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Research paper

Quasi-linear correlation between shear and young's moduli in some polycrystalline ceramics

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Abstract

This work aims to investigate the correlation between the shear modulus and the Young's modulus of some pore-free polycrystalline ceram-ics. Our study shows that the shear modulus correlates quasi-linearly with the Young's modulus. The best fit was obtained using the linear model. The fit of the shear modulus G as a function of the Young modulus E obeys this linear expression: G = 0.43E - 7.7 (where both G and E are expressed in GPa). The coefficient of the correlation was found at around 0.994. Our expression was used to predict the shear modulus G of some other polycrystalline ceramics, especially: Dy_2O_3, Er_2O_3, and Y_2O_3 materials, which are estimated at around 65.6, 72.4, and 51.8 GPa, respectively. We attempt also to estimate the Vickers hardness of our materials of interest using an empirical expression of the literature. Unfortunately our predicted results are larger than those reported previously in the literature.

Keywords: *Polycrystalline Ceramics; Young's Modulus; Shear Modulus; Quasi-Linear Correlation.*

1. Introduction

Elastic deformation under external stress is one of the most important considerations in structural applications of solids [1]. Indeed, elastic properties of materials are commonly required in computer aided design and manufacturing techniques to simulate a product's behavior under variable conditions of external stress and temperature [1].
Using different theoretical approaches, semi-empirical and empirical models, many works [2-28] investigated and analyzed the relations between different parameters for several materials with different crystallographic structures.
Until now, reported literature showed very little attention has been paid to the investigation of the correlation between the different elastic moduli of polycrystalline ceramics and the relation between the different elastic moduli is still to be discussed in comparison with these reported for the porosity.
Using a reactive sintering method, Zhang et al. [18] synthesized porous chromium carbide (Cr_3C_2) ceramics, which exhibit a uniform and accessible porous structure comprised of three-dimensional connected struts. Young's modulus of the ceramics synthesized was measured by dynamic mechanical analysis (DMA). They also developed a semi-empirical model basing on the generalized mixture rule (GMR), to describe the porosity dependence of Young's modulus for this ceramic.
Wachtman et al. [19] reported the essential data on the ceramic materials in their book 'Mechanical properties of ceramics', which is constituted from 25 chapters. They explained in detail the mechanical behaviors of ceramic materials under stress and high temperatures.
Shein et al. [20] have investigated the elastic constants $C_{ij}$and several other related properties of cubic binary phases of thorium based nonmetals, i.eThX (X = C, N, O, P, As, Sb, S, Se) using first-principles calculation with the full-potential linearized augmented plane wave (FLAPW) approach and the generalized gradient approximation (GGA) for the exchange-correlation potential. They found that the aggregate bulk modulus B of the polycrystalline ceramics decreases with increasing inter-atomic distances in the following sequences: ThN → ThP → ThAs and ThO → ThS → ThSe, respectively.
Using first principles calculations based on density functional theory (DFT), Qi et al. [25] have investigated the crystal structure, electronic and elastic properties, and mechanical anisotropy of XB_2 (X = V, Nb, Ta, Cr, Mo, and W) binary compounds. They found that the bonding behaviors of XB_2 (X = V, Nb, Ta, Cr, Mo, and W) are the combination of covalent and metallic bonds.
Using Niobium-doped lead zirconate-titanate (PNZT), Biswas and Fulrath [29] investigated the effect of porosity on the mechanical properties of a polycrystalline ceramic. They found that the Young's modulus showed a linear relationship with increase in porosity.
In the present work, we investigate the correlation between the bulk modulus, the shear modulus G for some pore-free polycrystalline ceramic materials based on some data reported by Wachtman et al. [19].

2. Theory and discussion of the results

Young's modulus E is a key mechanical property of isotropic brittle materials such as polycrystalline ceramics [18]. Values for Young's modulus E and shear modulus G for some pore-free polycrystalline ceramics are given in Table 1 [19], which are in some cases averages of measurements from several authors. The values of the Young's modulus E and shear modulus G of pore-free polycrystalline ceramics summarized in Table 1 are plotted in Figure 1.

Table 1: Values of Young'sand Shear Moduli of Pore-Free Polycrystalline Ceramics [19]

Material	Al_2O_3	MgO	ThO_2	TiO_2	ZnO
E (GPa)	402.8	310.9	261.0	284.2	123.5
G (GPa)	163.0	133.4	100.6	111.5	45.6

The values of the Young's modulus E and the shear modulus Gare also plotted in Figure 1.From Figure 1, we can observe clearly that the shear modulus Gincreases quasi-linearly with increase of the Young's modulus E. The data plotted in Figure 1 were fitted using the linear model, the obtained linear expression is given as follows: G = 0.43 E - 7.7, where both G and E are expressed in GPa. The linear coefficient of the correlation was found at around 0.994, while the average error on the estimation of the shear modulus G is only around 2.83%. Using the previous model, the errors on the estimation of the shear modulus G are around 1.54 % for Al_2O_3, 5.56 % for MgO, 3.91 % for ThO_2, 2.70 % for TiO_2 and 0.43 % for ZnO, respectively. So, the maximum error (5.56 %) was found for MgO, while the minimum error (0.43 %) was reported for ZnO material. It is very important to that a quasi-linear correlation between Young's and shear moduli was also obtained for several intermetallic compounds: X_3Ir (X = Ti, V, Cr, Nb and Mo) [5].

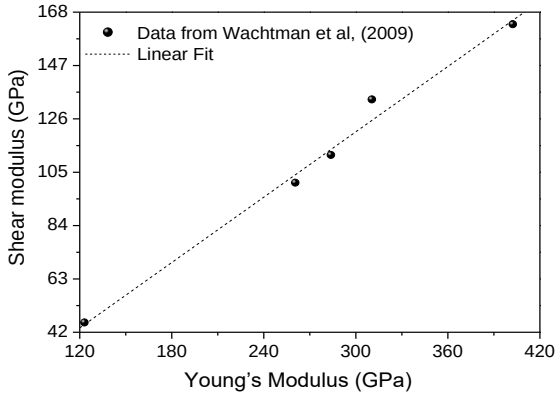

Fig. 1: Quasi-Linear Correlation between Young's and Shear Moduli in Pore-Free Polycrystalline Ceramics.

In the following section, we use our proposed model to predict the shear modulus G of some other polycrystalline ceramics based on their Young's modulus E values reported in the literature [19], [30], [31]. Using the C_{ij} single crystal of Ref [31] and Voigt–Reuss–Hill approximation [32], the obtained values of the shear modulus G for different polycrystalline ceramics are summarized in Table 2.

Table 2: Predicted Values of Shear Modulus for Some Ceramics, *Using C_{ij} Single Crystal of Ref [31] and Voigt–Reuss–Hill Approach [32].

Material	Dy_2O_3	Er_2O_3	Y_2O_3	ZrO_2	BeO	CaO
E (GPa)	170.5 [19]	186.3 [19]	138.3 [19]	230 [19]	379.2 [30]	197.7 [31]*
G (GPa)	65.6	72.4	51.8	91.2	155.4	77.3

There are different relationships frequently employed to predict the hardness H and the fracture toughness K_{IC} of the materials [33-37]. We calculate the Vickers hardness H_V of pore-free polycrystalline ceramics according to the following empirical expression: $H_V = 0.92(G/B)^{1.137}G^{0.708}$ [32], [38], whereG is the shear modulus and B is the bulk modulus. Frequently, the elastic moduli of the polycrystalline materials are calculated [39-48]. Iuga et al. [45] have investigated the elastic constants C_{ij} of ceramic crystals using an Ab-initio calculation. For aggregate polycrystalline materials, the bulk modulus B is expressed as a function of the Young's modulus E and the shear modulus G as follows: B = (1/3)EG/(3G-E) [19]. The obtained values of the bulk modulus B for different ceramics are summarized in Table 3, along the experimental one (210 GPa) for BeO material [49].

Table 3: Predicted Values of Bulk Modulus B for Some Polycrystalline Ceramics, [a]from Ref [1], [b]from Ref [45], [c]from Ref [49].

Material	Dy_2O_3	Er_2O_3	Y_2O_3	ZrO_2	BeO	CaO
B (GPa)	141.55, 144[a]	145.39,160[a]	140.33, 166[b]	160.37, 170 [a]	226.06, 210 [c]	148.95, 112.3[b]

The Poisson's ratioυis expressed as a function of E and G as follows: υ = (E/2G) -1[19]. The obtained values of thePoisson's ratioυ and $H_V$for different ceramics are reported in Table 4. In the case of MgO and Y_2O_3, we present a comparison of our calculations values with theoretical data of Iuga [45] on Poisson's ratioυ (Table 4). Furthermore, it is very clear that our obtained value (22.8 GPa) of the Vickers hardness for Al_2O_3 ceramic is very higher than the experimental one (13 GPa) reported by Wachtman et al [19].

Table 4: Predicted Values of Poisson's RatioY and Vickers Hardness H_V for Pore-Free Polycrystalline Ceramics, *from Ref [45].

Material	Al_2O_3	MgO	ThO_2	TiO_2	ZnO	Dy_2O_3	Er_2O_3	Y_2O_3	ZrO_2	BeO	CaO
υ	0.22	0.23, 0.18*	0.25	0.24	0.36	0.30	0.29	0.34, 0.31*	0.26	0.22	0.28
H_V(GPa)	22.8	17.2	14.0	15.5	3.6	7.4	8.6	4.8	11.8	21.4	8.8

Our value (11.8 GPa) of H_V for ZrO_2 material is also higher than the experimental one (9 GPa) reported by Wachtman et al [19]. Our obtained value (21.4 GPa) of H_V for BeO material is also very higher than the predicted one (9.95 GPa) reported by Yang et al [50]. The calculated values of the Poisson's ratioυ and Vickers hardness H_V forceramics are also plotted in Figure 2. We could see clearly that the

H_V decreases exponentially with increasing Poisson's ratio υ. Bioud and Benchiheub [51] studied the pressure effect on some physical properties of calcium oxide material, and found a correlation between the bulk modulus B and the microhardness H. Zhang et al. [18] have mensioned that the Young's modulus is correlated with most mechanical properties including tensile strength, hardness, bending strength, and fracture toughness, while Mezouar and Logzit [52] have studiedthe microhardness of $B_xAl_{1-x}Sb$ alloys using semi-empirical approach. It is well know that the Diamond is the hardest material on earth having H_V in the range of 70 –150 GPa [53]. The values of H_V for ceramics are very smaller than that of the diamond, and higher than that (3.57 GPa) of GaSb [54].

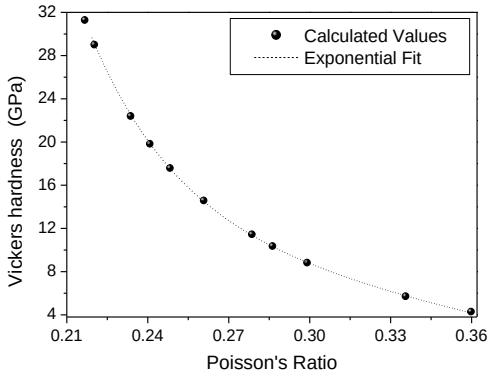

Fig. 2: Exponential Correlation between Poisson's Ratio υ and Vickers Hardness H_V in Pore-Free Polycrystalline Ceramics.

3. Conclusion

Based on some data reported previously in the literature, we have investigated the correlation between the shear modulus G andthe Young's modulus E for some pore-free polycrystalline ceramics. Our investigation shows that the shear modulus correlates quasi-linearly with the Young's modulus. The best fit between G andE was obtained using the linear model as follows: G = 0.43E - 7.7 (where both G and E are expressed in GPa). The coefficient of the correlation was found at around 0.994, while the average error is only around 2.83%. Our expression was used to predict the shear modulus of some other isotropic polycrystalline ceramic materials. The shear modulus of Dy_2O_3, Er_2O_3, Y_2O_3 and CaO ceramics are estimated at around 65.6, 72.4, 51.8 and 77.3 GPa, respectively. We calculated also the Vickers hardness (H_V) of some polycrystalline ceramics; our obtained values are very larger than other experimental data of the literature. The calculated Vickers hardness H_V of polycrystalline ceramics decreases exponentially with increasing Poisson's ratio υ.

References

[1] R. G. Munro, "Analytical representations of elastic moduli data with simultaneous dependence on temperature and porosity", Journal of Research of the National Institute of Standards and Technology, Vol. 109, No. 5, (2004), pp. 497-503. https://doi.org/10.6028/jres.109.036.

[2] S. Daoud, "Correlation study of optical, mechanical and thermal properties of BAs material and its experimental energy gap", International Journal of Physical Research, Vol.5, No.2, (2017), pp. 79-82. https://doi.org/10.14419/ijpr.v5i2.8314.

[3] N. Bioud and R. Mezouar, "Crystal density of CaS under pressure up to 40 GPa", International Journal of Advanced Chemistry, Vol. 10, No 1, (2022), pp. 29-31. https://www.sciencepubco.com/index.php/IJAC/article/view/32063. https://doi.org/10.14419/ijac.v10i1.32063.

[4] S. Daoud, P. K. Saini, and H. Rekab-Djabri, "Elastic constants and optical phonon frequencies of BX (X= P, As, and Sb) semiconductors: Semi-empirical prediction", International Journal of Physical Research, Vol. 8, No.2, (2020), pp. 45-49. https://doi.org/10.14419/ijpr.v8i2.31001.

[5] D. Chen, J. Geng, Y. Wu, M. Wang and C. Xia, " Insight into physical and thermodynamic properties of X_3Ir (X = Ti, V, Cr, Nb and Mo) compounds influenced by refractory elements: A first-principles calculation", Crystals, Vol. 9, No. 2, (2019), pp. 104 (15 pages). https://doi.org/10.3390/cryst9020104.

[6] S. Daoud, 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.

[7] S. Daoud, A. Bencheikh and L. Belagraa, "Quasi-linear correlation between high-frequency and static dielectric constants in II-VI and III-V semiconductors ", International Journal of Physical Research, Vol. 5, No.1, (2017), pp. 4-6. https://doi.org/10.14419/ijpr.v5i1.6961.

[8] F. Bounab, N. Bouarissa, A. Merrouche, A. Benmakhlouf, S. Daoud, and N. Chelali, "Theoretical investigation of elastic constants and related properties of compressed PbO_2",Journal of Computational Electronics, Vol. 18, No. 4, (2019), pp. 1111-1118. https://doi.org/10.1007/s10825-019-01372-w.

[9] 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.

[10] S. Daoud and A. Latreche, "Optical properties and electronic polarizability of boron-antimonide semiconductor ", International Journal of Physical Research: Vol. 5, No.2, (2017), pp. 43-45. https://doi.org/10.14419/ijpr.v5i2.7910.

[11] M. Kazan, E. Moussaed, R. Nader, and P.Masri, "Elastic constants of aluminum nitride", Physica Status Solidi C, Vol.4, (2007), pp. 204-207. https://doi.org/10.1002/pssc.200673503.

[12] S. Daoud, A. Latreche, and P. K. Saini, "Theoretical investigation of acoustic wave velocity of aluminum phosphide under pressure", International Journal of Physical Research, Vol. 7, No. 1, (2019), pp. 3-6. https://doi.org/10.14419/ijpr.v7i1.23681.

[13] S. Daoud, "Sound velocities and Debye temperature of BeSe under high pressure up to 50 GPa", International Journal of Physical Research, Vol. 5, No. 1, (2017), pp. 7-10. https://doi.org/10.14419/ijpr.v5i1.7013.

[14] A. Das Majumdar, P. Padmakumar, Munjal N. Rajni, and U. Kamboj, "First principle study on structural properties of boron compounds". In: C. Prakash, S. Singh, and G. Krolczyk, (eds) "Advances in functional and smart materials", Lecture Notes in Mechanical Engineering, Springer, Singapore (2023). https://doi.org/10.1007/978-981-19-4147-4_19.

[15] S. Kadri, M. Tourab, M. Berkani, R. Amraoui, Z. Bordjiba, "Study of structural, elastic, thermal and transport properties of ternary X (X = Co, Rh and Ir) MnAs obtained by DFT", East European Journal of Physics, Vol. 1, (2022), pp. 47-57. https://doi.org/10.26565/2312-4334-2022-1-07.

[16] 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.

[17] S. Daoud, "Simplified expressions for calculating Debye temperature and melting point of II-VI and III-V semiconductors", International Journal of Scientific World, Vol. 3, No.2, (2015), pp. 275-279. https://doi.org/10.14419/ijsw.v3i2.5314.

[18] L. Zhang, K. Gao, A. Elias, Z. Dong, W. Chen, " Porosity dependence of elastic modulus of porous Cr_3C_2 ceramics ", Ceramics International, Vol. 40, No. 1, (2013), pp. 191-198. https://doi.org/10.1016/j.ceramint.2013.05.122.

[19] J. B. Wachtman, W. R. Cannon, and M. J. Matthewson, "Mechanical properties of ceramics ", John Wiley & Sons Ltd, (2009). ISBN: 978-0-471-73581-6. https://doi.org/10.1002/9780470451519.

[20] I. R. Shein, K. I. Shein, and A. L. Ivanovskii, "Elastic properties of thorium ceramics ThX (X = C, N, O, P, As, Sb, S, Se)", Technical Physics Letters, Vol. 33, No. 2, (2007), pp. 128-131. https://doi.org/10.1134/S1063785007020113.

[21] J. Y. Baro and S. T. Tonga, "First principal calculations to predict the preferred crystal and structural parameter of indium phosphate", International Journal of Engineering and Applied Physics (IJEAP), Vol. 2, No. 3, (2022), pp. 502-514. https://ijeap.org/ijeap/article/view/89

[22] S. Daoud, "EOS parameters and elastic properties of cubic rock-salt BP", International Journal of Physical Research: Vol. 7, No. 1, (2019), pp. 7-10. https://doi.org/10.14419/ijpr.v7i1.25863.

[23] 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/10.14419/ijpr.v7i1.25863.

[24] 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/10.21272/jnep.13(1).01008.

[25] C-J. Qi, Y-H. Jiang, Y-Z. Liu, and R. Zhou, " Elastic and electronic properties of XB_2 (X = V, Nb, Ta, Cr, Mo, and W) with AlB_2 structure from first principles calculations ", Ceramics International, Vol. 40, (2014), pp. 5843– 5851. https://doi.org/10.1016/j.ceramint.2013.11.026.

[26] M. Anani, C. Mathieu, S. Lebid, Y. Amar, Z. Chama and H. Abid, "Model for calculating the refractive index of a III-V semiconductor", Computational Materials Science, Vol.41, No. 4, (2008), pp. 570-575. https://doi.org/10.1016/j.commatsci.2007.05.023.

[27] 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.

[28] S. Daoud, R. Mezouar, and A. Benmakhlouf, " Equation of state and some other properties of rock-salt AlN ", International Journal of Physical Research, Vol. 6, No. 1, (2018), pp. 49-52. https://doi.org/10.14419/ijpr.v6i1.10754.

[29] D. R. Biswas and R. M. Fulrath,"Mechanical properties of porous PNZT polycrystalline ceramics ", Lawrence Berkeley Laboratory, 1, 1977; Berkeley, California. https://digital.library.unt.edu/ark:/67531/metadc1063724/

[30] Substrates, 2nd, Edition, Chapter 2, doi:10.1016/b978-081551423-7.5000. In Hybrid Microcircuit Technology Handbook, edited by J. J. Licari and L. R. Enlow, William Andrew Inc., (1998). ISBN 978-0-8155-1423-7

[31] A. L. Dragoo, and I. L. Spain, "The elastic moduli and their pressure and temperature derivatives for calcium oxide", Journal of Physics and Chemistry of Solids, Vol. 38, No. 7, (1977), pp. 705–710. https://doi.org/10.1016/0022-3697(77)90061-0.

[32] 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.

[33] 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/10.21272/jnep.12(6).06008.

[34] 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, (2022), pp. 22-36. https://doi.org/10.2478/awutp-2022-0002.

[35] V. Kumar, A.K. Shrivastava, and V. Jha, "Bulk modulus and microhardness of tetrahedral semiconductors", Journal of Physics and Chemistry of Solids, Vol.71, No.11, (2010), pp. 1315 – 1320. https://doi.org/10.1016/j.jpcs.2010.07.012.

[36] M. A. Berding, A.Sher, M. Van Schilfgaarde, and An-Ban Chen, "Fracture and hardness characteristics ofsemiconductor alloys", Final Report, SRI International, November 1988. http://www.dtic.mil/dtic/tr/fulltext/u2/a204807.pdf.

[37] H. Niu, S. Niu, and A. R. Oganov, " Simple and accurate model of fracture toughness of solids", Journal of Applied Physics, Vol. 125, No. 6, (2019), pp. 065105(6 pages). https://doi.org/10.1063/1.5066311.

[38] S. Daoud, N. Bouarissa, A. Benmakhlouf and O. Allaoui, "High-pressure effect on elastic constants and their related properties of MgCa intermetallic compound", Physica Status Solidi B, Vol. 257, No. 6, (2020), pp. 1900537 (10 pages). https://doi.org/10.1002/pssb.201900537.

[39] 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.

[40] 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.

[41] 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.

[42] P. Ravindran, L. Fast, P.A. Korzhavyi, B. Johansson, J. Wills and O. Eriksson, "Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to $TiSi_2$", Journal of Applied Physics, Vol. 84, No. 9, (1998), pp. 4891–4904. https://doi.org/10.1063/1.368733.

[43] 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. 26–30. https://www.sciencepubco.com/index.php/IJAC/article/view/32462

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

[45] M. Iuga, G. Steinle-Neumann, and J. Meinhardt, "Ab-initio simulation of elastic constants for some ceramic materials", The European Physical Journal B, Vol. 58, (2007), pp. 127–133. https://doi.org/10.1140/epjb/e2007-00209-1.

[46] 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.

[47] Y. Bourourou, S. Amari, I.E. Yahiaoui and B. Bouhafs, "First principles predictions of electronic and elastic properties of $BaPb_2As_2$ in the $ThCr_2Si_2$ -type structure", Physica C: Superconductivity and its applications, Vol. 544, (2018), pp. 18–21. https://doi.org/10.1016/j.physc.2017.10.013.

[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] R. M. Hazen and L. W. Finger, "High pressure and high temperature crystal chemistry of beryllium oxide", Journal of Applied Physics, Vol. 59, No. 11, (1986), pp. 3728–3733. https://doi.org/10.1063/1.336756.

[50] W. Yang, R. G. Parr and L. Uytterhoeven, "New relation between hardness and compressibility of minerals", Physics and Chemistry of Minerals, Vol. 15, (1987), pp. 191-195. https://doi.org/10.1007/BF00308783.

[51] N. Bioud and N. Benchiheub, "Pressure effect on some physical properties of calcium oxide material ", Chemical Physics Impact, Vol. 7, (2023), pp. 100342 (5 pages). https://doi.org/10.1016/j.chphi.2023.100342.

[52] R. Mezouar and N.Logzit," Plasmon energy and microhardness of $B_xAl_{1-x}Sb$ alloys: semi-empirical prediction", International Journal of Physical Research, Vol. 11, No 1, (2023), pp. 1-4. https://doi.org/10.14419/ijpr.v11i1.32245.

[53] R. Khatun, M. A. Rahman, M. Z. Hasan and K. M. Hossain, "Effects of pressure on the structural, mechanical, anisotropic, and electronic properties of $MgTi_2O_4$ via density functional theory", The European Physical Journal B, Vol. 94, (2021), pp. 113 (9 pages). https://doi.org/10.1140/epjb/s10051-021-00119-6.

[54] F. Bengasmia, A. Benamrani, L. Boutahar, H. Rekab-Djabri, and S. Daoud, " Hydrostatic pressure effect on the structural parameters of GaSb semiconducting material: Ab-initio calculations", Journal of Physical & Chemical Research, Vol. 1, No. 2, (2022), pp. 25 – 30. https://doi.org/10.21272/jnep.12(6).06008.