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Research paper

Directional dependency of mechanical properties in gallium phosphide semiconducting material

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Abstract

The aims of this contibution is to investigate the directional dependency of mechanical properties of gallium phosphide (GaP) semiconduct-ing material using the experimental stiffness elastic constants C_{ij} reported in the litterature. These characteristics are visible by analysis and visualization of elastic tensors. The spatial dependencies of the Young's modulus, linear compressibility, shear modulus, and Poisson's ratio in GaP binary compound were calculated and schematized in graphical representations. Data analysis shows that the maximum value E_{max} of Young's modulus was estimated at around 166.7 GPa, while its minimum value E_{min} was estimated at around 102.5 GPa, which gives a ratio of approximately $E_{max}/E_{min} \approx 1.63$, while for the Poisson's ratio υ, the maximum value υ_{max} of υ was estimated at around 0.43, while its minimum value υ_{min} was estimated at 0.025, which gives a rate of approximately $\upsilon_{max}/\upsilon_{min} \approx 17.5$. The Debye temperature was also calculated, it is estimated at about 482.4 K, it is in good agreement with the experimental one (493 K) reported in the litterature, and the deviation between these two values is less than 2.2%.

Keywords: *Mechanical Properties; Gallium Phosphide; Elastic Anisotropy; Graphical Representation.*

1. Introduction

The elastic constants are important for determining the structural and thermal properties as well as the mechanical stability of materials. Furthermore, these quantities provide much information on the mechanical behaviour of the material to both the intrinsic and extrinsic forces applied to its crystal structure [1]. Mechanical stability was obtained by confiming the elastic constants C_{ij} [1].
Different theoretical approaches [1-22] and experimental technics [23-25] were used to study the elastic constants, thermel properties and some other physical properties of materials.
Using first-principle calculations, Moin and co-authors [6] have investigated structural, electronic, mechanical, optical, and thermodynamic features of promising (La, In)-doped AlSb for optoelectronic applications. Daoud [7] has investigated the mechanical behavior of aluminum phosphide under high pressure, while in other work Daoud and co-authors [20] have investigated the elastic constants and optical phonon frequencies of BX (X= P, As, and Sb) semiconductors using semi-empirical approach. Maaitah [21] has investigated the mechanical, optical, and lattice vibrational properties of gallium antimonide (GaSb) semiconductor under the influence of temperature using the empirical pseudopotential method (EPM), while Mezouar and co-authors [22] have investigated the mechanical properties of $B_xAl_{1-x}Sb$ ternary semiconducting alloys.
Weir [26] has investigated the high pressure phase transitions in the II-VI and III-V compounds, barium selenide, barium sulfide, barium oxide, gallium antimonide, gallium arsenide, and gallium phosphide, while Bouarissa and co-authors [27] have reported on the pressure-effects on band structure and chemical bonding of GaP semiconducting compound using the empirical pseudopotential method (EPM).
Benalia et al. [28] have studied the band gap behavior of scandium aluminum phosphide and scandium gallium phosphide ternary alloys and superlattices, Benamrani et al. [29] have studied structural, elastic and thermodynamic properties of ScP compound, while Rekab-Djabri et al. [30] have studied the ground state parameters, electronic properties and elastic constants of $CaMg_3$ intermetallic compound.
In the present contribution, we investigate the spatial dependencies of some engeniring moduli, especialy: the Young's modulus, linear compressibility, shear modulus, and Poisson's ratio in GaP binary semiconducting compound based on the experimental stiffness elastic constants C_{ij} reported in the litterature [31].

2. Theory and discussion of the results

In the case of cubic crystals, there are only three independent constants (C_{11}, C_{12} and C_{44}) that characterize the material [32-35]. For an arbitrary crystallographic direction m, the Young modulus E of single crystal may be given by this relationship [31]:

$$E^{-1} = S_{11} - 2(S_{11} - S_{12} - 0.5S_{44})(m_1^2 m_2^2 + m_2^2 m_3^2 + m_1^2 m_3^2) \quad (1)$$

Where S_{ij} are the compliance elastic constants and the m_i are the cosines of the direction m.
The Young modulus E for the direction of the cube axes $\langle 100 \rangle$ is readily given by: $E = 1/S_{11}$ [31].

Using the experimental elastic constants C_{ij} (C_{11} = 140.5 GPa,C_{12} = 62.03 GPa, and C_{44} = 70.33 GPa) reported in the litterature [31], and based on the expression describing the direction dependence of the Young's modulus of crystals [31] and the procedure presented by Gaillac et al. [18], the values obtained for the Young's modulus E as a function of the direction for the GaP semiconductor are presented in 2 dimensions (2D) and 3 dimensions (3D) in Figure 1 (A) and (B), respectively.The degree of anisotropy is dependent on the deviation of geometrical body (3D) from the spherical shape in this case, represented in a 2D shape. Data analysis shows that the maximum value E_{max} of Young's modulus was estimated at around 166.7 GPa (within (110) crystallographic plane and in [111] direction) [31], while its minimum value E_{min} was estimated at around 102.5 GPa (both within (100) crystallographic plane and in [001] direction, an within (110) crystallographic plane and in [001] direction) [31], which gives a ratio of approximately $E_{max}/E_{min} \approx 1.63$.

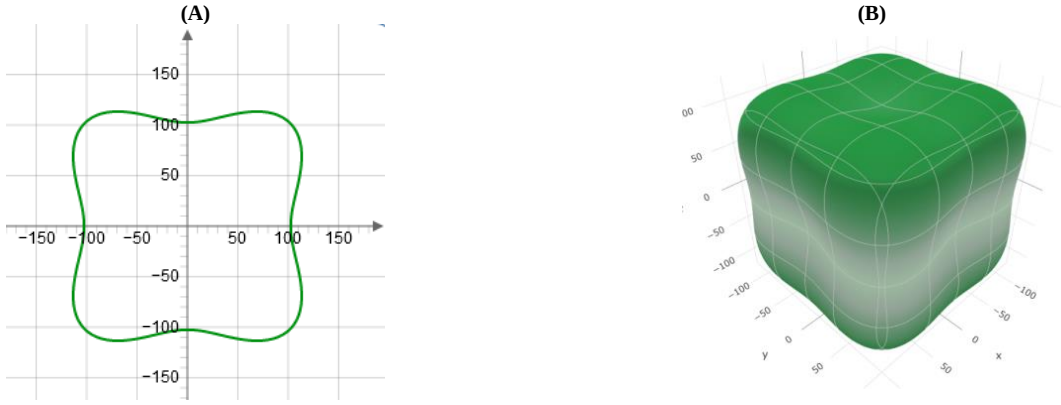

Fig. 1: The Spatial Dependency of Young Modulus in GaP Binary Compound: (A) in XY, XZ and YZ Planes, (B) in 3 Dimensions (3D).

The linear compressibility $\beta = 1/(C_{11} + 2C_{12})$ [31]. The implication of the previous definition is that a value of unity corresponds to the isotropic compressibility. The values obtained for the linear compressibility β as a function of the direction for the GaP binary compound are represented in 2 dimensions (2D) in Figure 2 (A). Data analysis shows that the maximum value β_{max} of β is equal to its minimum value β_{min} which is estimated at around 3.78 TPa^{-1} [31]. Since $\beta_{max} = \beta_{min}$ which gives the ratio $\beta_{max}/\beta_{min} = 1$. In order to understand the spatial dependency of the linear compressibility, the values obtained for the linear compressibility β as a function of the direction for GaP binary compound are represented in 3 dimensions (3D) in Figure 2 (B).

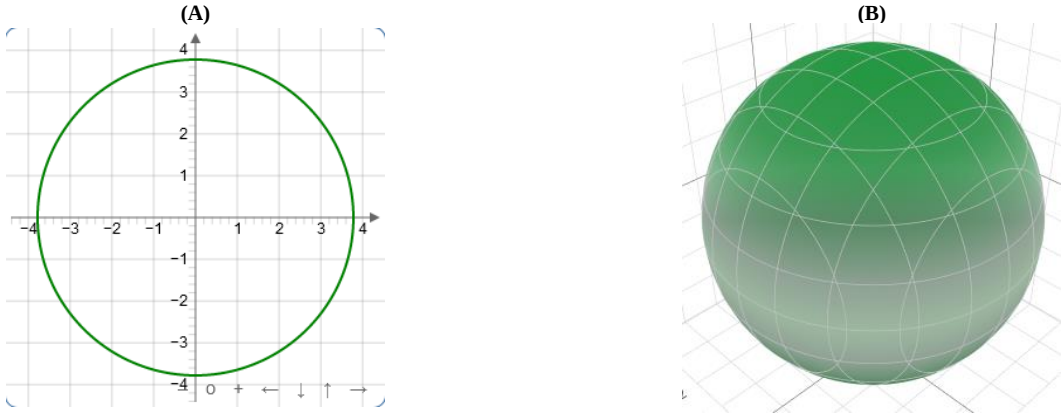

Fig. 2: Linear Compressibility in GaP Compound: (A) in XY, XZ and YZ Planes, (B) in 3 Dimensions (3D).

The values obtained for the shear modulus G as a function of the direction for GaP binary compound are presented in 2 dimensions (2D) and 3 dimensions (3D) in Figure 3 (A) and (B), respectively. A perfect circle (blue colour) represents the isotropy of the crystal structure plane; otherwise, it demonstrates the degree of anisotropy. Data analysis shows that the maximum value G_{max} of the linear compressibility G was estimated at around 70.33 GPa, while the minimum value G_{min} was estimated at around 39.24 GPa, which gives a ratio of approximately $G_{max}/G_{min} = 1.79$. Unfortunately, to our knowledge, no theoretical values or experimental data on G_{min} and $G_{max}$are available to make comparison.Thus, further theoretical predictions and experimental investigations are significantly needed.

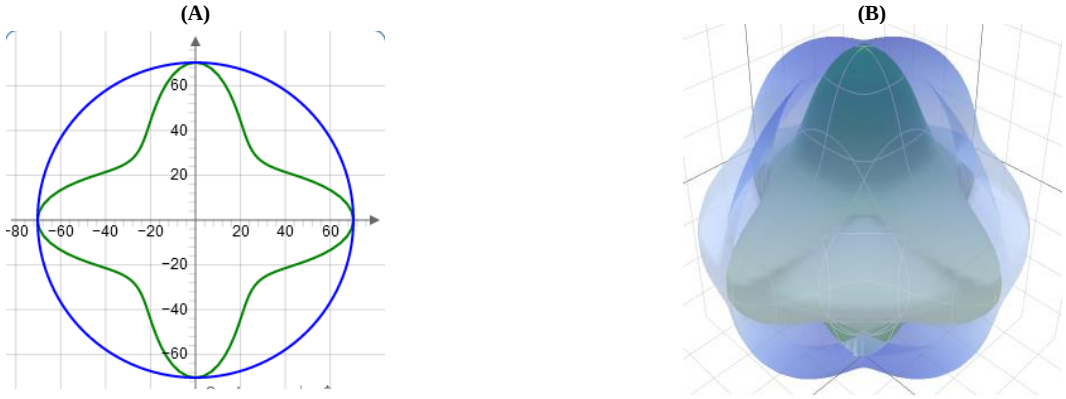

Fig. 3: The Spatial Dependency of Shear Modulus G in GaP Compound: (A) in XY, XZ and YZ Planes, (B) in 3 Dimensions (3D).

For an arbitrary crystallographic direction m and another perpendicular direction n, the Poisson's ratioυ is given by this relation [31]:

$$\nu = -\frac{S_{12} + (S_{11} - S_{12} - 0.5S_{44})(m_1^2 n_1^2 + m_2^2 n_2^2 + m_3^2 n_3^2)}{S_{11} - 2(S_{11} - S_{12} - 0.5S_{44})(m_1^2 m_2^2 + m_2^2 m_3^2 + m_1^2 m_3^2)} \quad (2)$$

where S_{ij} are the elastic compliance, the m_i are the cosines of the direction m and the n_i are the cosines of the direction n. Using the experimental elastic constants C_{ij} reported in the litterature [31], the values obtained for the Poisson's ratioυ as a function of the direction for the GaP binary compound are represented in 2 dimensions (2D) and 3 dimensions (3D) in Figure 4 (A) and (B), respectively. Data analysis shows that for the Poisson's ratio υ, the maximum value υ_{max} of υ was estimated at around 0.43 (within (100) crystallographic plane and in m = [010] and n = [001] directions) [31], while its minimum value υ_{min} was estimated at around 0.025 (within (100) crystallographic plane and in m = [011] and n = [0$\bar{1}$1] directions) [31], which gives a ratio $\upsilon_{max}/\upsilon_{min} \approx 17.5$.

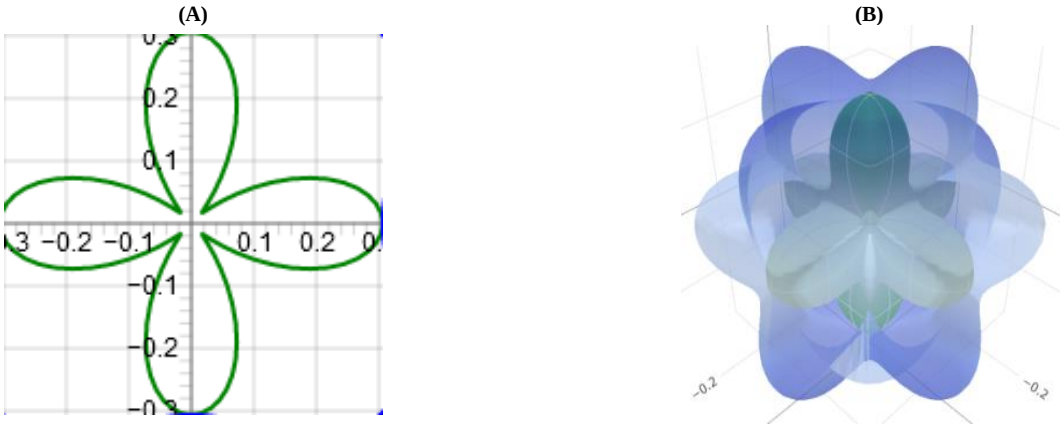

Fig. 4: The Spatial Dependency of Poisson's Ratio in GaP Compound: (A) in XY, XZ, YZ and Planes, (B) in 3 Dimensions (3D).

If the second-order elastic stiffness constants C_{ij} and the mass density ρ of the crystal areknown, it is possible to predict the acoustic sound velocities and the Debye temperature θ_D of materials [36, 37]. Many researchers have extensively employed ab initio methods to investigate the elastic constants C_{ij} and structural, electronic and piezoelectric properties of materials [38-54]. Bioud [54] has used the elastic constants C_{ij} to calculate the wave velocities andthe Debye temperature of CuX (X = Cl, Br) binary compounds Blackman's [55] proposed a formula which is usually used to predict the θ_D of a material from its elastic constants C_{ij}. In cubic systems, θ_D can also be expressed in terms of the elastic constants C_{ij} and the mass density ρ by the following expression [56-59]:

$$\theta_D^3 = \frac{3.15}{8\pi}\left(\frac{h}{k}\right)^3\left(\frac{n}{\rho^{3/2}V_a}\right)(C_{11} - C_{12})^{1/2}(C_{11} + C_{12} + 2C_{44})^{1/2}(C_{44})^{1/2} \quad (3)$$

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 ρ is the density.
Using the experimental elastic constants C_{ij} (C_{11} = 140.5 GPa, C_{12} = 62.03 GPa, and C_{44} = 70.33 GPa) and the lattice constant (a = 5.4508 Å) reported in the litterature [31], and using the formula of Eq. (3), the calculated value of $\theta_D$is estimated to be about: 482.4 K. The obtained value is in good agreement with the experimental one (493 K) quoted by Adachi [31], the deviation between these two values is estimated to be less than 2.2%.
The concept of the Debye frequency w_D, which is defined as the maximum vibrational frequency of a given mode in a crystal is of fundamental importance in the heat transport in a lattice [60]. For compounds with rocksalt, diamond and zincblende structures, the Debye frequency w_D retated to θ_D as follows: $w_D = 16.5374\times10^9\ \theta_D$ [60]. For GaP compound, the calculated value of w_D is about: 8 THz.
The acoustic impedance (Z) has been analyzed by the following equation $Z = (\rho G)^{1/2}$ [14], [61], [62], where G is the shear modulus and is the mass density. High values of the shear modulus G and the mass density ρ result in high acoustic impedance [14, 61]. Our obtained value of the acoustic impedance Z for GaP compound is estimated to be about: 15.16×10^6 Rayl. Unfortunately, to the best of our knowledge, there is no other data available in the literature on Z for GaP to compare with our results.

3. Conclusion

Using the experimental stiffness elastic constants C_{ij} reported in the litterature [31], we studied the spatial dependencies of the Young's modulus, linear compressibility, shear modulus, and Poisson's ratio in GaP semiconducting compound. The program used [18] detect the input structure's crystal symmetry and test the mechanical stability of the crystal. Data analysis shows that the maximum value E_{max} of Young's modulus was estimated at around 166.7 GPa (within (110) crystallographic plane and in [111] crystallographic direction) [31], while its minimum value E_{min} was estimated at around 102.5 GPa (for both within (100) crystallographic plane and in [001] direction, an within (110) crystallographic plane and in [001] crystallographic direction) [31], which gives $E_{max}/E_{min} \approx 1.63$, while for the Poisson's ratio υ, the maximum value υ_{max} of υ was estimated at around 0.43 [31], while its minimum value υ_{min} was estimated at around 0.025 [31], which gives $\upsilon_{max}/\upsilon_{min} \approx 17.5$. This result indicates that gallium phosphide (GaP) semiconducting material exhibits a large anisotropy on the Poisson's ratio υ. Furthermore, the Debye temperature and the acoustic impedance of GaP material are computed.

References

[1] S. Wafula, R. Musembi, and F. Nyongesa, "Analysis of K_4ZnAs_2 Zintl phased ternary semiconductor compound for optoelectronic application", Results in Materials, Vol. 20, (2023), pp. 100469. https://doi.org/10.1016/j.rinma.2023.100469.

[2] S. Daoud, N. Bioud, N. Lebga, and R. Mezouar, "Optoelectronic and thermal properties of boron- bismuth compound", International Journal of Physical Research, Vol. 2, No. 2, (2014), pp. 27-31. https://doi.org/10.14419/ijpr.v2i2.2760.

[3] Y. El Krimi and R. Masrour, " First-principles calculations of electronic, magnetic, mechanical and thermoelectric properties of tetragonal Mn_2PtSn-Ferromagnetic phase: Ab initio calculations", Modern Physics Letters B, Vol. xx, No xx, (2024), pp. 2450080 (22 pages). https://doi.org/10.1142/S0217984924500805.

[4] S. Daoud, R. Mezouar and A. Benmakhlouf, " Structural and piezoelectric coefficients of AlP under pressure ", International Journal of Physical Research, Vol. 6, No. 2, (2018), pp. 53-55. https://doi.org/10.14419/ijpr.v6i2.11020.

[5] Y. El Krimi and R. Masrour, " Study of structural, elastic, electronic, optical and magnetic properties of Heusler Mn_2NiAl: Ab initio calculations", Modern Physics Letters B, Vol. xx, No xx, (2024), pp. 2450081 (19 pp). https://doi.org/10.1142/S0217984924500817.

[6] M. Moin, A.W. Anwar, M.A. Ahmad et al, " First-principle calculations to investigate structural, electronic, mechanical, optical, and thermodynamic features of promising (La, In)-doped AlSb for optoelectronic applications ", Journal of Molecular Modeling, Vol. 29, No. 7, (2023), pp. 219 (18 pages). https://doi.org/10.1007/s00894-023-05622-4.

[7] S. Daoud, "Mechanical behavior of aluminum phosphide under high pressure", Acta Physica Polonica A, Vol. 133, No.1, (2018), pp. 23-27. https://doi.org/10.12693/APhysPolA.133.23.

[8] S. Daoud, P. K. Saini, and H. Rekab-Djabri, "Theoretical prediction of some physical properties of $B_xAl_{1-x}Sb$ ternary alloys", Journal of Nano- and Electronic Physics., Vol. 12, No. 6, (2020), pp. 06008 (5 pages). https://doi.org/10.2478/awutp-2022-0002.

[9] S. Daoud and N. Bioud,"Semi-empirical prediction of physical prop (B3) TlP compound", International Journal of Physical Research, Vol. 2, No. 2, (2014), pp. 72-77. https://doi.org/10.14419/ijpr.v2i2.3361.

[10] F. Okba and R. Mezouar, " Some physical parameters of calcium chalcogenides at high pressures: Semi-empirical approach", Journal of Nano- and Electronic Physics, Vol. 14, No 4, (2022) pp. 04004 (4 pages). https://doi.org/10.21272/jnep.14(4).04004.

[11] S. Daoud, "Linear correlation between Debye temperature and lattice thermal conductivity in II-VI and III-V semiconductors", International Journal of Scientific World, Vol. 3, No.2, (2015), pp. 216-220. https://doi.org/10.14419/ijsw.v3i2.4793.

[12] N. Bioud, "Debye temperature of CaO under high pressure up to 65.2 GPa ", International Journal of Advanced Chemistry, Vol. 11, No 1, (2023), pp. 6–9. https://doi.org/10.14419/ijac.v11i1.32228.

[13] S. Daoud, N. Bioud, and P. K. Saini, "Finite temperature thermophysical properties of MgCu intermetallic compound from quasi-harmonic Debye model", Journal of Magnesium and Alloys, Vol. 7, No. 2, (2019), pp. 335-344. https://doi.org/10.1016/j.jma.2019.01.006.

[14] N. Bioud, " Some physical properties of K_2TlAsX_6 (X = Cl, Br) and $CsPbBr_3$ semiconducting compounds", International Journal of Advanced Chemistry, Vol. 12, No 1, (2024), pp. 26–3**0.** https://www.sciencepubco.com/index.php/IJAC/article/view/32462.

[15] M. L. Cohen, "Calculation of bulk moduli of diamond and zinc-blende solids", Physical Review B, Vol. 32, No. 12, (1985), pp. 7988–7991. https://doi.org/10.1103/PhysRevB.32.7988.

[16] S. Daoud, "Empirical prediction of thermal properties, microhardness and sound velocity of cubic zinc-blende AlN", Semiconductor Physics, Quantum Electronics and Optoelectronics: Vol. 22, No. 4, (2019), pp. 404 – 409. https://doi.org/10.1007/s12043-020-01966-1.

[17] R. Masrour, A. Jabar, S. Labidi, Y. El Krimi, M. Ellouze, M. Labidi, and A. Amara, " Study of structural, elastic, thermal, electronic and magnetic properties of heusler Mn_2NiGe: An Ab initio calculations and Monte Carlo simulations ", Materials Today Communications, Vol. 26, No 3, (2021), pp.101772(10 pages). https://doi.org/10.1016/j.mtcomm.2020.101772.

[18] R. Gaillac, P. Pullumbi, and F-X. Coudert, "ELATE: an open-source online application for analysis and visualization of elastic tensors", Journal of Physics: Condensed Matter, Vol. 28, No 27, (2022), pp. 275201. https://doi.org/10.1088/0953-8984/28/27/275201.

[19] A. Benmakhlouf, A. Benmakhlouf, O. Allaoui, and S. Daoud, "Theoretical study of elastic and thermodynamic properties of CuSc intermetallic compound under high pressure", Chinese Journal of Physics, Vol. 57, (2019), pp. 179–188. https://doi.org/10.1016/j.cjph.2018.11.017.

[20] S. Daoud, N. Bioud, and N. Lebga, " Erratum to elastic and piezoelectric properties, sound velocity and Debye temperature of (B3) BBi compound under pressure", Pramana Journal of Physics, Vol. 86, No. 4, (2016), pp. 945 – 946. https://doi.org/10.1007/s12043-015-1099-0.

[21] I. F. Al Maaitah, "Mechanical, optical, and lattice vibrational properties of gallium antimonide (GaSb) semiconductor under the influence of temperature", Physica Scripta, Vol. 98, No.5, (2023), pp. 055904. https://doi.org/10.1088/1402-4896/acc76c.

[22] R. Mezouar, N. Bioud, H. Rekab-Djabri, N. Beloufa, and Z. Rouabah, " Theoretical prediction of mechanical properties of $B_xAl_{1-x}Sb$ ternary semiconducting alloys", Annals of West University of Timisoara Physics, Vol. 64, No. 1, (2022), pp. 22–36. https://doi.org/10.2478/awutp-2022-0002.

[23] N. Benkara-Mohammed, R. Md Nor, and N. Benouattas, "Electrons extraction from MWCNT/PEO composites ", Journal of Nano-and Electronic Physics, Vol. 10 No 4, (2018) 04006 (5pp). https://doi.org/10.21272/jnep.10(4).04006.

[24] N. Benkara Mohammed and S. Benkara Mahammed, " Space radiation environment of ALSAT-2 and its degradation effect on InGaP/InGaAs/Ge solar cells ", African Journal of Science, Technology, Innovation and Development, Vol. 7, No. 6, (2015), pp. 475–479. https://doi.org/10.1080/20421338.2015.1096673.

[25] J. B. Wachtman, W. E. Tefft, D. G. Lam, and C. S. Apstein, "Exponential temperature dependence of Young's modulus for several oxides", Physical Review, Vol. 122, No.6, (1961), pp. 1754–1759. https://doi.org/10.1103/PhysRev.122.1754.

[26] S. T. Weir, "High pressure phase transitions in the II-VI and H I-V compounds barium selenide, barium sulfide, barium oxide, gallium antimonide, gallium arsenide, and gallium phosphide", Doctor of Philosophy Dissertation, Cornell University, New York (1989).

[27] N. Bouarissa, H. Algarni, F. Mezrag, and M. Ajmal Khan,"Band structure and chemical bonding of GaP: pressure-induced effects", Phase Transitions, Vol. 93, No. 10–11, (2020), pp. 973–980. https://doi.org/10.1080/01411594.2020.1817452.

[28] S. Benalia, M. Merabet, D. Rached, Y. Al-Douri, B. Abidri, R. Khenata, and M. Labair, "Band gap behavior of scandium aluminum phosphide and scandium gallium phosphide ternary alloys and superlattices", Materials Science in Semiconductor Processing, Vol. 31, (2015)), pp. 493–500. https://doi.org/10.1016/j.mssp.2014.12.021.

[29] A. Benamrani, S. Daoud, and P. K. Saini, " Structural, elastic and thermodynamic properties of ScP compound: DFT study ", Journal of Nano- and Electronic Physics, Vol. 13, No 1, (2021), pp. 01008 (5pp). https://doi.org/10.21272/jnep.13(1).01008.

[30] H. Rekab-Djabri, Manal M. Abdus Salam, S. Daoud, M. Drief, Y. Guermit, and S. Louhibi-Fasla, " Ground state parameters, electronic properties and elastic constants of $CaMg_3$: DFT study ", Journal of Magnesium and Alloys, Vol. 8,No. 4, (2020), pp. 1166 - 1175. https://doi.org/10.1016/j.jma.2020.06.007.

[31] S. Adachi, "Properties of Group-IV, III-V and II-VI semiconductors", John Wiley & Sons, New York, (2005). https://doi.org/10.1002/0470090340.

[32] R. Dholpuria, A. Rani and R. Kumar, "DFT study of ScP and AlP in B1, B2 and B3 phases at ambient pressure", ECS Transactions, Vol. 107, No. 1, (2022), pp. 12693-12704. https://doi.org/10.1149/10701.12693ecst.

[33] S. Amari and S. Daoud, "Structural phase transition, elastic constants and thermodynamic properties of TmAs: An ab-initio study", Computational Condensed Matter, Vol. 33, (2022), pp. e00764 (8 pages). https://doi.org/10.1016/j.cocom.2022.e00764.

[34] S.A. Dar, V. Srivastava, S.N. Tripathi, and U. K. Sakalle, "A complete DFT description on structural, electronic, elastic, mechanical and thermodynamic properties of some intermetallic AuX_2 (X = Al, Ga, In) compounds", The European Physical Journal Plus, Vol. 133, (2018), pp. 541 . https://doi.org/10.1140/epjp/i2018-12397-x.

[35] S. Daoud, N. Bioud, L. Belagraa, and N. Lebga, "Elastic, optoelectronic and thermal properties of boron phosphide", Journal of Nano-and Electronic Physics: Vol. 5, No.4, (2013), pp. 04061 (6pp). https://doi.org/10.14419/ijpr.v7i1.23681.

[36] C. K. Singh, A. K. Pandey and B. K. Pandey, "Theoretical prediction of Debye temperature & elastic constants of geophysical mineral", AIP Conference Proceedings, Vol. 1728, No.1, (2016), pp. 020047. https://doi.org/10.1063/1.4946097.

[37] S. Daoud, " Empirical study of elastic properties of BX (X = As, Sb) materials", International Journal of Scientific World, Vol.3, No.1, (2015), pp. 37- 42. https://doi.org/10.14419/ijsw.v3i1.4022.

[38] S. Amari, H. Rekab-Djabri, and S. Daoud, "Mechanical, thermal, electronic, and magnetic properties of $Ca_{0.75}Er_{0.25}S$ alloy from a DFT approach: a promising material for spintronic applications", Materials Today Communications, Vol. 33, (2022), pp. 104237 (9 pages). https://doi.org/10.1016/j.mtcomm.2022.104237.

[39] S. Daoud, N. Bioud, and N. Lebgaa, "Elastic and piezoelectric properties, sound velocity and Debye temperature of (B3) boron–bismuth compound under pressure", Pramana Journal of Physics, Vol. 81, No. 5, (2013), pp. 885–892. https://doi.org/10.1007/s12043-013-0596-2.

[40] L. Shi, Y. Duan and L. Qin, "Structural phase transition, electronic and elastic properties in TlX (X = N, P, as) compounds: Pressure-inducedeffects", Computational Materials Science, Vol.50, (2010), pp. 203-210. https://doi.org/10.1016/j.commatsci.2010.07.027.

[41] Y. O. Ciftci, K. Colakoglu, and E. Deligoz, "A First Principles Studies on TlX (X=P, As)", Central European Journal of Physics, Vol. 6, No. 4,(2008), pp. 802-807. https://doi.org/10.2478/s11534-008-0109-y.

[42] S. Daoud, "Mechanical and piezoelectric properties, sound velocity and Debye temperature of thallium-phosphide under pressure", International Journal of Advanced Research in Physical Science, Vol. 1, No. 6, (2014), pp. 1-11. www.arcjournals.org/pdfs/ijarps/v1i6/1.pdf.

[43] E. Viswanathan, M. Sundareswari, S. Krishnaveni, M. Manjula and D. S. Jayalakshmi, "Theoretical investigation on effect of boron on improving the hardness of zincblende-aluminium nitride and its mechanical, thermal and thermoelectric properties", Journal of Superhard Materials, Vol. 41, No. 5, (2019), pp. 321–333. https://doi.org/10.3103/S1063457619050046.

[44] L. Boutahar, A. Benamrani, Z. Er, N. Bioud and Z. Rouabah, "Elastic constants of tetragonal Cu_2ZnSnS_4 semiconductor: Ab-initio calculation ", Annals of West University of Timisoara-Physics, Vol. 64, No. 1, (2022), pp. 55-67. https://doi.org/10.2478/awutp-2022-0004.

[45] S. T. Tonga and J. Y. Baro, "Structural and electronic properties of gallium phosphate semiconductor in wurtzite, rock salt and zinc blende", International Journal of Engineering and Applied Physics (IJEAP), Vol. 2, No. 3, (2022), pp. 555-565. https://ijeap.org/ijeap/article/view/88/94.

[46] S. Daoud, "Structural and piezoelectric properties of BSb under high pressure: A DFT study", Journal of Nano- and Electronic Physics, Vol. 11, No. 5, (2019), pp. 05004 (4pp). https://doi.org/10.21272/jnep.11(5).05004.

[47] R. Boulechfar, A. Trad Khodja, Y. Khenioui et al., " First-principal study of the structural, mechanical, electronic and thermodynamic properties of intermetallic compounds: Pd_3M (M=Sc, Y) ", International Journal of Modern Physics B, Vol. 33, No 27, (2019), pp.1950321(14 pages). https://doi.org/10.1142/S0217979219503211.

[48] N. Lebga, S. Daoud, X-W. Sun, N. Bioud, and A. Latreche, "Mechanical and thermophysical properties of cubic rock-salt AlN under high pressure", Journal of Electronic Materials, Vol. 47, No. 7, (2018), pp. 3430-3439. https://doi.org/10.1007/s11664-018-6169-x.

[49] S. Amari and B. Bouhafs, "Ab initio full-potential study of mechanical properties and magnetic phase stability of californium monopnictides (CfN and CfP) ", Journal of Nuclear Materials, Vol. 478, No. 9, (2016), pp. 149–157.https://doi.org/10.1016/j.jnucmat.2016.06.012.

[50] Y. El Krimi, R. Masrour and A. Jabar, "A comparative study of structural electronic and magnetic properties of full-Heusler's Co_2MnZ (Z=Al, Ge and Sn) ", Journal of Molecular Structure, Vol. 1220, (2020), pp. 128707–128717. https://doi.org/10.1016/j.molstruc.2020.128707.

[51] Y. El Krimi et al., "Structural, electronic, magnetic and thermoelectric properties of Full-Heusler Fe_2MnSi: ab initio calculations", Results in Physics, Vol. 18, (2020), pp. 103252–103260. https://doi.org/10.1016/j.rinp.2020.103252.

[52] Y. El Krimi, R. Masrour and A. Jabar, "Structural, electronic and magnetic properties of full- Heusler alloy Co_2CrAl", Inorganic Chemistry Communications, Vol. 121, (2020), pp. 108207. https://doi.org/10.1016/j.inoche.2020.108207.

[53] Ibtisam F. Al Maaitah and Elkenany B. Elkenany, "Sound velocity, electronic, optical, and mechanical properties for nano semiconductor materials (CdTe, ZnTe) under the influence of pressure", ECS Journal of Solid-State Science and Technology, Vol. 11, No. 2, (2022), pp. 023013. https://doi.org/10.1149/2162-8777/ac5578.

[54] N. Bioud, "Comment on structural, electronic, elastic, optical and thermodynamic properties of copper halides CuCl, CuBr and their ternary alloys $CuCl_{1-x}Br_x$ ($0.0 \leq x \leq 1.0$) using full-potential linear muffin-tin orbital (FP-LMTO) method",Optik, Vol. 127, (2016), pp. 11395-11397. https://doi.org/10.1016/j.ijleo.2016.08.020.

[55] M. Blackman, " On the calculation of characteristic temperatures from the elastic constants", The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, Vol. 42, No. 335, (1942), pp. 1441-1442. https://doi.org/10.1080/14786445108560963.

[56] S. Daoud, " Sound velocities and thermal properties of BX (X = As, Sb) compounds", International Journal of Scientific World, Vol. 3, No. 1, (2015), pp. 43-48. https://doi.org/10.14419/ijsw.v3i1.4039.

[57] S. Daoud, "Mechanical properties of BBi compound under pressure", International Journal of Scientific World, Vol. 3, No.1, (2015), pp. 69-75.https://doi.org/10.14419/ijsw.v3i1.4218.

[58] S. Daoud," Sound velocities and thermal properties of BeX (X=S, Se and Te) alkaline-earth chalcogenides ", International Journal of Scientific World, Vol. 5, No. 1 (2017), pp. 9-12. https://doi.org/10.14419/ijsw.v5i1.6929.

[59] N. Bioud, "Etude des propriétés structurales, élastiques et thermodynamiques des halogénures à base de cuivre", Thèse de doctorat, Université de Sétif 1, (2018). http://dspace.univ-setif.dz:8888/jspui/handle/123456789/1378.

[60] S. Daoud, N. Bioud, N. Lebga,"Mechanical, piezoelectric and some thermal properties of (B3) BP under pressure", Journal of Central South University of Technology, Vol. 21, No. 1, (2014), pp. 58–64. https://doi.org/10.1007/s11771-014-1915-6.

[61] S. Islam, M.R. Rana, K. Hoque, G.G. Biswas, M.E. Hossain, M.M. Hossain, M.M. Uddin, S.H. Naqib and M.A. Ali, " A comprehensive exploration of the physical properties of M_2GaB (M = Ti, Zr, Mo, Hf) through DFT method ", Results in Materials, Vol. 19, (2023), pp. 100438 (14 pages). https://doi.org/10.1016/j.rinma.2023.100438.

[62] N. Benkara-Mohammed, N. Bioud, and N. Benchiheub," Hydrostatic pressure response of semiconducting GaSb applyinga semi-empirical approach ", Computational Condensed Matter, Vol. 39, No.2, (2024), pp.e00895. https://doi.org/10.1016/j.cocom.2024.e00895.