International Journal of Nanoelectronics and Materials
Volume 16, No. 4, October 2023 [853-864]

The Influence of Pressure on the Electronic and Elastic Characteristics of GaP Nanocrystals using Density Functional Theory

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Received 21 August 2022, Revised 30 January 2023, Accepted 2 March 2023

ABSTRACT

The electronic structural and mechanical properties of III-V Gallium Phosphide (GaP) nano-crystals zinc-blende stable (ZB) phase under pressure dependence have been studied via the model of the density functional theory (DFT) in combination with the large unit cell (LUC) approach at (8, 16, 54 & 64) atoms. The exchanges and correlations (XC) energy has been defined in all approaches through generalized gradient approximations of the Perdew-Burke-Ernzerhof (GGA-PBE), and determination of GaP characteristics in the case where the pressure has been increased from 0GPa to ±50GPa. Elastic parameters like elastic constants (C_{11}, C_{12} & C_{44}), Kleinmann parameter (ξ), Zener anisotropic factor (A), shear modulus (G), Young's modulus (E), Poisson's ratio (v), Bulk modules (B) of GaP-ZB structure have been calculated and showed systematic variation with a pressure increase. Our calculations show that Bulk modules and sound speed increase with an increase in the number of core atoms. In this systematic approach, it has been found that the B/G ratio is 1.58 for this compound and it exhibits a negative Cauchy pressure, classifying GaP as brittle. The results were discovered to be consistent with other theoretical as well as experimental results. The present study directly relates to the latest experimental works on the III-phosphide compounds. The current results provide information and direction for further investigation into the fundamentals and potential applications of gallium phosphate (GaP) nanocrystals. In addition, we attempted to compare the results of the investigation with some similar types of compounds that are already documented in the literature. We believe that our study will have a significant impact on both the field of research and contemporary technology based on semi-conducting materials.

Keywords: DFT, pressure dependence, mechanical properties, GaP.

1. INTRODUCTION

One of the significant parts of the science of computational materials is the prediction of some new material forms and the description of their various properties, affected by their electronic structures. Narrow-gap semi-conducting materials represents a significant material with numerous applications, which include lasers, ultra-sonic multipliers, infrared detectors, solar cells, magnetic sensors, electrically driven light sources, and thermo-photovoltaic cells [1]. Gallium phosphide (GaP) that is a typical 2nd-generation compound semi-conductor material is mainly utilized for the productions of high-power, high-frequency, high-speed, and light-emitting electronic devices. GaP is an excellent type of material as well for the production of light-emitting devices and high-performance millimeter-wave and microwave devices. With the rise of information highways and internet, it was widely utilized as well in the areas of mobile and satellite communications, GPS navigation and solar power technology [2].

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One of the important motivations for the high-pressure investigations in the semi-conductor complexes stems from the fact that the semi-conductor layers are usually subjected to the large built-in strains due to the fact that they're usually grown on various substrates that have noticeable lattice mismatches within the difference in coefficients of thermal expansion between the substrate and the epitaxial layer. In the case of superlattices and heterostructures, this case becomes of a higher complexity and mutual influences between various material layers could appear [3]. Therefore, it's quite important to know the evolutions of physical characteristics under the strain effects.

There are several theoretical and experimental computations for elastic and structural constants of the GaP utilizing various approaches. Weil et al [4] have specified elastic GaP constants by ultra-sonic measurements. Ultrasonic wave velocity values were utilized by Nichols et al. [5], Yogurtcu et al. [6] and Rimai et al [7] for the purpose of measuring elastic constants of the gallium and indium phosphide. Besides experimental measurements, some progress was made in the theoretical descriptions of elastic characteristics of the GaP. Hierrera- Cabrerra et al. [8], Rodriguez-Hernandez et al. [9, 10] and Wang et al. [11] have utilized an ab initio pseudopotential approach for the simulation of III-P compounds' elastic constants. Meyer & Vurgaftman [12] have utilized envelope function approximations (i.e. multi-band KP approach) for studying elastic constant values of the AlP, InP and GaP compounds. Kamal et al. [13] had researched static dipole polarizability of stoichiometric GaP clusters (Gan Pn with n=2–5) through the use of a variety of the ab initio the wave function- based approaches and density functional time/theory dependent density functional theory (DFT/TDDFT). Arbouche et al. [14] conducted the first total-energy calculation principles based upon full-potential augmented plane-wave plus local orbitals (FP-LAPW+lo) approach for the purpose of investigating phase transformation under the high pressures of the III-phosphide (BP, AlP, GaP, InP) in zinc-blende, CsCl, cmcm, sc 16, NiAs, NaCl, d- β- tin, Imm2 and Immm structures. Structural, electronic, mechanical, and thermal characteristics, in addition to elastic anisotropy and stability, of XP (X = Al, Ga, or In) in the P $6_4$22 phase had been researched through the density functional theory (DFT) by J. Miao et al.[15].

In the present work, the structural, mechanical and elastic characteristics of GaP based Gauss.09 program having face-centered cubic in zinc-blende (B3) structure, with Wyckoff positions Ga at (0, 0, 0), (0.5, 0.5, 0.5), and P at (0.25, 0.25, 0.25), (0.75, 0.75, 0.75) and position coordinates with space group $F43m$, where the value of its experimental lattice constant is approximately 5.451 Å was researched [16]. The 3-D crystal structure view has been displayed with the use of the Gaussian View 5.0 w [17, 18] as shown in Figure 1.

Thus, it is thought that it's worthwhile to conduct those computations by using DFT-GGA that has been coupled with an LUC and results have been found to be in good agreement with available experimental and theoretical information [14].

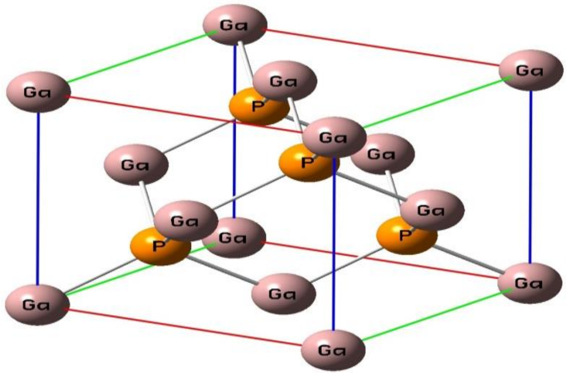

Figure 1. Zinc-blende crystalline structure of GaP (by GaussView3.0w).

2. MATERIAL AND METHODS

The calculation of GaP has been performed with first-principles calculations (Ab-initio) through employing a large unit cell method (LUC) [19, 20], within the DFT framework [21-23] with the Perdew-Bruke-Ernzerhof-Generalized Gradient Approximation (PBE-GGA) for potentials of exchanging correlations [24] as it has been carried out in the Gaussian 09 program [25].

Within the DFT formalism, total energy may be represented as the density of electron system function, $E[\rho(\mathbf{r})]$ and the functional form of the $F_{HK}[\rho(\mathbf{r})]$ has been expressed as the summation of non-interacting electrons' kinetic energy (T_s), Columbic electron-electron contribution, which has been referred to as Hartree electrostatic energy (E_{Hartree}) as well, and all of the many-body quantum impacts have been put together into exchange and energy of correlation (E_{xc}) [26]. Therefore, the energy function will be expressed as follows:

$$\begin{aligned} E[\rho(\boldsymbol{r})] &= \int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r} + F_{\text{HK}}[\rho(\boldsymbol{r})] \\ &= \int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r} + T_S[\rho(\boldsymbol{r})] + E_{Hartree}[\rho(\boldsymbol{r})] + E_{xc}[\rho(\boldsymbol{r})] \end{aligned} \tag{1}$$

The following step in the electronic structure issue is defining effective potentials V_{eff} [26],

$$\begin{aligned} V_{eff} &= \frac{\delta\{\int \rho(\boldsymbol{r})v(\boldsymbol{r})d\boldsymbol{r} + E_{Hartree}[\rho(\boldsymbol{r})] + E_{xc}[\rho(\boldsymbol{r})]\}}{\delta\rho(\boldsymbol{r})} \\ &= v(\boldsymbol{r}) + \int \frac{\rho(\mathbf{r}')}{|r - r'|} d\mathbf{r}' + v_{xc}(\boldsymbol{r}) \end{aligned} \tag{2}$$

here $v_{xc}(\mathbf{r})$ represents potential of exchange-correlation that may be represented as:

$$v_{xc}(r) = \frac{\delta E_{xc}[\rho(\boldsymbol{r})]}{\delta\rho(\boldsymbol{r})} \tag{3}$$

which results in central equation in the Kohn-Sham DFT that represents 1-electron Schrodinger such as equation that has been represented by:

$$\left[-\frac{1}{2}\nabla^2 + V_{eff}\right]\phi_i = \epsilon_i\phi_i \tag{4}$$

where the 1st term denotes non-interacting electrons' kinetic energy and $\{\phi_i\}$ represent Kohn-Sham 1-electron orbitals and electron density can be expressed by,

$$\rho(r) = \sum_{i=1}^{N} |\phi_i|^2 \tag{5}$$

ϵ_i's represent energy values of Kohn-Sham 1-electron orbitals.

Geometry optimization is a reliable method for DFT at the level of generalized gradient approximations, coupled with the LUC-DFT for the purpose of gaining stable configuration for the periodic system or molecule via inexpensive and sufficient energy calculations. A process of optimization involves repeated sampling of the possible energy surface to a point where possible energy would reach a minimum value where all of the forces on all of the atoms have been 0 [27, 28], 4 cores of LUC have been taken under consideration in this work 8, 16, 54, and

64 atoms for the GaP nano-crystals.

From derivatives of energy as a function of lattice strain elastic moduli may be obtained. It's common that a cubic system has three independent values of the elastic constant only, which areC_{11}, C_{12} andC_{44}. That is why, a set of 3 equations is required for the determination of all the constants. The 1st eq. involves the calculations of bulk modulus (B), related to elastic constants as: [29]

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{6}$$

Here, C_{11}, C_{12} and C_{44} represent 2nd order elastic constant values ($C_{11} = 140.5$, $C_{12} = 62$, $C_{44} = 70.3$) [30].

3. RESULTS AND DISCUSSION

Elastic constants (C_{ij}) measure crystal structure stiffness under applications of the external strains. For crystals' cubic symmetries, 3 independent constant values, which are namely C_{11}, C_{12} and C_{44} are needed for the determination of mechanical stability. For the purpose of confirming the criteria of the mechanical Born-Haung stability must be satisfied, which include 4 equations, which are: $-(C_{11} - C_{12}) > 0$ and$(C_{11} + 2C_{12}) > 0$, $C_{44} > 0$. These conditions lead also to restrictions on bulk modulus B value that has to be between C_{11} and C_{12}, in other words, $C_{11} > B > C_{12}$. [31]

Zener anisotropy factor (A) indicates the anisotropy degree in solid structures. For an entirely isotropic material, A factor is assigned a value of 1, in a case where A value is smaller or higher than the unity it measures elastic anisotropy degree. Shear modulus, Poisson's ratio, and Young's modulus that represent the most significant elastic characteristics for the applications, have usually been assessed for poly-crystalline materials in a case where their hardness value was researched. Those amounts are estimated based on computed data with the use of the following set of the equations [31]:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{7}$$

$$v = \frac{3B - 2G}{6B + 2G} \tag{8}$$

and,

$$E = \frac{9GB}{G + 3B} \tag{9}$$

where G_V represents Voigt's shear modulus that corresponds to upper bound of the G values, G_R represents Reuss'es shear modulus that corresponds to lower bound of the G values, $G = \frac{G_V + G_R}{2}$ represents isotropic shear modulus and may be expressed as [32]:

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{10}$$

and,

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \tag{10}$$

Estimated Zener anisotropy factor (A), shear modulus and Young's modulus, Poisson ratio have been summarized in Table 1. Estimated (A) values for the GaP under the ambient temperatures and pressures were 1.79, where the value of 1 is considered to be isotropic. The Poisson ratio value (v) for the covalent materials has been small (where it equals 0.10), while for the ionic materials, 0.250 represents the typical value [33]. In this case, a value of v equals 0.27, which reveals that higher ionic contributions in the intra-atomic bonding for that compound have to be estimated. Bulk modulus (B) denotes resistance to fractures, whereas shear modulus (G) represents resistance to plastic deformations [33, 34].

High value of Pugh B/G ratio has been associated to the ductility, while low values represent a brittle nature. The critical value which separates the ductile materials from the brittle ones is 1.750; in other words, in the case where $B/G > 1.750$, then the material's behavior has been ductile, and in the opposite its behavior becomes brittle [35]. Now it is found that the B/G ratio is 1.58 for this complex, which classifies the GaP as brittle.

The other criterion that has been utilized is Frantsevich's ratio of modulus G/B, in a case where $G/B > 0.570$ [36], and materials have brittle behavior.

Table 1 Calculated values of shear modulus, Pugh's ratio, Young's modulus, Poisson's ratio, and Frantsevich's ratio of GaP.

Parameter	Calculated value
Young modulus (E)	141.536
Shear modulus (G)	55.640
Pugh Ratio (B/G)	1.584
Poisson Ratio (v)	0.274
Frantsevich ratio (G/B)	0.631

The estimated Shear modulus value from the elastic constant values has been 55.64 GPa, signifying GaP hardness. Cauchy pressure (C_P). Kleinman parameter (ξ), Anisotropy index (A), and Lames' coefficient values $(\mu \ \& \ \lambda)$ have been estimated as well for mono chalcogenide of the lanthanum have been calculated with the use of the relation [37]:

$$C_p = C_{12} - C_{44} \tag{12}$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{13}$$

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \tag{14}$$

$$\mu = \frac{Y}{2(1 + \sigma)} \tag{15}$$

$$\lambda = \frac{Y\sigma}{(1 + \sigma)(1 - 2\sigma)} \tag{16}$$

Table 2 The estimated value of Cauchy pressure, Kleinman parameter, Anisotropy index, and Lames' coefficients (μ and λ) of GaP.

Parameters	Calculated values
Cauchy pressure (C_P)	-8.3
Kleinman parameter (ξ)	0.574
Anisotropy index (A)	1.791
Lames' coefficients (μ)	55.542
Lames' coefficients (λ)	67.575

However, the bulk modulus isn't the only mechanical amount determining the material utility for the hard coatings. The Cauchy pressure was suggested that it might be utilized for the description of the angular character of the atomic bonding in the compounds and the metals. In the case where the Cauchy pressure value is negative, then this material becomes non-metallic with the directional bonding, however, in the case where the value of the Cauchy pressure value is positive, then this material is probably metallic. GaP has negative Cauchy pressure indicating its brittle nature [38].

Figure 2 illustrates the numberof atoms in the core of GaP nanocrystal versus Bulk modulus. This figure shows that the bulk modulus value increases with an increase in the number of atoms in the core. Such correlation could simply be due to the fact that the lattice constant for the crystal's core part decreases with increasing number of atoms, latter equation indicates that lattice constant decrease entails the decrease in inter-atomic distance (d) that results in the increases of bulk modulus based upon the Cohen empirical formula [39]:

$$B_0 = \frac{(1970 - 200I)}{d^{3.5}} \tag{17}$$

where I denotes ionicity factor that equals 0, 1 & 2 for lV, lll-V & ll-V groups, d represents inter atomic distances [39, 40].

$$d = \frac{\sqrt{3}}{4} a_0 \tag{18}$$

Here, a_0 lattice constant at pressure (P) and temperature (T) of 0.
And sound speed equals:

$$v_0 = \frac{\sqrt{B_0}}{\rho} \tag{19}$$

where v_0 represents sound speed, ρ represents density of Gallium phosphid (4.138 g/cm^3) [16].

And this relation is shown in Figure 3 for sound speed with number of the core atoms, which appear speed of sound depends upon atom arrangements [41].

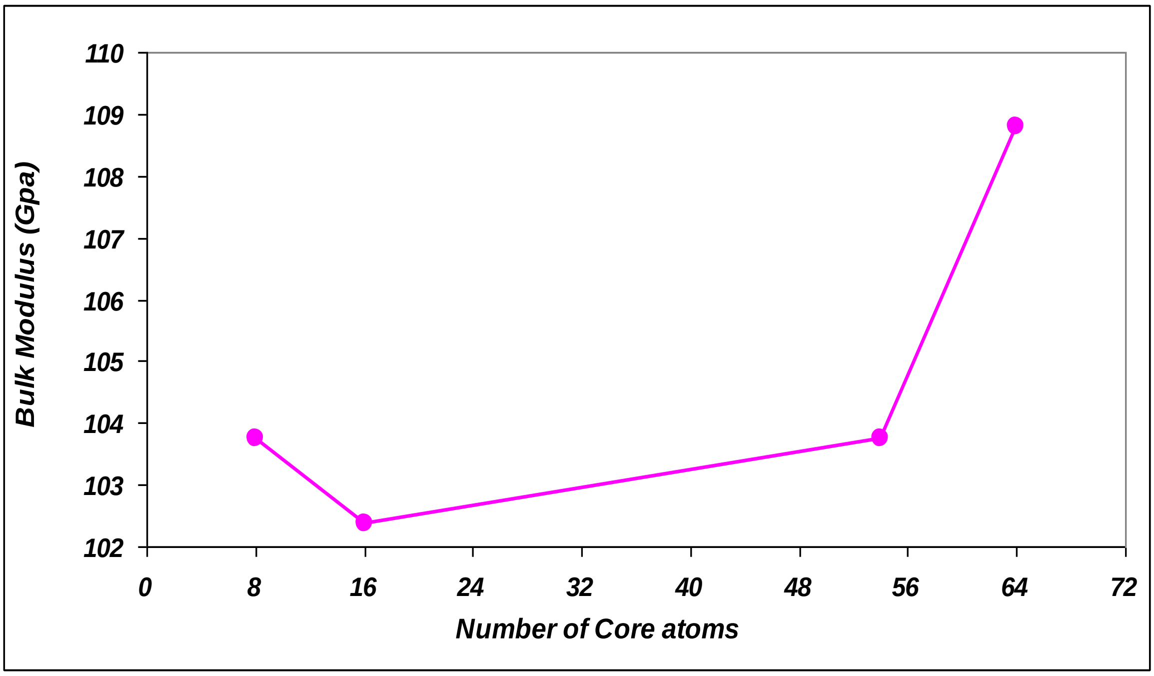

Figure 2. Bulk modulus of GaP nano-crystals alloy as function of number of core atoms per LUC

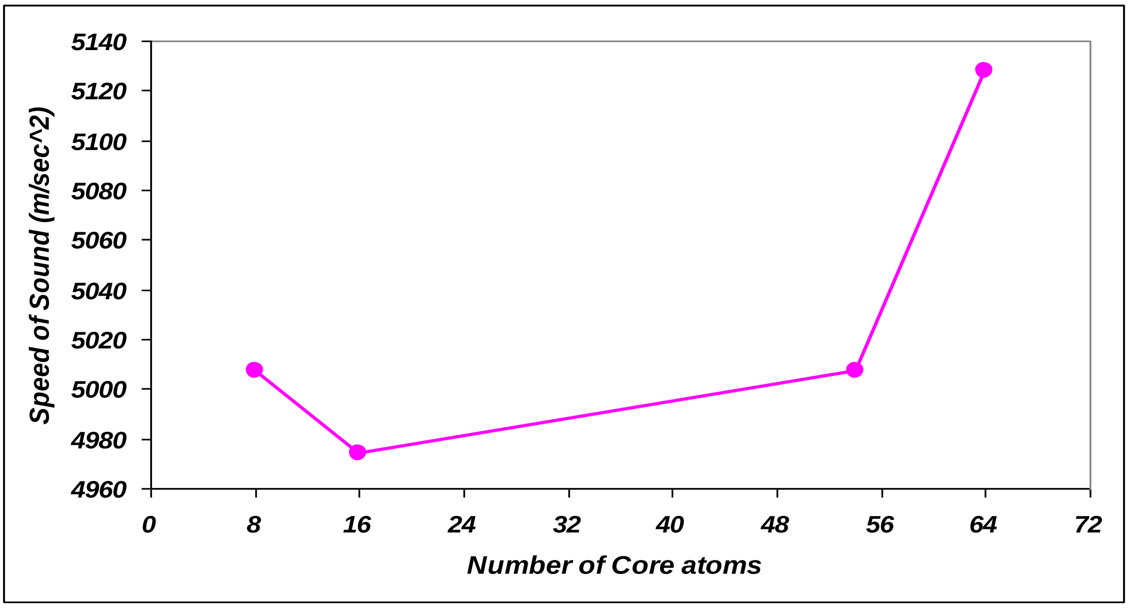

Figure 3. Sound speed of GaP nanocrystal as function of number of core atoms per an LUC.

Compression stress leads to an increase in the density and a decrease in volume due to orbital shrinkage, which is seen in Figure 4, it has been noticed that the ratio V/V_0 is decreased smoothly with the increases in pressure, on the other hand, change of the is getting smaller because of mutual repulsion of atoms, resulting in difficulty of compressing crystals under the high pressures [42].

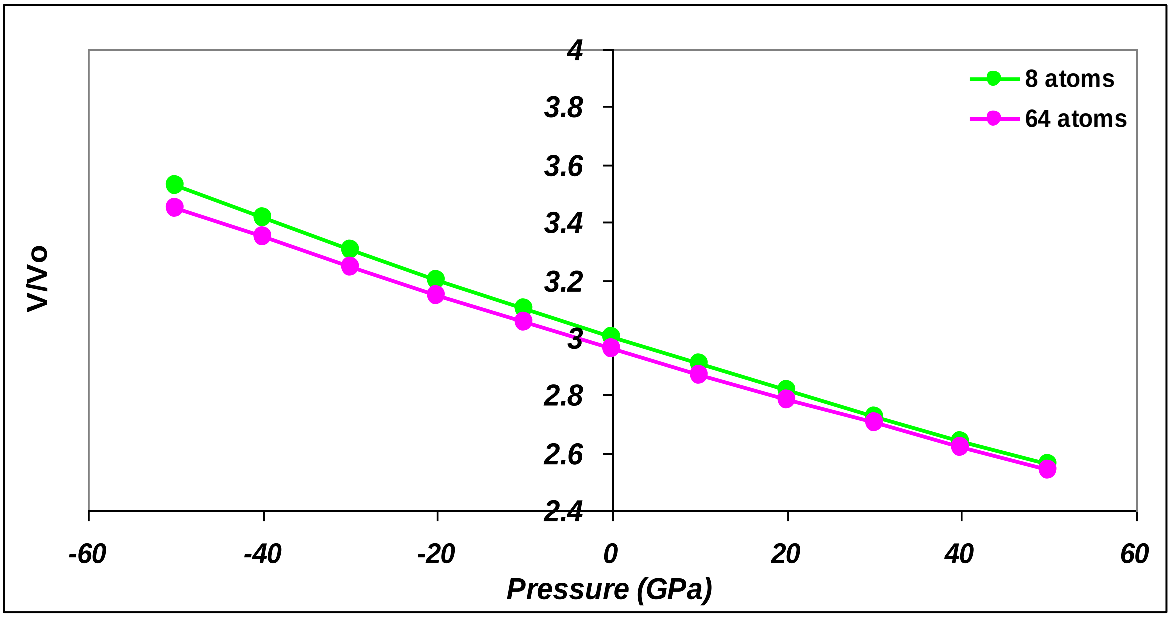

Figure 4. Volume of GaP nanocrystal versus pressure for core atoms per LUC.

Moreover, the average phonon velocity which representation in the speed of sound can be shown in Figure 5.

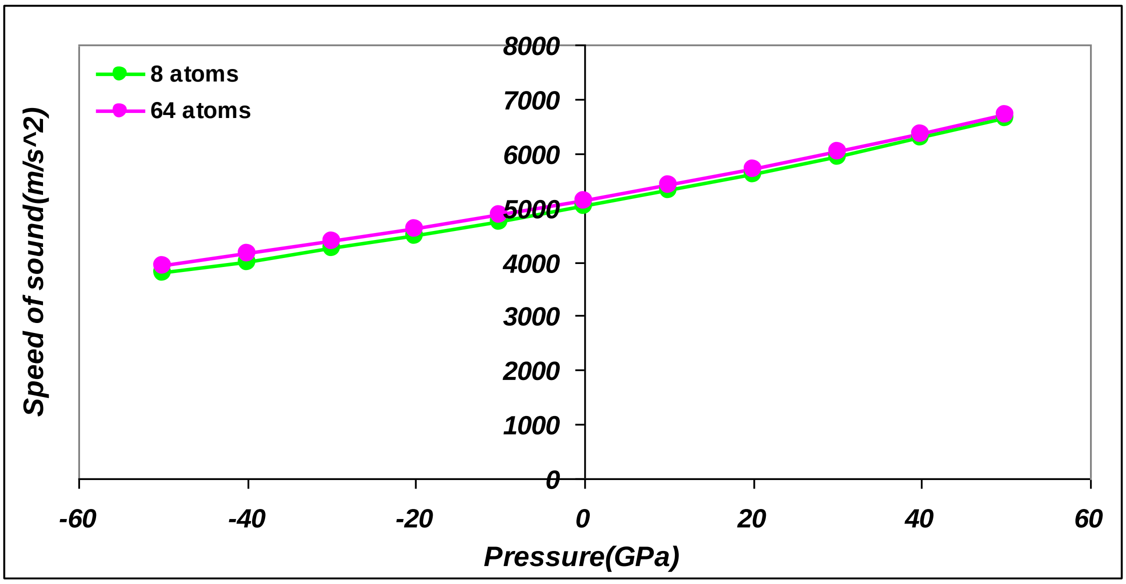

Figure 5. Pressure dependence of speed sound in GaP nanocrystal for the core atoms per LUC.

The pressure dependence of Bulk modulus in GaP when pressure is changed from 0GPa to ±50 GPa is shown in Figure 6. As pressure increases, bulk modulus has the same changes. Bulk modulus directly depends on the value of the density, and Young modulus which is dependent on bulk modulus, and vice versa around for value of tensile stress [43]. One can predicate an increasing for Bulk modulus based on the knowing physical equation ($B = \Delta P = \Delta V$), because it depends on the influence of pressure.

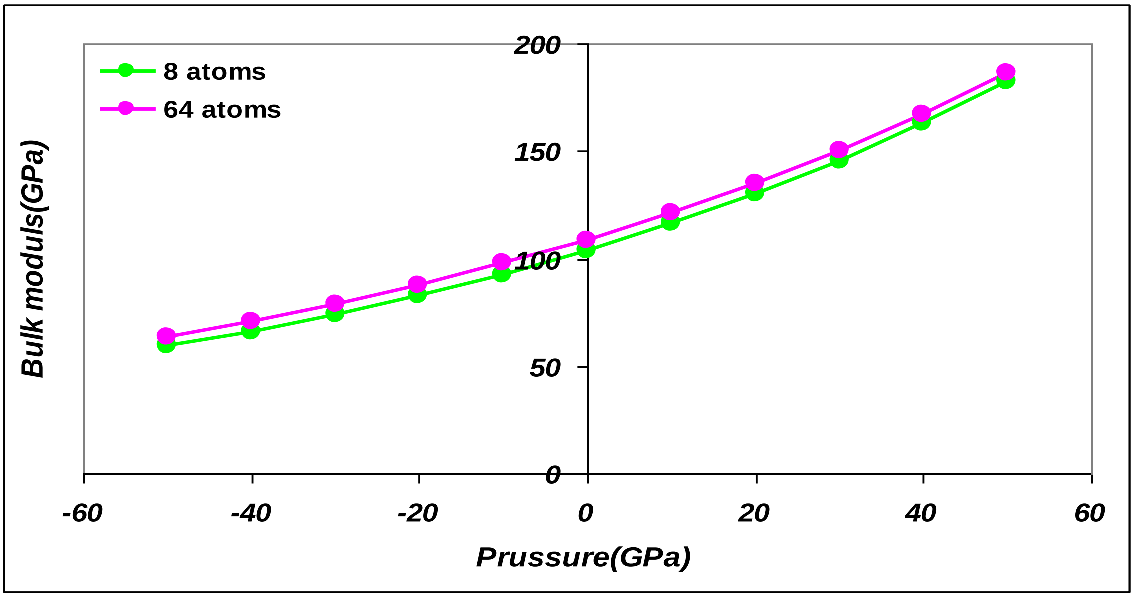

Figure 6. Pressure dependence of Bulk modulus in GaP nanocrystal for core atoms per LUC.

The material is stiffer with an increment Young modulus (E), according to (E) which represents resistance to the uniaxial tensions and indicates the degree of stiffness [**44**]. Similarly bulk, shear and Young moduli of GaP, in addition to that, an identical behavior appears with the Pressure's effect as can be revealed from Figure 7.

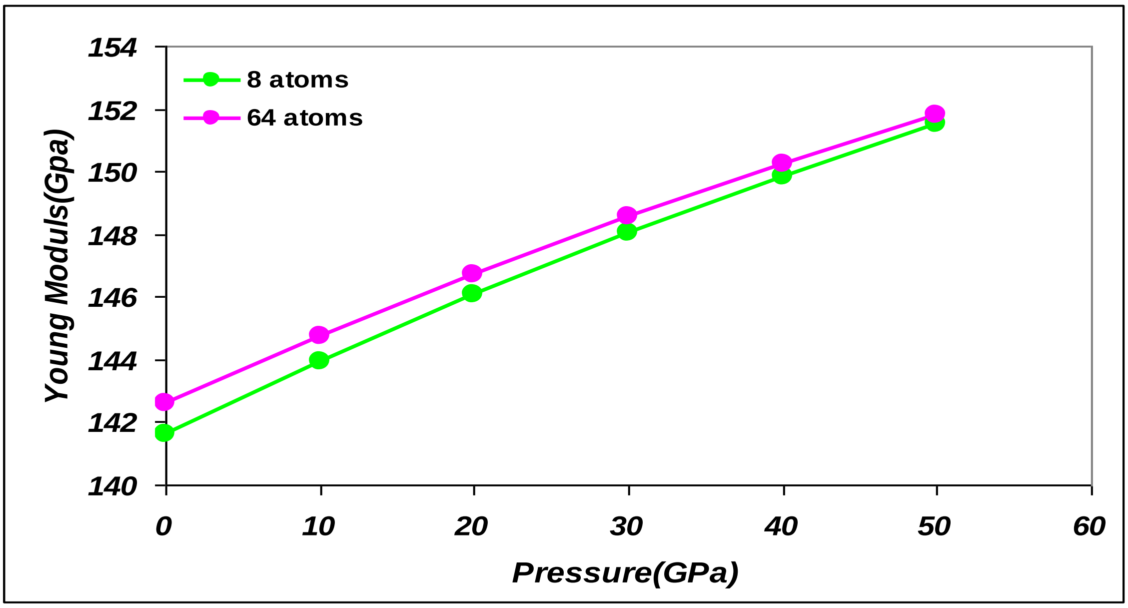

Figure 7. Pressure dependence of Young modulus in GaP nanocrystal for core atoms per LUC.

Our computations have shown that with an increased value in the pressure value of the Poisson ratio (v) changed from 0.293 to 0.363, which shows that by the increase of the value of the pressure, ionic contribution to inter atomic bonding turns as dominant, which was shown in Figure 8. Poisson ratio of GaP at 0GPa was 0.274 that predicates metal nature of GaP.

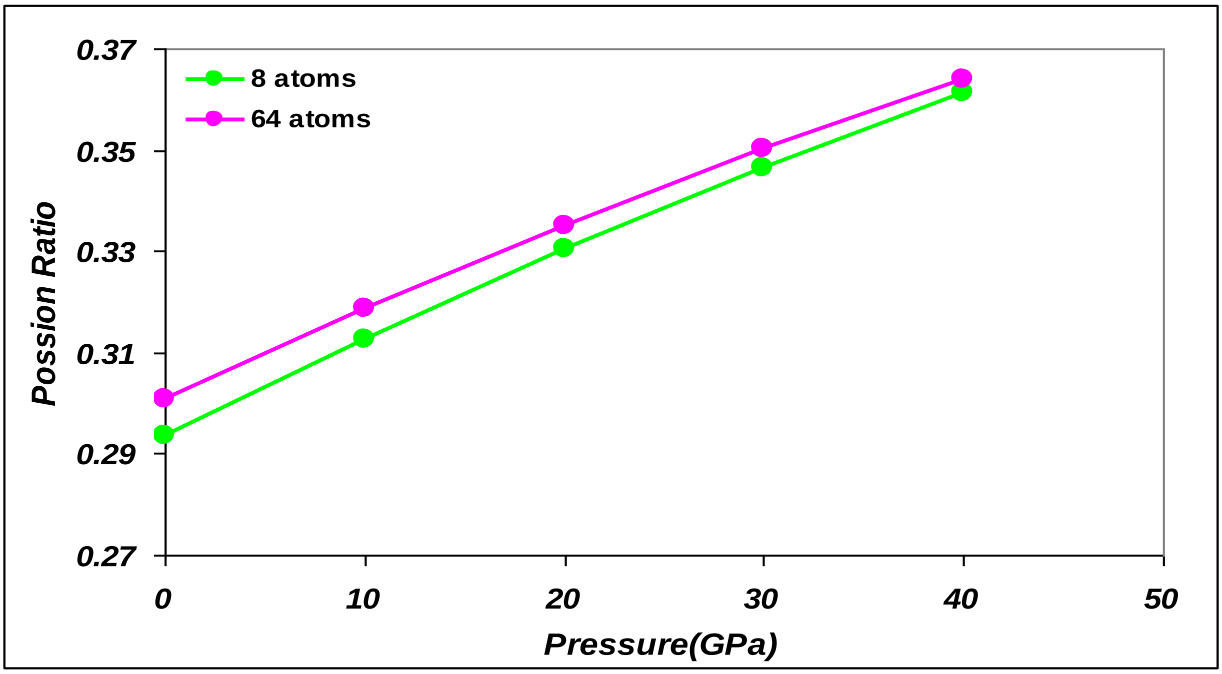

Figure 8. Behavior of the Poisson ratio under pressure for GaP nanocrystal for core atoms per LUC.

4. CONCLUSION

In this systematic approach, elastic, structural, and mechanical characteristics of the zinc-blende GaP nanocrystals alloys' had been researched under pressure effects by employing first-principles combining via DFT within generalized gradient approximation. Bulk modulus and sound speed have been found to increase with increasing number of core atoms. Several mechanical characteristics like sound speed, Poisson ratio, bulk and young moduli increases by increasing pressure. Moreover, it had been discovered that the B/G ratio was 1.58 for this compound, categorizing GaP as brittle. Our calculations in this work are presented to be in good agreement with the other experimental and theoretical researches.

STATEMENT OF DISCLOSURE

No potential conflicts of interests had been reported by authors.

REFERENCES

[1] Han Liu , Yaqian Dan , Ao Zhang , Siyuan Liu , Jincheng Yue , Junda Li , Xuejiao Ma , Yanping Huang , Yanhui Liu1, and Tian Cui ," First-Principles Study of High-Pressure Phase Stability and Electron Properties of Be-P Compounds", Materials, 15, (2022),1255.
[2] Jiao, Z.-Y.; Ma, S.-H.; Guo, Y.-L. "Simulation of optical function for phosphide crystals following the DFT band structure calculations". Comput. Theor. Chem., 970, (2011) 79–84.
[3] H. Gleize, F. Demangeot, J. Frandon, M.A. Renucci, F. Widmann, B. Daudin, Appl. Phys. Lett. 74, (1999), 703.
[4] R. Weil, W.O. Groves, J. Appl. Phys. 39, 4049 (1968).
[5] D.N. Nichols, D.S. Rimai, R.J. Sladek, Solid State Commun. 36, (1980), 667.

[6] Y.K. Yogurtçu, A.J. Miller, G.A. Saunders, J. Phys. Chem. Solids 42, (1981), 49.
[7] D.S. Rimai, R.J. Sladek, Solid State Commun. 30, (1979), 591.
[8] M.J. Herrera-Cabrera, P. Rodriguez-Hernandez, A. Munoz, Phys. Stat. Sol. (b) 223, (2001),411.
[9] P. Rodrيguez-Hernلndez, A. Munoz, Semicond. Sci. Technol. 7, (1992), 1437.
[10] P. Rodrيguez-Hernلndez, M. Gonzalez-Diaz, A. Munoz, Phys. Rev. B 51, (1995), 14705.
[11] S.Q. Wang, H.Q. Ye, Phys. Stat. Sol. (b) 240, (2003), 4.5
[12] I. Vurgaftman, J.R. Meyer, L.R. Ram-Mohan, J. Appl. Phys. 89, (2001), 5815.
[13] C. Kamal, Tapan K. Ghanty, Arup Banerjee, and Aparna Chakrabarti, "ab initio study of stoichiometric gallium phosphide clusters", the journal of chemical physics 130, ,(2009), 024308.
[14] O. Arbouche , B. Belgoumène , B. Soudini , Y. Azzaz , H. Bendaoud , K. Amara , "First-principles study on structural properties and phase stability of III-phosphide (BP, GaP, AlP and InP)", Computational Materials Science, 47, (2010) pp.685–692.
[15] Junjie Miao, Changchun Chai,Wei Zhang , Yanxing Song and Yintang Yang, "First-Principles Study on Structural, Mechanical, Anisotropic, Electronic and Thermal Properties of III-Phosphides: XP (X = Al, Ga, or In) in the P6422 Phase", Materials 13, (2020), 686.
[16] R. Weil, W.O. Groves, "The Elastic Constants of Gallium Phosphide",J. Appl. Phys. 39, (1968), 4049.
[17] Mohammed T. Hussein and Hamid A. Fayyadh, Chalcogenide Letters journal, Vol. 13, No. 12(2016) pp.537 – 545.
[18] A. Frisch, H.P. Hratchian, R.D. Dennington, II, T.A. Keith, J. Millam, A.B. Nielsen, A.J. Holder, J. Hiscocks. GaussView Version 5.0 (Gaussian Inc., 2009).
[19] Hamid A. Fayyadh, "Stability, Structural and Electronic properties of Indium Phosphide Wurtzite-Diamantane Molecules and Nanocrystals: A Density Functional Theory Study", Journal of Nano Research, Vol. 69, (2021) pp1-9.
[20] H. A. FAYYADH, T. H. MAHMOOD, E. K. HASAN, " Journal of Non-Oxide Glasses Vol. 12, No. 2, (2020) pp.13 – 19.
[21] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas", Phy. Rev. B, vol. 136, no. 3, (1964) pp. B864-B871.
[22] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects", Phys. Rev., vol. 140, no. 4A, (1965) pp. 1133-1138.
[23] S. Cottenier, Density Functional Theory and the family of (L) APW-methods: a step-by-step introduction, Belgium, ISBN 90-807215-1-4, (2002).
[24] J. P. Perdew, K. Burke and M. Ernzerhof, "Generalized Gradient Approximation Made simple", Phys. Rev. Lett., vol. 77, pp. 3865-3868 (1996).
[25] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka and J. Luitz, Wien2k. Techn. Universitat, Wien, Austria, ISBN 3- 9501031-1-2, (2001).
[26] B. Santra, "Density-Functional Theory Exchange-Correlation Functionals for Hydrogen Bonds in Water", Ph.D. Thesis, Berlin University, (2010).
[27] J. D. Gale and J. Chem. Soc. Faraday 93, 629 (1997).
[28] M. T. HUSSEIN, A. RAMIZY , B. K. AHMED, H. A.FAYYADH, "Study the Electronic Properties of AlAsxP1-x Nanocrystalalloying Composition, using Density Functional Theory", Journal of Non-Oxide Glasses Vol. 8, No 2 , (2016) pp.37 – 45.
[29] E.Schreiber, O.L.Anderson, N.Soga,"Elastic constants and their measure", MC. Graw-Hill, New York (1973).
[30] Y.K. Yogurtçu, A.J. Miller, G.A. Saunders, " PRESSURE DEPENDENCE OF ELASTIC BE~AVIOUR AND FORCE CONSTANTS OF GaP ", J. Phys. Chem. Solids, Vol.42, (1981) pp.49-56.
[31] B. Mayer, H. Anton, E. Bott, M. Methfessel, J. Sticht, P.C. Schmidt, Intermetallics 11, (2003), 23.
[32] M. Mattesini, R. Ahuja, B. Johansson, Phys. Rev. B 68, (2003), 184108.
[33] J. Haines, J.M. Leger, G. Bocquillon, Annu. Rev. Mater. Res. 31, (2001), 1.

[34] F. Boufadi, K. Bidai, M. Ameri, A. Bentouaf, D. Bensaid, Y. Azzaz and I. Ameri," First Principles Study of Mechanical Stability and Thermodynamic Properties of K2S under Pressure and Temperature Effect", Acta Physica Polonica A Vol. 129 , No. 3, (2016).

[35] R.D. Eithiraj, G. Jaiganesh, G. Kalpana, M. Rajagopalan, Phys. Status Solidi B 244, (2007), 1337.

[36] Pugh S.F., Philos. Mag. Ser. 7, 45, (1954), 823.

[37] Tavneet Kaur and M.M. Sinha, "A DFT Based Computation of Structural, Elastic and Mechanical Properties of VCo2Al", Advanced Materials and Radiation Physics (AIP Conf. Proc. 2352, 020027-1–020027-5, (2020).

[38] Peltiifor DG. ,"Theoretical predications of structure and related properties of intermetallic" J. of Mat. Sci. and Tech., 8, 345-9 (1992).

[39] J.Zheng, C.H.A.Haun, A.T.S.Wee, R.Wang and Y.Zheng,"Ground State Properties of Cubic C-BN Solid Solutions,"Journal of Physics; Condensed Matter, Vol.11, No.3, (1999), pp.927-935.

[40] S. Q. Wang and H. Q. Ye, “Plane-Wave Pseudopotential Study on Mechanical and Electronic Properties for IV and III-V Crystalline Phases with Zinc-Blende Structure,” Physical Review B, Vol. (2002), 66.

[41] T. Iitaka and T. Ebisuzaki, “First-Principles Calculation of Elastic Properties of Solid Argon at High Pressures”, Physical Review B 65(1) (2001).

[42] Young Liu, et al., "First principles investigation of structural and electronic properties of MgCu2 lave, phase under pressure”, Intermetallics Vol.31, (2012) pp. 257-263.

[43] B. T. Wang, P. Zhang, H. L. Shi, B. Sun and W. D. Li,“Mechanical and Chemical Bonding Properties of Ground State BeH2,” The European Physical Journal B, Vol. 74, No. 3, (2010) pp.303-308.

[44] E. Guler and M. Guler , Mater. Res. Ibero. Am. J.17, (2014), 1268.