International Journal of Physical Research, 7 (1) (2019) 7-10

International Journal of Physical Research

Website: www.sciencepubco.com/index.php/IJPR

Research paper

EOS parameters and elastic properties of cubic rock-salt BP

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Abstract

The present work aims to study the equation of state (EOS) under compression up to 100 GPa, and the elastic properties of cubic rocksalt Boron phosphide (BP) material. The EOS parameters and the elastic constants of our material of interest were predicted using plane wave-pseudopotential (PW-PP) approach in the framework of the density functional theory (DFT) and the density functional perturbation theory (DFPT) with the generalized gradient approximation (GGA) for the exchange-correlation functional. The Young modulus, the Poisson's ratio, the sound velocity, the Debye temperature and the melting temperature of the aggregate material were also presented. The results obtained are in general in good agreement compared to other data of the literature.

Keywords: *Ab-Initio Calculation; BP Material; Equation of State; Elastic Constants; Thermal Properties.*

1. Introduction

Because of the good performance of boron phosphide (BP) semiconducting compound, such as high melting points, high hardness, dielectric and thermal characteristics as well as its unusual behavior, it attracts more attention in recent years [1]. Using the linear muffin-tin orbitals (LMTO) approach and the pseudopotential - plane waves (PP-PW) method, the structural and electronic properties of BP with three different structures (cubic zinc-blende, β-Sn and cubic rock-salt phases) were systematically investigated by Kocinski and Zbroszczyk [1]. Theirs calculations indicate that the boron phosphide material crystallizes in the cubic zinc-blende phase, and it has an indirect gap of approximately 1.5 eV, which decreases quadratically under compression. They found also that the phase transition from zinc-blende to rock-salt phase occurs at extremely high pressure (approximately 150 GPa).
Using first principles total-energy calculations based on the full-potential augmented plane-wave plus local orbitals (FP-LAPW+lo) method, Bouhemadou et al. [2] have studied the effect of the high pressure on the structural and mechanical properties of some III-phosphide compounds (BP, GaP, AlP, InP). They found a linear dependence between the elastic constants and the applied pressure. They calculated also the sound velocity and the Debye temperature θ_D of the aggregate materials.
Using the same approach, Arbouche et al. [3] have studied the effect of high pressure on the phase transition of the same materials (BP, GaP, AlP, InP). For BP material, they found that this compound transforms from the zinc-blende structure to the rock-salt phase at around 133 GPa, then from the rock-salt phase to the NiAs phase at a pressure of around 212 GPa.
In our previous work [4-6], the elastic constants, the piezoelectric coefficients, the electronic properties and some other physical properties of zincblende BP material under high pressure were studied using ab-initio calculations. We found that the elastic constants increase monotonously with increasing pressure, while the piezoelectric coefficients decrease with the increase of pressure.
Although the cubic rock-salt phase of boron phosphide material is not synthesized until now, we will test to extent our study on the cubic rock-salt phase of this compound, so some other properties of this phase have been systematically studied here. In the present work, we compute the structural parameters, the elastic constants and some other physical quantities of BP material in cubic rock-salt phase.

2. Computational method

The structural parameters and the elastic constants calculated in the present study were carried out using ABINIT code [7], which based on the PP-PW approach in the framework of the DFT and the DFPT. To describe the interactions between the valence electrons and the nuclei and core electrons, the Troullier-Martins type pseudopotentials which have been generated thanks to the FHI98PP code [8] were employed. The exchange-correlation energy was evaluated in the generalized gradient approximation (GGA) [9]. The total energy was found converged near the energy cutoff of 80 Ha. The Brillouin zone was sampled by (12x12x12) Monkhorst and Pack mesh of k points [10]. For more detail on the calculation of the structural parameters, and the elastic constants of materials, please see for example our previous works [4-6].

3. Results and discussion

3. 1. EOS parameters and crystal density

To predict the equilibrium structural parameters of cubic rock-salt BP, the pressure-volume (P-V) data was employed. The unit cell volumes at fixed values of applied pressure were used to construct the equation of state (EOS). The normalized lattice parameter (a_p/a_0) versus pressure in the range from 0 to 100 GPa for cubic rock-salt BP was plotted in Fig. 1, along with the theoretical one reported by Arbouche et al. [3].
From figure 1, we observe that the normalized lattice parameter (a_p/a_0) of our material of interest decreases with the increase of pressure, where it is started with the value 1 at zero-pressure, and it reaches the value 0.896 at 100 GPa.

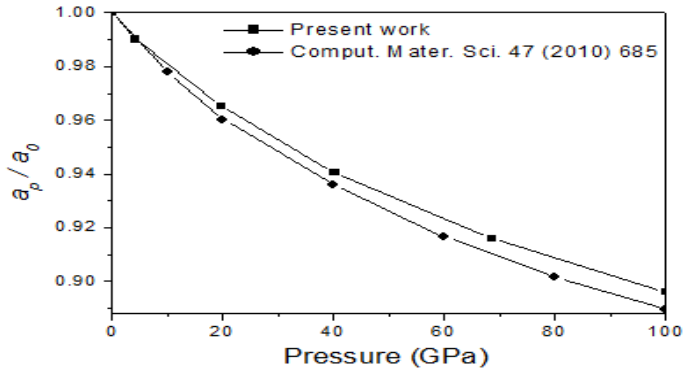

Fig. 1: Normalized Lattice Parameter (a_p/a_0) Versus Pressure.

The calculated normalized volume (V_p/V_0) versus pressure is plotted in Fig. 2, along with the theoretical one reported by Arbouche et al. [3]. From figure 2, we observe that V_p/V_0 of BP decreases also with increasing pressure, where it is started with the value 1 at zero pressure, and it reaches the value 0.716 at 100 GPa.

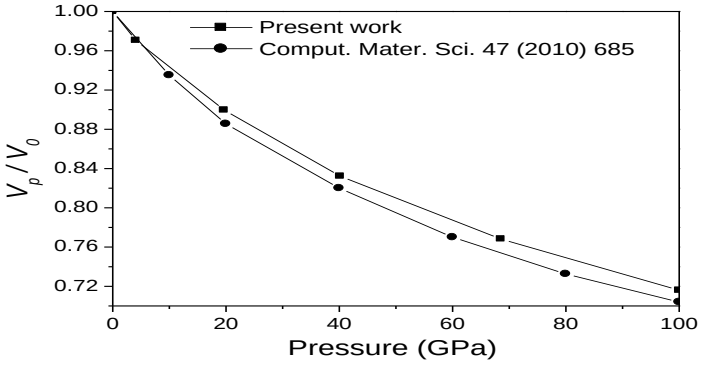

Fig. 2: Normalized Volume (V_p/V_0) Versus Pressure.

The EOS parameters (equilibrium lattice constant a_0, bulk modulus B_0, and its pressure derivatives B_0') can be determined through the well-known pressure-normalized volume (P-(V/V_0)) third-order Vinet EOS, which is given as follow [11], [12]

$$P(V) = 3B_0 \left[\frac{1-(V/V_0)^{1/3}}{(V/V_0)^{2/3}}\right] exp\left\{\tfrac{3}{2}(B_0' - 1)\left[1-(V/V_0)^{1/3}\right]\right\} \quad (1)$$

Where: V is the volume at pressure P, and V_0 is the volume at zero-pressure, respectively.
The calculated data (P-(V/V_0)) of BP material with B1 structure was plotted in Fig. 3.

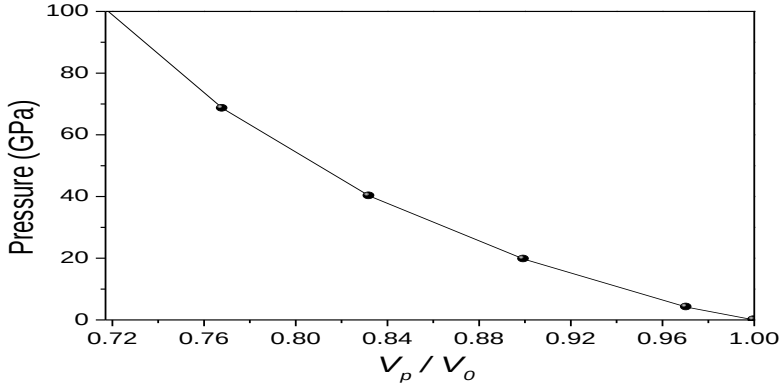

Fig. 3: Pressure versus (V_p/V_0) of BP with B1 Phase.

The obtained value of a_0, B_0, and B_0' are given in Table 1, and compared with other theoretical data [1], [3] and [13] of the literature. In general, our calculated values of a_0, B_0 and B_0' are agreed with other theoretical data [1], [3] and [13].

Table 1: Equilibrium Lattice Constant a_0, Bulk Modulus B_0, and Its Pressure Derivatives B_0' of BP with Rock-Salt Structure, Compared to other Theoretical Data of The Literature. [a] PP-PW, [b] LMTO, [c] LDA, [d] GGA

Parameter	a_0 (Å)	B_0 (GPa)	B_0'
This work	4.282	148.4	4.64
Ref. [1][a]	4.30	152	-
Ref. [1][b]	4.27	176	-
Ref. [3]	4.32	163.2	3.58
Ref. [13][c]	4.268	177	3.32
Ref. [13][d]	4.332	161	3.60

The deviation between our calculation (148.4 GPa) of B_0 and the theoretical one (152 GPa) reported by Kocinski and Zbroszczyk [1] is only about 2.4%. It can be seen that our value (4.64) of B_0' is slightly higher than the previous results 3.58 and 3.32 (3.6) reported by Arbouche et al. [3], and Meradji et al. [13], respectively.
We further investigate the high-pressure crystal density g of our compound of interest. The calculated crystal density at different values of pressure is plotted in Fig. 4. An analytical relation for the pressure dependence of the crystal density is given by the following a quadratic fit:

$$g = 3.554 + 1.932\times10^{-2}\, p - 0.55\times10^{-4} p^2 \quad (2)$$

Where p is given in GPa, and g in g/cm^3.
At zero-pressure, our calculated value of the crystal density g was found at around 3.534 g/cm^3.

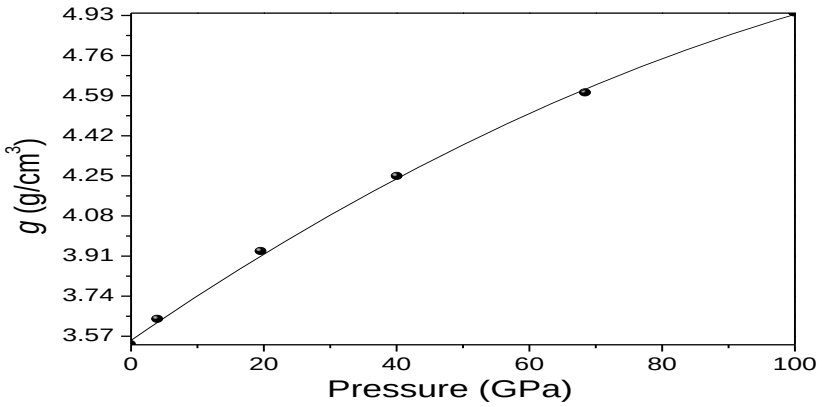

Fig. 4: Crystal density Versus Pressure of BP Up to 100 GPa.

3.2. Elastic constants, young modulus and poisson's ratio

The elastic constants obtained here were calculated by the density functional perturbation theory (DFPT) method. For more detail on the calculation of the elastic constants of materials by the DFPT, please see for example our previous works [6, 14]. The obtained value of C_{11}, C_{12} and C_{44} for BP material with B1 structure are given in Table 2, and compared with other theoretical data [15].

Table 2: Elastic Constants C_{ij} (in GPa) of BP with Rock-Salt Structure, Compared to Other Theoretical Data [15]

Parameter	C_{11}	C_{12}	C_{44}
This work	326.4	68.2	274.9
Ref. [15]	341	86	248

From the Table 2, it is observed that our obtained values of C_{11}, C_{12}, and C_{44} are in general in agreement compared to other theoretical ones [15]. Our value (326.4 GPa) of C_{11} underestimate the theoretical one (326.4 GPa) [15] obtained from the full potential linearized augmented plane wave (FP-LAPW) method by only about 4.3%. To the best of our knowledge, there are no other data (except the work [15]) available in the literature on the elastic constants for BP compound with rock-salt structure.
For the aggregate polycrystalline materials, the average quantities of the mechanical properties are usually used. The Young modulus E and the Poisson's ratio σ are usually expressed as function of the bulk modulus B and the isotropic shear modulus G as follow [16]

$$E = 9BG/(3B + G), \text{ and } \sigma = (3B - 2G)/(6B + 2G) \quad (3)$$

Our calculated values of B, G, E and σ of BP aggregate polycrystalline material are: 154.25 GPa, 202.97 GPa, 423.26 GPa and 0.04, respectively. Our calculated value (154.25 GPa) of B agreed well with the value (148.4 GPa) obtained previously in the present work from the P-V data. It is also in good agreement with the theoretical result (152 GPa) reported by Kocinski and Zbroszczyk [1]. The deviation between these two values is only around 1.5%.

3.3. Sound velocity, Debye temperature and melting temperature

The longitudinal v_l, transverse v_t, and average v_m sound velocities as well as the Debye temperature are calculated, the details are described elsewhere [17-20]. The calculated values of v_l, v_t and v_m of BP compound with B1 structure are: 10.965, 7.579 and 8.244 km/s, respectively. The calculated value of the Debye temperature θ_D of BP with rock-salt structure is around 1147 K. This value is slightly

higher than the value 1095 K of the zinc-blende phase reported by Bouhemadou et al. [2]. For crystals with cubic structure symmetry, the melting temperature T_m and the elastic constant C_{11} are related by [5], [16]

$$T_m = 553 + (591 / \text{Mbar})\, C_{11} \pm 300 \text{ K} \quad (4)$$

The value of T_m for BP with B1 structure has been found 2482 ± 300 K. To the best of our knowledge, there are no other data available in the literature on the sound velocity and the melting temperature T_m for BP compound with B1 structure.

4. Conclusion

Using PW-PP approach in the framework of the DFT and the DFPT, we determine the EOS parameters of cubic rock-salt BP material using the pressure-volume data. The values obtained are in general in agreement with other theoretical ones of the literature.
The pressure dependence of the crystal density under high pressure up to 100 GPa was also studied.
The elastic constants, the bulk modulus, the isotropic shear modulus, the Young modulus and the Poisson's ratio are also predicted. In addition, the longitudinal, transverse and average elastic wave velocities and also the Debye temperature θ_D of the aggregate material were also presented. It was found that the Debye temperature θ_D of the cubic rock-salt structure is slightly higher than the value of the cubic zinc-blende phase reported in the literature.
To the best of our knowledge, there are no data available in the literature on the longitudinal, transverse and average elastic wave velocities, and the Debye temperature θ_D for BP compound with B1 structure. So, future experimental and theoretical results are needed to valid our finding data of B1 phase.

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