1)$$

Where a is expressed in Å, and the elastic stiffness constant C_{ij} are expressed in 10^{10} Pa, respectively.

The proposed relations of Eq. (1) have been applied to evaluate the elastic stiffness constants C_{ij} of BP, BAs and BSb compounds.

Replacing the experimental values: (4.5383 Å) [14] for BP, (4.777 Å) [14] for BAs, and (5.30 Å) [3] for BSb, respectively of the equilibrium lattice parameters a in the relations of Eq. (1), the obtained values of elastic stiffness constants C_{11}, C_{12} , and C_{44} are summarized in Table 1, along the results obtained in Refs. [9], [14], [15] and [16]. In general, our values of the elastic constants C_{ij} of BP and BAs are in agreement with other data of the literature. For BSb compound, except the value of C_{12} (62.59 GPa), the values of C_{11} (145.16) and C_{44} (68.07 GPa) are slightly lower than the theoretical ones 203.90 and 90.36 GPa, respectively as reported in Ref. [9].

The compressibility β of material is defined as the reciprocal of the bulk modulus B . A substance that is difficult to compress has a small compressibility, but a large bulk modulus [7]. In cubic crystals, the bulk modulus B is expressed as a function of the elastic constants C_{11} and C_{12} as follow [13, 16]: $B = (C_{11} + 2C_{12})/3$. Our calculated values of B for BP, BAs and BSb are around 160.51, 132.28, and 90.11 GPa, respectively. They are also summarized in Table 1, along the results obtained in Refs. [9], [12], [14], [15] and [16]. Like the elastic constants C_{ij} , our values of the bulk modulus of BP and BAs are also in general in agreement with other data of the literature. For example the deviation between our value (132.28 GPa) and the theoretical one (129 GPa) reported by Tian et al. [16] is only around 2.54%. Although the first (160.51 GPa) and the second (132.28 GPa) values are in general well agreement with other data of the literature, it is very clear that the later value (90.11 GPa) is slightly lower than the theoretical values 106.8 and 108 GPa reported in Ref. [9]. To the best of our knowledge there is no experimental data on the elastic constants C_{ij} and the bulk modulus B for BSb compound.

The Cauchy's pressure C_p is quantity which used to study the ductility and brittleness of solids. This quantity is defined as the difference between C_{12} and C_{44} ($C_p = C_{12} - C_{44}$). If C_p is positive (i.e. $C_p > 0$), the material is expected to be ductile in nature, and in another case, i.e. if $C_p < 0$, the material is expected to be brittle [17]. For BP, BAs and BSb compounds, our calculated values of C_p are: -59.70, -35.34, and -5.48, respectively. Our obtained values of C_p are negative, which show that all these compounds behave as brittle materials.

In cubic diamond and cubic sphalerite structures, the relative position of the cation and anion sub-lattices under volume-conserving strain distortions for the positions which are not fixed by symmetry, was described by the Kleinman parameter (called also the internal strain parameter) ζ [18]. For crystals with cubic diamond and cubic zinc-blende structures; the internal strain parameter and the elastic constants are related by following expression [18]: $\zeta = (C_{11} + 8C_{12}) / (7C_{11} + 2C_{12})$. For BP, BAs and BSb compounds, our calculated values of ζ are around: 0.46, 0.49, and 0.57, respectively. Our obtained values of ζ are slightly higher than the previously calculated results 0.368, 0.39, and 0.445, respectively reported by Ustundag et al. [18].

We can obtain different anisotropy parameters using the elastic stiffness constants. For cubic crystals, the Zener anisotropy parameter Z is usually used. This latter is expressed as function of the elastic stiffness constants C_{ij} as follow [7], [19]:

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

For isotropic media $Z = 1$, while if $Z \neq 1$ the crystal possesses an elastic anisotropy [19]. In addition, if $Z < 1$, the crystal is stiffest along $\langle 100 \rangle$ cube axes, and when $Z > 1$, it is stiffest along the $\langle 111 \rangle$ body diagonals [7]. The Zener anisotropy parameter based on our present reported elastic constants obtained for BP, BAs and BSb, respectively, 1.50, 1.53, and 1.65; which indicate that all these materials are stiffest along the $\langle 111 \rangle$ body diagonal (the direction of the nearest-neighbor bond). Our calculated values of the Zener anisotropy ratio for BP, BAs and BSb are lower than the results: 2.64 and 2.35 reported for ZB-AlN and RS-AlN, respectively [19], which indicates the lowest elastic anisotropy in BP, BAs and BSb compared to AlN in both zinc-blende and rock-salt phases.

The hardness is related to the crystal structure of the material as well as the concentration of defects (dislocations, etc). There are different model related the hardness with other elastic moduli. For cubic group-IV, III-V and II-VI materials, the Knoop microhardness H and the bulk modulus B are related by the following linear formula [14]:

$$H = 0.16 B - 5.74 \quad (3)$$

Replacing our obtained values of B in this equation; the obtained values of H for BP, BAs and BSb are: 19.94, 15.42 and 8.68 GPa, respectively. They are also summarized in Table 1, along the results obtained in Refs. [9], [12], [14] and [16]. We note that the use of the empirical method slightly underestimates the Knoop microhardness H of BSb compared to the available values, while the discrepancy becomes more important for BP and BAs.

Table 1: Elastic Constants C_{ij} (in GPa), Bulk Modulus B (in GPa), and Knoop Microhardness H (in GPa) of BP, BAs and BSb Semiconducting Compounds, Compared to Other Data [9], [12], [14 - 16]

		C_{11}	C_{12}	C_{44}	B	H
BP	This work	295.88	92.82	152.52	160.51	19.94
	Ref. [14]	315	100	160	170	32
	Ref. [15]	356	83.5	194.6	174.6	-
	This work	233.85	81.49	116.83	132.28	15.42
BAs	Ref. [9]	289.56	77.25	129.62	-	23.82(17.94)
	Ref. [14]	279	120	113	173	19
	Ref. [16]	263	62	143	129	22
	This work	145.16	62.59	68.07	90.11	8.68
BSb	Ref. [9]	203.90	60.05	90.36	106.8 (108)	9.73(11.49)
	Ref. [12]	-	-	-	95.30	9.80

The Debye temperature θ_D is a useful parameter in solid-state problems, this because of its inherent relationship to lattice vibration [14]. The calculated structural parameters and elastic constants of crystals are usually used to predict their Debye temperature θ_D [20]. At low temperature, θ_D can be obtained from the sound velocity [20]. For binary crystals with cubic zinc-blende structure, θ_D can be obtained from the average sound velocity v_m (expressed in km/s), and the lattice constant a (expressed in Å) as follow [21], [22]:

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

Using the same formulas used in our previous works [21, 22], the average sound velocities v_m of BP, BAs and BSb semiconducting compounds were found at around: 7.279, 4.793 and 3.404 km/s, respectively. Replacing these values of v_m in Eq (4); the obtained value of θ_D are around: 955, 597 and 382 K, respectively. Our obtained values of θ_D for BP and BAs compounds are slightly lower than the experimental 1025 K (measured at $T = 320$ K) for BP [14], and 681 K for BAs [16], respectively. The deviation between our calculated value (955K) and the experimental one (1025 K) reported in Ref. [14] is around 6.83%. Although the Debye temperature θ_D of BSb has been extensively studied by the theoretical calculation [6], [10], and [12]; to the best of our knowledge there is no experimental data on this parameter for BSb compound. Our computed value of θ_D of BSb is slightly lower than the theoretical one 456.07 K reported in Ref. [10], but excellent agreement with the theoretical data 384.9 K reported by Bioud et al. [12]. We have also calculated the Debye temperature θ_D using a semi-empirical formula expressed as follow [23]:

$$\theta_D = C_B (a G_B / M)^{1/2} \cdot G_B = [C_{44}(C_{11} - C_{12})(C_{11} - C_{12} + 2C_{44})]^{1/3} \quad (5)$$

where a is the lattice parameter, $C_B = 3.89 \times 10^{11} n^{-1/6} h / k_B$ is a model parameter, h is Planck's constant, k_B is Boltzmann's constant, n is the number of atoms in the unit cell, and M is the atomic weight (arithmetical average of the masses of the species), respectively.

Using Eq. (5), the Debye temperature θ_D of BP, BAs and BSb semiconducting compounds were found at around: 1025.9, 644.4 and 416.6 K, respectively. Although our values (1025.9 and 644.4 K) of BP and BAs are slightly higher than the values (955 and 597 K) obtained from Eq. (4), they are in very good agreement with the experimental ones (1025 K for BP [14], and 681 K for BAs [16]). The deviation between our calculated value (1025.9 K) of θ_D and the experimental one (1025 K) reported by Adachi [12] is less than 0.09%, while that between our value (644.4 K) and the experimental one (681 K) reported by Tian and co-workers [16] is only around 5.4%. For BSb material, our obtained value of θ_D is slightly higher than that (382 K) obtained from Eq. (4) and slightly lower than the theoretical data 495 K reported by Lindsay and coworkers [6] and the value (491.88 K) reported in our previous work [10], so it is localized between these two theoretical data.

The melting point is one of the most essential thermophysical parameters of solid [14]. There are different expressions usually used to predict the melting point T_m . For materials with cubic structure, the melting point T_m correlates with the elastic constants C_{ij} as follow [24]: $T_m = 560.4 + 7.805 C_{11} - 3.094 C_{12} - 1.086 C_{44}$, where the elastic constants C_{ij} are expressed in GPa, and the melting point T_m is expressed in K. Replacing our values of C_{ij} in the previous expression, the melting point T_m of BP, BAs and BSb compounds were estimated at around: 2416.94, 2006.59 and 1425.8 K, respectively. Like bulk modulus B and the microhardness H , our values of T_m for BP, BAs and BSb compounds are also slightly lower than the experimental (> 3300 K for BP [14], 2300 K for BAs [14]) and other theoretical (1758.05 \pm 300 K and 1500 K reported in Ref. [10], and by Bioud et al. [12], respectively for BSb) values. The deviation less than 5% between our calculated value (1425.8 K) of T_m and the theoretical one (1500 K) reported by Bioud and coworkers [12].

2. 3. Thermodynamic properties

Applying an approach based on the correlation between thermodynamic properties and melting point T_m , Vassiliev et al. [25] have calculated several thermodynamic properties of certain III-V semiconducting materials. The dependence of the standard enthalpy of formation $\Delta_f H_{298}^0$ and the standard entropy S_{298}^0 on melting point T_m can be approximately described by the following equations [25]:

$$\Delta_f H_{298}^0 = 11.38 - 0.0343 T_m \quad (6)$$

$$S_{298}^0 = 167.664 - 18.68 \ln(T_m) \quad (7)$$

Where the enthalpy of formation $\Delta_f H_{298}^0$ is expressed in kJ/mol-at, the standard entropy S_{298}^0 is expressed in J/(K mol-at), while the melting point T_m is expressed in K.

The enthalpy of formation $\Delta_f H_{298}^0$ of BP, BAs and BSb semiconducting compounds were estimated at around: -71.52, -57.45 and -37.52 kJ/mol-at, respectively; while these of the standard entropy S_{298}^0 were found: 22.14, 25.62 and 32 J/(K mol-at), respectively. Our value of S_{298}^0 for BAs semiconducting compound is slightly higher than the experimental values (from 15.76 ± 0.6 to 20.5 ± 2) J/(K mol-at) reported by Vassiliev and coworkers [25].

2. 4. Longitudinal and transverse optical phonon frequencies

Phonons play a major role in many physical properties of solids, such as thermal property, superconducting and electrical conductivity [26]. Under consideration of the scarce data on the dynamic properties of BP, BAs and BSb, the present work investigates the longitudinal and transverse optical phonon frequencies of BP, BAs and BSb materials. We have calculated the longitudinal optical (LO) and transverse optical (TO) phonon frequencies, following the method of Harrison [27] and Wolverson and coworkers [28]. The calculation of LO phonon frequency at the zone-center has been geared up using the following expression [23]:

$$\omega_{LO}^2 = (8/3\mu d^2)(C_0 + 8C_1) \quad (8)$$

Where μ is the reduced mass of an BX (X= P, As, and Sb) formula unit cell ($\mu = M_1 M_2 / (M_1 + M_2)$), d is the interatomic separation, C_0 is the bond stretching force constant and C_1 is the bond bending force constant. The force constants can be expressed:

$$C_0 = (3a^3/16)(C_{11} + 2C_{12}), \text{ and } C_1 = (a^3/32)(C_{11} - C_{12}) \quad (9)$$

The zone-center LO phonon frequency of BP, BAs, and BSb using this procedure has been obtained as: 866.6, 731.3 and 598.3 cm^{-1} , respectively. They are also summarized in Table 2, along the results obtained in Refs. [3], [5], [14] and [29]. Our value (598.3 cm^{-1}) of the zone-center LO of BSb is slightly lower than the calculated values 621, 623 cm^{-1} , and the observed Raman spectroscopy value 623 cm^{-1} reported by Touat et al. [29], Bouamama and coworkers [5], and Das et al. [3], respectively. The zone-center TO phonon frequency can be calculated by the Lydanne - Sachs -Teller relation [30] (well-known LST relation), which is expressed as follow [31]:

$$\omega_T^2 = (\varepsilon(\infty) / \varepsilon(0)) \omega_L^2 \quad (10)$$

Where ω_T is the transverse optical frequency, ω_L is the longitudinal optical frequency (both at low wave vector), $\varepsilon(\infty)$ is the high-frequency limit of the dielectric constant and $\varepsilon(0)$ is the low-frequency (static) limit.

Replacing in Eq. (10) the values 10.2 and 11 of $\varepsilon(\infty)$ and $\varepsilon(0)$ reported by Adachi [14] for BP, the values 9.56 and 9.67 of $\varepsilon(\infty)$ and $\varepsilon(0)$ reported by Bouamama et al. [5], and Labidi et al. [32], respectively for BAs, and the values 10.72 and 11.17 of $\varepsilon(\infty)$ and $\varepsilon(0)$ reported by Bouamama et al. [5], and Labidi et al. [32], respectively for BSb; the zone-center TO phonon frequency of BP, BAs and BSb semiconducting compounds have been obtained as : 834.5, 727.1 and 586.2 cm^{-1} , respectively. These values are also summarized in Table 2, along the results obtained in Refs. [3], [5], [14] and [29].

The value 586.2 cm^{-1} is slightly lower than the calculated values 611 and 605 cm^{-1} , and the observed Raman value 605 cm^{-1} reported by Touat et al. [29], Bouamama et al. [5], and Das et al. [3], respectively. The optical phonon frequency difference $\Delta\omega_{op} = \omega_{LO} - \omega_{TO}$ of BP is 32.1 cm^{-1} , that of BAs is 4.2 cm^{-1} , while in case of BSb (narrow-gap semiconducting compound) has been obtained at around 12.1 cm^{-1} . They are also summarized in Table 2, along the results obtained in Refs. [3], [5], [14] and [29].

Table 2: Longitudinal Optical (LO) and Transverse Optical (TO) Phonon Frequencies (In cm^{-1}) of BP, BAs and BSb Compounds, Compared to Other Data [3], [5], [14], [29]

		ω_{LO}	ω_{TO}	$\Delta\omega_{op}$
BP	This work	866.6	834.5	32.1
	Ref. [14]	828.9	798.9	30
BAs	This work	731.3	727.1	4.2
	Ref. [5]	705	701	4
BSb	This work	598.3	586.2	12.1
	Ref. [3] Exp	623	605	18
	Ref. [5]	623	605	18
	Ref. [29]	621	611	10

From data reported in Table 2, we can notice that our values of $\Delta\omega_{op}$ are in good agreement with other results reported in Refs. [3], [5], [14] and [29]. For example, the deviation between our value (32.1 cm^{-1}) and the value (30 cm^{-1}) reported by Adachi [14] is 7%, while the deviation between our value (4.2 cm^{-1}) and the value (4 cm^{-1}) reported by Bouamama et al. [5] is around 5% only.

3. Conclusion

Based on some simple semi-empirical and empirical formulas, and some experimental and theoretical data reported in literature, we tried to predict the elastic constants and related properties of cubic zinc-blende BP, BAs and BSb materials. Except the values of C_{12} and C_{44} , these of C_{11} and B are slightly lower than the experimental and other theoretical values reported in the literature.

The Kleinman parameter was determined. In general, our obtained values are slightly higher than other calculated results of the literature. The analyses of the Zener anisotropy parameter indicates that BP, BAs and BSb are stiffest along the $\langle 111 \rangle$ body diagonals, while the Cauchy's pressure shows that all these compounds behave as brittle materials.

The Debye temperature was also calculated using two different formulas; generally the data obtained in this work are in agreement with other experimental and theoretical values of the literature. The standard enthalpy of formation, the entropy, the Knoop microhardness, the

melting point, and the zone-center longitudinal optical (LO) and transverse optical (TO) phonon frequencies were also obtained. Except the standard entropy, our obtained values of other parameters are slightly lower than the experimental values and other calculated data of the literature.

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