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Research Paper

Mechanical properties of BBi compound under pressure

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Abstract

In several research activities, the ab-initio calculations have become a vital tool for many research scientists (especially the physicists and the chemists). Pseudopotential plane wave method based on density functional perturbation theory within the Teter and Pade exchange-correlation functional form of the local density approximation is applied to study the anisotropy and pressure dependency of the mechanical properties of Boron-bismuth compound. The independent elastic compliance constants, the mechanical behavior, the phase transition, the volume collapse, the Young's modulus and the Poisson's ratio for directions within the important crystallographic planes under pressure are studied. The Debye temperature and the melting point are also predicted.

Keywords: *PP-PW Method; Mechanical Properties of Semiconductors; Boron-Bismuth Compound.*

1. Introduction

The mechanical properties such as: plasticity, hardness and brittleness of semiconductor materials are no less important than the thermoelectric and other physical properties of those materials to assure high reliability of respective products, instruments and devices [1]. The elastic constants of semiconductor materials provide a link between the mechanical and dynamical behavior of crystals, and give important information concerning the nature of the forces operating in solids [2]. In particular, they provide information on the brittleness and stiffness of materials, and their ab initio calculation requires precise methods [2]. So the mechanical properties of semiconductor materials play an important role on the fabrication of modern semiconductor instruments and devices. And because there are no data available in the literature of the effect of hydrostatic pressure on several of these quantities for boron bismuth (BBi) compound, we used density functional perturbation theory (DFPT) and as implemented in the ABINIT code to calculate series of mechanical constants and moduli under pressure of this compound.
The structural parameters and electronic behavior of boron-bismuth (BBi) in its zincblende phase have been studied by Madouri et al [3] using the full potential linearized augmented plane wave method. Under hydrostatic pressure the low pressure phase of material is destabilized and structural phase transition occurs. For BBi material, the phase transition appears at pressure of 31.74 GPa [4]. Singh et al. [5] used the three-body interactions potential (TBIP) approach to study the elastic properties of this compound; they have also studied the phase transition pressure from zincblende (B3) phase to Rock-salt (B1) phase of BBi compound, and they found a value of pressure at about 34 GPa. In the present work, we report ab-initio calculations of the hydrostatic pressure effect on the elastic compliance constants and some others mechanical quantities of BBi compound in its structure (B3) phase using the pseudopotential plane wave method in the framework of the density functional perturbation theory [6], within the local density approximation (LDA). The mechanical stability criteria and the volume collapse are also studied.

2. Computational methods

Our calculations were performed by using the density functional perturbation theory and implemented in the ABINIT code [7-9]. ABINIT code is a package whose main program allows one to find the total energy, electronic structure and other properties such as elastic, optic, and dynamic of periodic solids within density functional theory, using

pseudopotentials and a plane-wave basis-set. It is a common project of the Université Catholique de Louvain, Corning Incorporated, the Université de Liège, the Commissariat à l'Energie Atomique, Mitsubishi Chemical Corp., the Ecole Polytechnique Palaiseau and other contributors.
The pseudopotentials of Trouiller-Martins [10] in the context of the LDA are employed in the computation. The electron-electron interaction was considered within the LDA by Teter-Pade parameterization [11], which reproduces the correlation scheme of Perdew and Wang [12].
The two parameters that affect the accuracy of calculations are the kinetic energy cutoff which determines the number of plane-waves in the expansion and the number of special k-points used for the Brillouin zone (BZ) integration. The BZ integrations were replaced by discrete summations over a special set of k-points, using the standard k-point technique of Monkhorst and Pack [13] where the k-point mesh used is (8 × 8 × 8). The plane-wave energy cut-off to expand the wave functions is set to be 90 Hartree. Careful convergence tests show that with these parameters, the relative energy is converged to better than 10^{-5} Hartree.

3. Results and discussions

3.1. Elastic compliance constants

The first goal of the present work is to report the pressure dependency of the elastic compliance constants for (B3) BBi material. In the case of the cubic crystals, the elastic compliance tensor [S] contains only three elastic compliance constants (S_{11}, S_{12} and S_{44}) [14]. The obtained values of the compliance constants S_{11}, S_{12} and S_{44} in (10^{-2} GPa^{-1}) of (B3) BBi at zero pressure are: 0.887, -0.231 and 1.340 respectively. Unfortunately, there are no data available in the literature on the elastic compliance constants S_{ij} for this compound. Future experimental work or other theoretical calculations will contribute with more tests for the validating of our calculated results of these parameters.
The pressure variation of the elastic compliance constants S_{ij} of (B3) BBi material up to 48 GPa is depicted in figure1. We observe that the constants S_{11}, S_{12} and S_{44} decrease gradually with the increasing of the hydrostatic pressure and with a negative sign for the constant S_{12}.

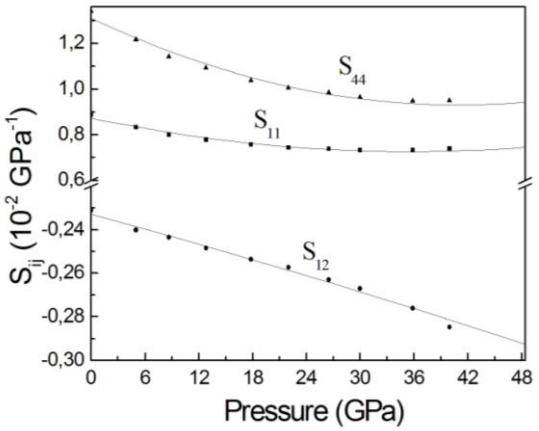

Fig. 1: Elastic Compliance Constants S_{ij} versus the Hydrostatic Pressure of the (B3) BBi.

3.2. Young's modulus and Poisson's ratio

The second goal of this work is to report the pressure dependency of the Young's modulus Y and Poisson's ratio ν for (B3) BBi compound. Young's modulus which is a measure of longitudinal elongation for isotropic solids, it is a very important mechanical coefficient in engineering of materials science; it is a quantity which is anisotropic for cubic zinc blende crystals (i.e.: strongly dependent with the directions) [14]. The Young's modulus Y for an arbitrary crystallographic direction x can be given as a function of the elastic compliance constants S_{ij} by the following expression [14]

$$1/Y = S_{11} - 2(S_{11} - S_{12} - 0.5S_{44})(x_1^2x_2^2 + x_2^2x_3^2 + x_1^2x_3^2) \quad (1)$$

Where the x_i values are the direction cosines for x.
The obtained values of the Young's modulus of BBi compound at different pressure p for the important directions are presented in figure 2. As shown on this figure, that all the curves increase with the increasing of the hydrostatic pressure. Three Analytical relations for the pressure dependency of (B3) Boron-bismuth Young's modulus Y are given by the following a quadratic fit, i.e.:

$$Y_{\{100\}/<001>} = 112.93 + 1.547p - 2.59\times10^{-2}p^2 \quad (2\text{-a})$$

$$Y_{\{100\}/<011>} = 151.18 + 3.285p - 4.4\times10^{-2}p^2 \quad (2\text{-b})$$

$$Y_{\{110\}/<111>} = 170.80 + 4.466p - 5.21\times10^{-2}p^2 \quad (2\text{-c})$$

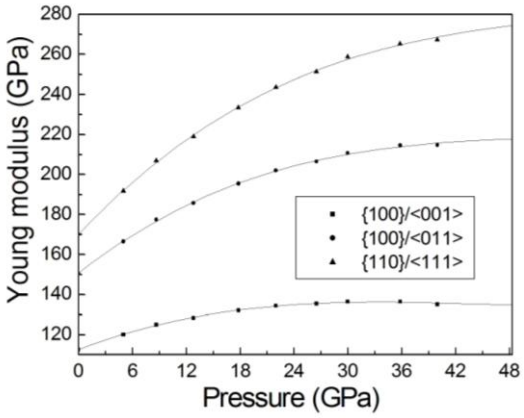

Fig. 2: Young's Modulus for Important Directions versus the Hydrostatic Pressure of (B3) BBi Compound.

Another important engineering coefficient in the fabrication of modern semiconductor devices is the Poisson's ratio ν, it is also varied with the orientation in the cubic zinc blende crystals [14]. For isotropic solids, the Poisson's ratio ν is a measure of the transverse contraction [15]. If a longitudinal stress in the direction x and the transverse strain along the orthogonal direction y are under consideration, the Poisson's ratio ν can be given by [14].

$$\nu = -\frac{\left[S_{12} + (S_{11} - S_{12} - 0.5S_{44})(x_1^2y_1^2 + x_2^2y_2^2 + x_3^2y_3^2)\right]}{\left[S_{11} - 2(S_{11} - S_{12} - 0.5S_{44})(x_1^2x_2^2 + x_2^2x_3^2 + x_1^2x_3^2)\right]} \quad (3)$$

The obtained values of ν at different pressure up to 48 GPa for important crystallographic directions are presented in figure 3. As shown on this figure, that also all the curves (except for the Plane {100} with direction m= <011>, and n= <0 $\bar{1}$ 1>) of the Poisson's ratio ν increase also gradually with the increasing of the hydrostatic pressure.

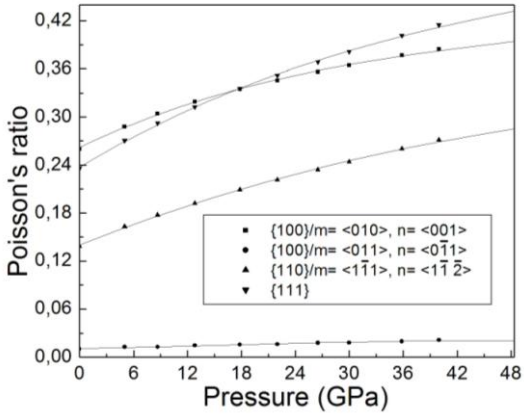

Fig. 3: Poisson's Ratio ν for Important Directions versus the Hydrostatic Pressure of (B3) BBi Compound.

Four Analytical relations for the pressure dependence of (B3) BBi Poisson's ratio ν are given by the following a quadratic fit, i.e.:

$$\upsilon_{\{100\}/m=<010>,\ n=<001>} = 0.262 + 5.27\times10^{-3}p - 6.34\times10^{-5}p^2 \quad (4\text{-a})$$

$$\upsilon_{\{100\}/m=<011>,\ n=<0\bar{1}1>} = 1.05\times10^{-2} + 3.57\times10^{-4}p - 3.23\times10^{-6}p^2 \quad (4\text{-b})$$

$$\upsilon_{\{100\}/m=<1\bar{1}0>,\ n=<1\bar{1}\bar{2}>} = 0.140 + 4.61\times10^{-3}p - 3.86\times10^{-5}p^2 \quad (4\text{-c})$$

$$\upsilon_{\{100\}} = 0.237 + 6.74\times10^{-3}p - 6.64\times10^{-5}p^2 \quad (4\text{-d})$$

In the following section, we will discuss some mechanical properties as ductility and brittleness of our material. The ductility and brittleness of materials are of substantial importance and can be obtained usually from the Pugh's index of ductility $R_{G/B}$ (called also the inverse ratio) or from the Poisson's ratio *v* (for more detail on the study of ductility and brittleness of materials, please see the Ref. [16]). The effect of pressure on the inverse ratio $R_{G/B}$ is illustrated in Fig. 4 (a). Based on $R_{G/B}$ quantity, for BBi compound, Fig. 4(a) shows that it is of brittle in nature from 0 to 24.7 GPa and it is ductile in nature with an increase in pressure up to 48 GPa.
The pressure dependency of Poisson's ratio (here the average Poisson's ratio is taken) is also illustrated in Fig. 4 (b). Based on Poisson's ratio rule, two different values (0.26 and 0.33) [16] of the exact border between the two types of mechanical behavior have been mentioned. So, if the value of the Poisson's ratio is less than 0.26 (0.33), the material is considered brittle; otherwise (i.e. if *v* is more than 0.26 (0.33)) the material behaves in a ductile manner [16]. For BBi compound, Fig. 4 (b) shows that it is of brittle in nature from 0 to 15 GPa (0 to 42 GPa) and it is ductile in nature with the increasing in pressure up to 48 GPa.

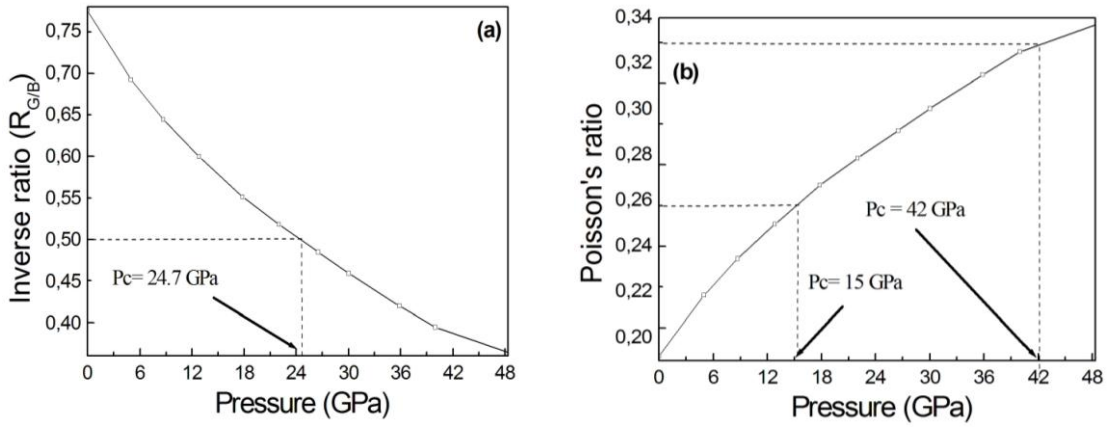

Fig. 4: Variation of Poisson's Ratio *v* (a), and The Inverse Ratio $R_{G/B}$ (b) of (B3) BBi Compound with Pressure.

Another quantity is also used to study the ductility and brittleness of materials; it is named the Cauchy's pressure. This quantity is defined as the difference between the elastic constants (C_{12} - C_{44}). If the pressure is positive (i.e.: C_{12} - C_{44} > 0), the material is expected to be ductile in nature, and in another case, i.e. if the pressure is negative (C_{12} - C_{44} < 0), the material is expected to be brittle [17].

3.3. Mechanical stability criteria

Usually the Gibbs-free energies (or the enthalpies at T= 0 K) are used to study the structural phase transition under pressure. But also the structural phase transition of crystal material can be investigated with the help of the elastic stability criteria. The structural stability under compressions of BBi compound was studied by using the generalized elastic stability criteria which are given by the following relations [18]:

$$K = \frac{1}{3}(C_{11} + 2C_{12} + P) > 0\,,\ G = \frac{1}{2}(C_{11} - C_{12} - 2P) > 0 \ \text{ and } \ G' = C_{44} - P > 0 \quad (5)$$

Where C_{ij} are the elastic stiffness constants and P is the pressure
The elastic stiffness constants C_{ij} and the elastic compliance constants S_{ij} are related by the following expressions [14]:

$$C_{11} = (S_{11} + S_{12})/[(S_{11} - S_{12})(S_{11} + 2S_{12})]\,, \quad C_{12} = (-S_{12})/[(S_{11} - S_{12})(S_{11} + 2S_{12})], \quad \text{and} \quad C_{44} = 1/S_{44} \quad (6)$$

At zero pressure, the elastic stability criteria are satisfied, indicating that this compound is elastically stable. As pressure is applied to (B3) BBi compound, it gets transformed from the (B3) phase into the site-ordered NaCl (B1) phase. Three Analytical relations for the pressure dependency of the generalized elastic stability criteria are given by:

$$K = 78.09 + 3.65p - 0.01p^2 \quad (7\text{-a})$$

$$G = 45.15 - 6.75\times10^{-1}p - 5.42\times10^{-3}p^2 \quad (7\text{-b})$$

$$G' = 75.64 + 4.07\times10^{-1}p - 1.58\times10^{-2}p^2 \quad (7\text{-c})$$

We find that G decreases gradually with the pressure and vanishes at about 48 GPa; so the phase transition occurs at pressure of 48 GPa. This value is listed in table 1 and compared with the available theoretical data [4], [5], [19-21]. Our calculated value of the transition pressure is very higher than the previously calculated data [4], [5], [19-21].

Table 1: Transition Pressure P_T (GPa) of (B3) BBi Material in Comparison with the Theoretical Data [4], [5], [19], [20] and [21].

Parameter	Our work	Other works				
Pt	48	31.74[4]	34[5]	35.38[19]DM	24.5[20]	56.37[21]

The equation of state curves of BBi compound (plotted between V (P) / V (0) and the pressure) for both zinc blende (B3) and Rock-salt (B1) phases obtained in this work are plotted in figure 5. From this curves, we can estimate the volume collapse in the point of transition (in our case at 48 GPa).

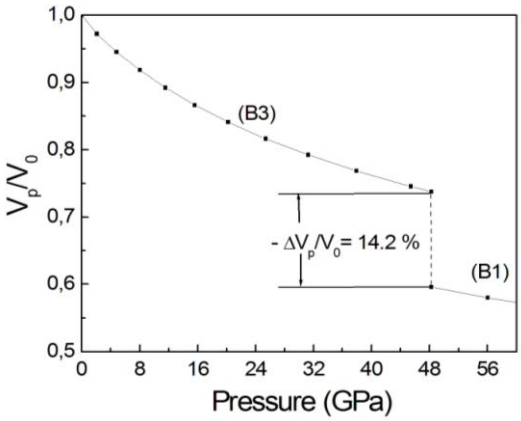

Fig. 5: Variations of the Ratio V_P/V_0 of (B3) and (B1) BBi with Hydrostatic Pressure.

Our result of the volume collapse for (B3) BBi compound is given in table 2 and compared with the available theoretical data [4], [5]. Unfortunately, to the best of our knowledge, there are a little theoretical data [4], [5] available in the literature on this parameter for this compound.

Table 2: Volume Collapse of (B3) BBi Compound, in Comparison with the Available Theoretical Values [4], [5].

	Our work	Other works	
Volume collapse (%)	14.2	6.6[4]	11.2[5]

The Debye temperature is usually obtained by using the average sound velocity. But other formulas are largely used; among those formulas largely used for calculation of the Debye temperature of the cubic crystal materials is that proposed by Blackman [22]. It relating the Debye temperature and the elastic stiffness constants C_{IJ}; it is given as [22]:

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

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 crystal density. The elastic stiffness constants C_{ij} are related to the elastic compliance constants S_{IJ} by the formula of Eq. (6). Our calculated values of θ_D of BBi compound is listed in table 3, and compared with the available theoretical data [19-21], [23-25]. Our obtained value is in agreement with other theoretical results. Our obtained value (337.75 K) is in good agreement with the theoretical value 331.56 K cited in the Ref. [20]; the deviation being only about 1.87 %.
For A^{III}-B^{V} binary semiconductor compounds, a linear relationship between the Debye temperature and the melting point T_m was proposed; it is given by the following formula [26]:

$$\theta_D = -C_1 + C_2 T_m \quad (8)$$

Where C_1 and C_2 are constants, the numerical values of the constants C_1 and C_2 are: 153.40K and 0.354 respectively. Using the formula of Eq. (8), we can estimate approximately the value of T_m from the following expression:

$$T_m = (\theta_D + C_1)/C_2 \quad (9)$$

The calculated T_m of BBi material is about 1387.43 K; it's listed in table 3, and compared with the available theoretical data [19], [20], [23-25]. Our obtained value of T_m is in excellent agreement with other theoretical values, especially the value 1424 ± 300 K cited in the Ref. [20] and the value 1312.866 K obtained by Ustundag et al. [24]; the deviations between our value and these cited in the Ref. [20] and in the Ref. [24] are only about 2.57 % and 5.68 % respectively.

Table 3: Debye Temperature and Melting Point f BBi Compound Along with Those Computed Through other Methods [19], [20], [21], [23], [24] and [25].

Parameter	Our work	Other works				
θ_D (K)	337.75	324.11[19] 370.23 [25]	331.56 [20]	311.85[21]	352.56 [23]	324.806 [24]
T_m(K)	1387.43	1467 [19]	1424 [20]	1522 [23]	1312.866[24]	1479.18 [25]

4. Conclusion

The effect of the hydrostatic pressure on the elastic compliance constants of BBi material are obtained, we found that these elastic compliance constants decrease almost quadratic with the increasing of hydrostatic pressure (with a negative sign for the constant S_{12}). The obtained values of the elastic compliance constants S_{ij} were used to predict the orientation dependency of two mechanical quantities: Young's modulus Y, and Poisson's ratio ν.
The value of pressure separates the ductile and brittle nature is also obtained; at zero pressure the BBi compound is of brittle in nature. In the investigation of the stability criteria, the results showed a phase transition pressure from the zinc blende to Rock-salt phase at around 48 GPa. The volume collapse, the Debye temperature and the melting point are also predicted. The percentage deviations of 1.87 % and 2.57 % were obtained in the cases of Debye temperature and melting point respectively.

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