SSRG International Journal of Applied Physics
ISSN: 2350 – 0301 /doi:10.14445/23500301/ IJAP-V8I1P106

Volume 8 Issue 1, 36-43, Jan-April 2021

Calculate And Study The Structural, Electronic, And Mechanical Properties of Cubic Zirconia By Using First-Principles Calculations

Hasan Abdullah H. Ali[1], Abdullah Hamoud Mohammad[2]

[1]*College of Education for pure Sciences – University of Kirkuk*
[2]*College of Education for pure Sciences – University of Kirkuk*

Received Date: 20 February 2021
Revised Date: 25 March 2021
Accepted Date: 06 April 2021

Abstract

In this study, we construct the crystal structure of cubic zirconia (c-ZrO2), then structural, electronic, and mechanical properties of cubic zirconia (c-ZrO2) were investigated using first-principles calculations by the Materials Studio software. Simulation of the X-ray diffraction of (c-ZrO2) showing the characteristic peaks that contain Miller indices [(111), (200), (220), (311), (222), (400), (331), (420)], and provided us with sufficient information to determine the inter distance between the crystal planes (d_{hkl}). We were also able to calculate the density per unit cell, which was (6.094 g/cm^3), unit cell size (134.297 Å^3), and bond length (2.2174 Å). The lattice constants were also studied using the materials studio 2017 software by approximating (LDA) (a= b= c= 5.025 Å), ($\alpha = \gamma = \beta = 90^\circ$). We obtained the bandgap of (c-ZrO2) by Castep code using (LDA) the value is (3.345 eV), and we found the width upper valence band (WUVB) as electronic properties. Mechanical properties, including elasticity properties, as the elastic stiffness constants (C_{ij}), elastic compliance constants (S_{ij}), and elastic moduli. And the Debye temperature (645.34 k), average sound velocity (4765.11 m/s), and compressibility (0.0043 1/Gpa).

Keywords: *cubic zirconia, materials studio, first-principles calculations, elastic moduli, structural properties, electronic properties*

I. INTRODUCTION

Zirconia (ZrO2) is an important modern ceramic material, one of the good materials where structure, phase transformations are related to mechanical properties [1] [2]. Because of their prominent physical and chemical properties, ZrO2 ceramic materials have been wide range used in modern engineering and industrial fields, including uses in ceramic engineering as an oxygen sensor in fuel cells, and it is used in refractory, cutting tools, and dental applications, also a technologically important catalytic support medium [3][4]. Zro2 is a Technologically important material because of its high strength and stability at high temperatures and its excellent dielectric properties [5]. As a typical advanced structural ceramic. However, zirconia ceramics is a material that is difficult to manufacture automatically because of its high hardness, strength, and low fracture toughness, high flexural, resistance to bending and scratches [6]. The search for energy storage material is still a global challenge for the progress of solutions to current industrial demands. In recent years, zirconia has arisen as a fascinating functional material because of its high strength, good thermal stability [4]. Zirconia exists under five different forms, which have been fully characterized crystallographically. The monoclinic phase (baddeleyite, space group P/c, below 1500 K), tetragonal phase, space group P/nmc (between 1500 and 2650 K), and cubic phase, space group Fmm, (above 2650 K) polymorphs are stable at room pressure, whereas the two orthorhombic, space group *Pbca* and space group *Pnma* polymorphs (respectively, to brookite TiO2 and cotunnite PbCl2) are stable between (3–5 GPa) and (12.5–20 GPa) and above (12.5–20 GPa), respectively [7], figure 1 [8]. The melting point of natural zirconia, like baddeleyite, is high, which is 2988 K, and its boiling point is 4573 K, which makes the hardness of zro2 very high [9]. In the present study, the structural, electronic, and mechanical properties of zro2 at room pressure have been investigated through first-principles methods for the cubic ZrO2 phase. For these calculations, we have used density functional theory (DFT) in the local density approximation (LDA) [7].

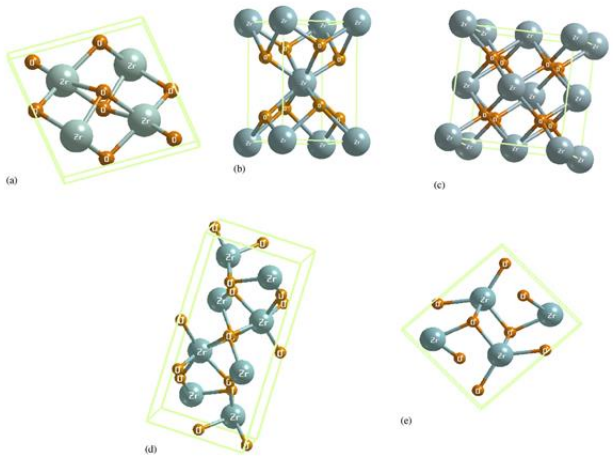

Figure 1. Represents the five phases of zirconia, where the zirconium atoms are dark gray, and the oxygen atoms are bronze, a/ monoclinic, b/ tetragonal, c/ cubic, d/ orthorhombic-Pbca (brookite), e/ orthorhombic- Pnma (cotunnite) [8].

II. Theoretical Computation methods

All the calculations in this paper are done in the ground State energy of cubic zirconia (c-ZrO2), the exchange-correlation functional is given by the local density approximation as (LDA). The atomic configurations are $4s^2$ $4p^6 4d^2 5s^2$ for Zr and $2s^2$ $2p^4$ for O. The k-point grid of Brillouin zone sampling in primitive cells, based on the Monkhorst–Pack scheme, is $9 \times 9 \times 9$ for c-ZrO2 [3]. These calculations were performed with Materials Studio 2017 software [10] by using Castep code and Forcite [11] [12].

A. Structural properties

First. Inter-Planar Spacing (d_{hkl})

We calculate the distances between crystalline planes (d_{hkl}) using (Bragg's law) and through the following relationship [13].

$$n\lambda = 2d \sin \Theta \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

n: An integer representing the degree of diffraction
λ: Wavelength
d: Inter-Planar Spacing
Θ:The angle between the crystal plane and the incident ray

Second. Lattice constants

The lattice constants (a, b, c) are calculated for the system cubic system (a = b = c) through the following equation [13].

$$a = d_{hkl} \sqrt{h^2 + k^2 + l^2} \quad \ldots\ldots\ldots\ldots (2)$$

hkl**:** Miller indices
d**:** Inter-Planar Spacing
(a, b, c): Lattice constants

B. Mechanical properties for solid

Mechanical properties include Elastic constants (Cij), Bulk modulus (B), shear modulus (G), Young's modulus (E), ductile characteristic (B/G), anisotropic factor (A^U) and Poisson's ratio (v), as all these mechanical properties are studied, as well as the mechanical stability of the cubic zirconia in the ground state [14].

a) Elasticity

In the small strain limit, the generalized Hooke's law describes stress (σ)as a linear function of strain (Ɛ), such that [15]

$$= C_{ij}\, \varepsilon_j \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)\sigma_i$$

$$= S_{ij}\, \sigma_j \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)\varepsilon_i$$

C_{ij}: elastic stiffness
S_{ij}: elastic compliance
σ: Stress
Ɛ: Strain

$i, j = 1, 2, \ldots\ldots$

The stiffness matrix, consisting of (81) compounds produced from (9x9) of the composites since when stressing the Stresses in the three directions on the material, we will have stress in each direction (x, y, z) σ_x, σ_y, σ_z and that each stress will generate two strains, as in Figure (2), which shows the effect of stresses on the material in every direction [16].

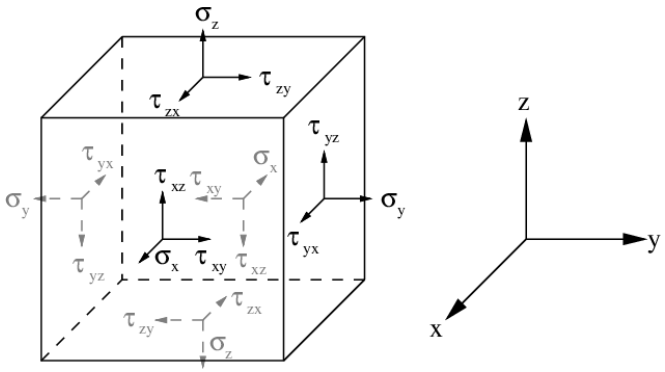

Figure 2. Stresses acting on a volume element [16]

The stiffness matrix of the cubic system is as follows [17],

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ sym. & C_{22} & C_{23} & 0 & 0 & 0 \\ sym. & sym. & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} \ldots(5)$$

Because of the lattice symmetry, there are three dependent variables in the stiffness matrix for the cubic system, C_{ij} (C_{11}, C_{12}, C_{44}) also for the compliance matrix S_{ij} (S_{11}, S_{12}, S_{44}) [17], is as follows [18].

$$[S]=\begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ sym. & S_{22} & S_{23} & 0 & 0 & 0 \\ sym. & sym. & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{66} \end{bmatrix} \ldots(6)$$

As for the Cubic System, we note that:
$C_{12} = C_{13} = C_{23} = C_{21} = C_{31} = C_{32}$, $C_{44} = C_{55} = C_{66}$, $C_{11} = C_{22} = C_{33}$.

The (C_{11}, C_{12}, C_{44}) compounds are used to find S_{ij} through the following relationships [15]

$$= \frac{C_{11}+C_{22}}{{C_{11}}^2+C_{11}C_{12}+2{C_{12}}^2} \quad \ldots\ldots\ldots\ldots (7) S_{11}$$

$$= \frac{C_{12}}{{C_{11}}^2+C_{11}C_{12}+2{C_{12}}^2} \quad \ldots\ldots\ldots\ldots (8) S_{12}$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9) S_{44} = \frac{1}{C_{44}}$$

b) Mechanical stability

We described it through the elasticity constants C_{ij}, and it is as follows [19],
For cubic system

$$> 0, \; C_{44} > 0, \; C_{11} - C_{12} > 0, \; C_{11}+2C_{12} > 0 \quad \ldots\ldots (10) C_{11}$$

***c) Elastic* moduli**

1) Bulk modulus (B): The Bulk modulus can be described by the elastic constants C_{ij}, and as follows [20]:

$$B = \frac{1}{3}(C_{11} + 2\,C_{12}) \quad \ldots\ldots\ldots\ldots\ldots (11)$$

2) Shear modulus (G): The Shear modulus can be described by the elastic constants C_{ij}, for three theories (Voigt (G_V), Reuss (G_R), Hill (G_H)) and as follows [14]:

$$= \frac{1}{5}(C_{11} - C_{12} + 3\,C_{44}) \ldots\ldots\ldots\ldots (12) G_V$$

$$= \frac{C_{44}\,(C_{11}- C_{12})}{4C_{44}+3(C_{11}- C_{12})} \quad \ldots\ldots\ldots\ldots\ldots (13) G_R$$

$$= \frac{1}{2}(G_V + G_R) \quad \ldots\ldots\ldots\ldots\ldots\ldots (14) G_H$$

3) Young's modulus (E): The isotropic Young's modulus can be described by Bulk modulus and Shear modulus and as follows [20]:

$$E = \frac{9\,BG}{3B+G} \quad \ldots\ldots\ldots\ldots\ldots (15)$$

4) Poisson's ratio (v): The isotropic Poisson's ratio can be described by Bulk modulus and Shear modulus and as follows [15]:

$$= \frac{3B-2G}{2(3B+G)} \quad \ldots\ldots\ldots\ldots\ldots (16) \bar{v}$$

5) Anisotropic factor (A^U): The anisotropic factor is used to determine the elastic contrast of the crystal, so the anisotropy relationship is written as follows [21]:

$$= 5\frac{G_V}{G_R} + \frac{B_V}{B_R} - 6 \quad \ldots\ldots\ldots (17) A^U$$

6) Ductile characteristic (B/G):

A higher B/G value indicates the ductility of the material, while a lower B / G value indicates the brittleness of the material. So the threshold is around 1.75. When the B/G value is less than 1.75, the material is brittle; otherwise, it is ductile [21].

III. Results and discussion

we constructed and modeled the 3D crystal structure of cubic zirconia by using material studio software then making the calculations on it to calculate the structural, electronic, and mechanical properties for c-ZrO2.

A. Structural properties

X-ray diffraction result:

When comparing our results obtained through simulation using the (Materials studio) program (figure 3) with the results of previous studies, they were very close to the experimental results that P.R. Rauta in 2012 (figure 4), the slight difference is due to the measurement conditions during which the calculations were made in our study and previous studies, as well as to the preparation method that the researcher worked by using a bottom-up approach for nanoparticles of zirconia and calcination at 600 C° [22].

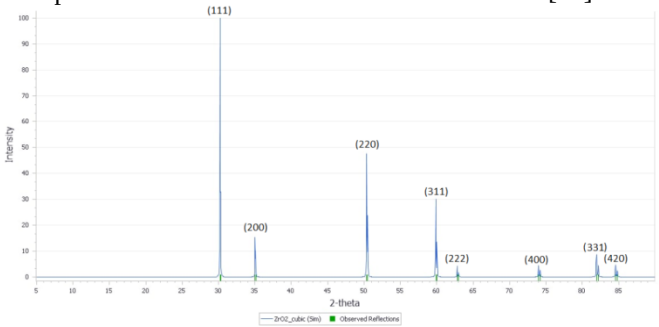

Figure 3. X-ray diffraction of c-ZrO2 was obtained by simulating XRD using the (Materials-studio software) at room temperature.

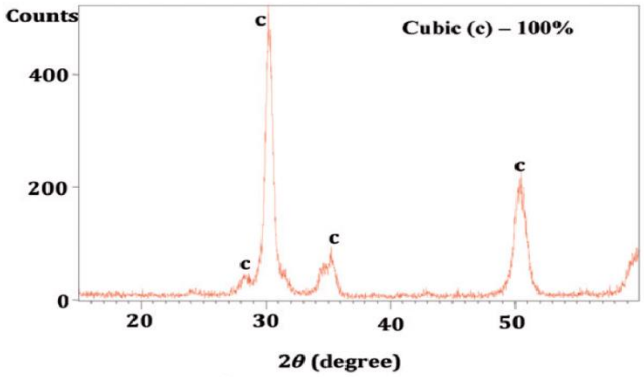

Figure 3. X-ray diffraction of c-ZrO2 experimentally obtained [22]

We compared the values of the distances between the crystalline planes (d_{hkl}) that were theoretically calculated (using equation 1) from the X-ray diffraction data obtained through simulation (XRD using the Materials studio program) for the c-ZrO2. With the experimental results of previous studies ($d_{EXP.}$), reached by Gerald Katz [23], as well as compared with the values of (d_{AMCSD}) taken from the international AMCSD card (American Mineralogist Crystal Structure Database) with the code [AMCSD 0011730]. As in table 1.

Table 1. Compare values of distances between crystalline planes (d_{hkl}) that we calculated using M.S and experimental results computed in previous studies and standard results [AMCSD 0011730] for c-ZrO2.

Peak No.	2Θ (deg.)	d present (Å)	$d_{EXP.}$ (Å) [23]	d_{AMCSD} (Å)	hkl	Intensity arb. (Unit)
1	30.34	2.943	2.93	2.927	111	100
2	35.10	2.554	2.55	2.535	200	16
3	50.40	1.809	1.801	1.792	220	48
4	60.00	1.540	1.534	1.528	311	30
5	62.90	1.476	1.471	1.463	222	4
6	74.00	1.279	1.270	1.267	400	4.5
7	82.00	1.174	1.167	1.163	331	9
8	84.80	1.142	1.135	1.133	420	5

We noticed that there is a great convergence in the results with a very slight difference, and the reason for the slight difference in the results is due to the surrounding conditions during which the measurements were made, as well as to the methods of calculation [14].

We also plotted the curve as a relationship between the scattering angle (2Θ) and the intermediate distances (d_{hkl}) for the results that we calculated using the materials studio software and the results of the international AMCSD card [AMCSD 0011730] as shown in figure 4.

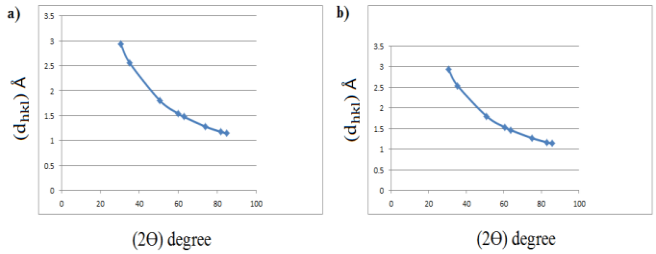

Figure 4. The relationship between (2Θ) and (d_{hkl}) for c-ZrO2, a / for the results that we reached through the materials studio software, b/ for the results obtained from the international card with code [AMCSD 0011730].

Through the above chart, we notice a clear decrease in the value of the distances between (d_{hkl}) gradually with the value of the angle (2Θ) [24].

Among the structural properties, we also calculated the lattice constants of cubic zirconia using the (LDA) approximation and compared the results we obtained using the M.S. With the results of previous theoretical and experimental studies As in table 2.

Table 2. Lattice constants for c-ZrO2 obtained using the M.S, by using the (LDA) with the theoretical and experimental results of previous studies and the values of the (AMCSD) card, [amcsd 0011730]

Lattice constants	Present study LDA (Å)	LDA (Å) [7]	LDA (Å) [5]	EXP. (Å) [25]	AMCSD (Å)
a = b = c	5.025	5.028	5.036	5.085	5.07
ɤ = β = α	90°	90°	90°	90°	90°

When comparing our results, we obtained using the (M.S) software, by the (LDA) for the lattice constants, as (a = b = c) and the value (a = 5.025), which is close to the results reached by G. Fadda in 2010 and Dash in 2004 through the calculations of the LDA and it was a value (a = 5.028 Å) and (a = 5.036 Å) respectively [7] [5]. It was also close to the experimental results reached by researcher C. J. Howard [25], and the results of the AMCSD card too, [amcsd 0011730].

We also calculated some of the constants related to the structural properties, such as unit cell volume (V), unit cell density (ρ), and bond length, and We compared our results with the experimental and theoretical results of previous studies and the AMCSD card with the code [amcsd 0011730], as in table 3.

Table 3. comparison in the values of the structural parameters of c-ZrO2 between the results obtained through simulations using the (materials studio software) and between the experimental and theoretical results of previous studies and the AMCSD card with the code [amcsd 0011730].

Structural parameters	Present a study (by M.S)	Theoretical	EXP.	AMCSD
Unit cell volume (V)	134.297 ($Å^3$)	135.5 ($Å^3$) [4]	-	130.324 ($Å^3$)
Unit cell density (ρ)	6.094 (g /cm^3)	6.08 (g /cm^3) [4]	6.27 (g /cm^3) [14]	6.279 (g /cm^3)
Bond length Zr-o	2.2174 (Å)	2.219 (Å) [4]	2.210 (Å) [25]	-

Our results were largely close to the results of previous theoretical and experimental studies of previous studies [4] [14] [25], as well as close to those of the AMCSD card.

B. Electronic properties

We calculate the Band structure after the formation of the Billion zone (as shown in figure 5) by simulation using the materials studio software, then we calculate the energy bandgap (as shown in figure 6) by using (LDA).

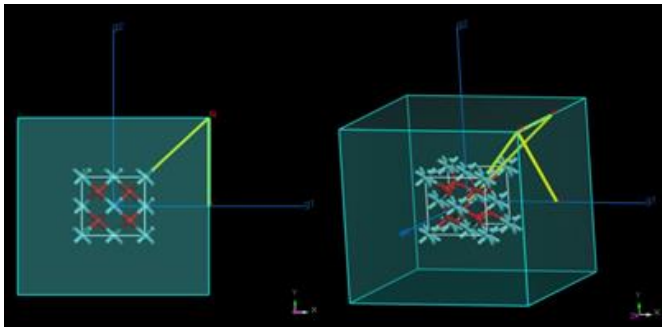

Figure 5. Billion zone of c-ZrO2 by using Materials studio

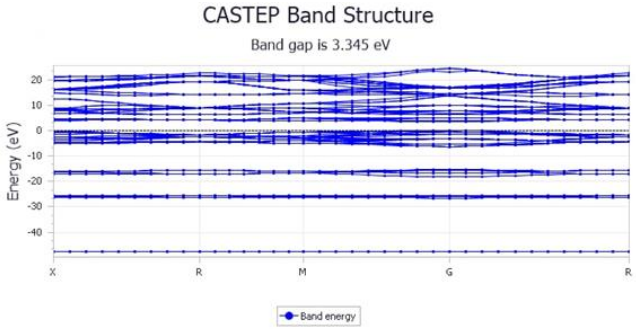

Figure 6. Band structure of c-ZrO2 by materials studio, using (LDA) and shown the bandgap.

The Fermi level was set at zero energy, and as we note, it appears as a dashed line. The calculated band structure using (LDA) shows that c-ZrO2 presents a direct bandgap of about 3.345 eV, so Zro2 is an insulator [26] [19]. When comparing our results with those of previous theoretical and experimental studies, there was a significant convergence of the results, as in table 4.

Table 4. comparison our results with those of previous theoretical and experimental studies

BG	Present Study LDA	Previous Study LDA [28]	Previous Study [4]	EXP. Study [27]
c-ZrO2	3.345 eV	3.67 eV	3.316 eV	6.10 eV

We ran simulations of Density of state, as the Brillouin zone sampling was performed using a Monkhorst-Pack with a k-point grid consisting of $9 \times 9 \times 9$
For c-ZrO2, we obtained the width upper valence band (WUVB) (as in figure 7.), we compared our result with previous studies (as in figure 8.) and (table 5.)

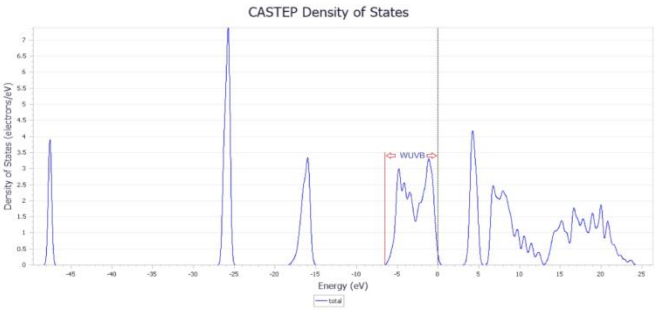

Figure 7. density of states of c-ZrO2

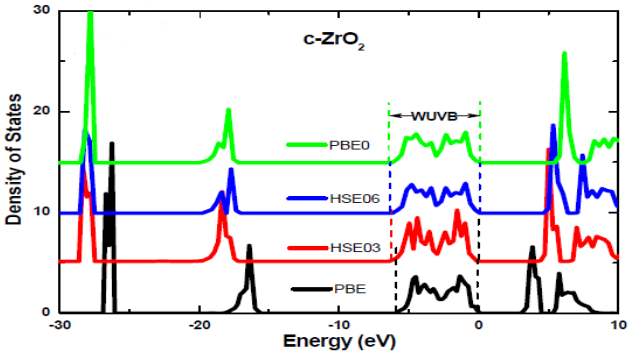

Figure 8. density of states of c-ZrO2 [30]

Table 5. comparison the width upper valence band (WUVB) that computed using the (materials studio) of the c-ZrO2 with the results obtained from previous theoretical and experimental studies.

WUVB	Preset study LDA (eV)	LCAO [32] (eV)	EXP. [31] (eV)
Cubic c-ZrO2	6.60	5.90	6.50

We note that our results are close to the results of previous studies, as shown in table 5, and the reason for the slight difference is due to the measurement conditions through which the calculation was performed, as well as the difference in the capabilities of the computers used for the calculation [30].

C. Mechanical properties

We calculated the elastic stiffness constants by the local density approximation (LDA) using the materials studio software and compared our results with the results of previous theoretical and experimental studies, as we noticed a great convergence between our results and the results of previous theoretical and experimental studies. As shown in table 6.

Table 6. Elastic stiffness constants (c_{ij}) for c-ZrO2 using the materials studio software, and results of previous theoretical and experimental studies

c_{ij} (Gpa)	Present LDA	LDA [15]	EXP. [29]
c_{11}	570.926	563	417
c_{44}	79.573	72	47
c_{12}	111.619	116	82

All ab initio calculations (in our and previous studies) for cubic phase zirconia c-ZrO2 c44 <c12 <c11, also we noticed that our results close to the results of previous studies, experimental studies generally show slightly lower results than the calculated values, but they show similar trends [33].

Also, for the Elastic compliance constants (Sij) (S_{11}, S_{12}, S_{44}), which we can obtain by using (equ. 7, equ. 8, equ. 9) respectively, as well as through the elastic compliance matrix that the Material Studio software provides for us [15]. We compare our results with previous studies, and we noticed a big convergence, as shown in table 7.

Table 7. elastic compliance constants Sij of c-ZrO2

s_{ij} (1/Gpa)	Present LDA	LDA [15]
s_{11}	0.00187	0.00191
s_{44}	0.01256	0.01395
s_{12}	-0.000306	-0.00032

Important factors in mechanical properties are elastic moduli such as Bulk modulus (B), Young's modulus (E), Poisson's ratio (ν), ductile characteristic (B/G), and shear modulus (G) (as in table 9.). As table 8. contains a comparison between the elastic moduli values of three theories (Voigt, Reuss, Hill) of our results with the results of previous studies.

Table 8. Shear moduli (G_V , G_R, G_H) and Bulk moduli (B_V , B_R, B_H)

Structure & Calculation	G_V Gpa	G_R Gpa	G_H Gpa	B_V Gpa	B_R Gpa	B_H Gpa
c-ZrO2 Present	139.6	107.7	123.6	264.7	264.7	264.7
c-ZrO2 [19]	132.4	98.4	115.4	265.4	265.4	265.4

The results that we reached by using the M.S software and through the Castep tool for the LDA approximation were very in convergence with the result in previous studies [19].

Table 9. comparison the isotropic moduli (shear modulus, Bulk modulus, Young's modulus, and Poisson's ratio) and ductile characteristic

Stru.	G (Gpa)	B (Gpa)	E (Gpa)	$\bar{v}$	B/G
c-ZrO2 Present	123.6	264.7	320.8	0.2979	2.14
c-ZrO2 Cal. [15]	115	265	302	0.3101	2.30
c-ZrO2 Exp. [29]	81	194	212	0.3173	-

Through the comparison in Table 9, we note that there is great convergence between our results and the results of previous theoretical and experimental studies.

The calculated *B*/*G* ratio for c-ZrO2 is larger than 1.75, which indicates ductile materials [34]. The value of the Poison ratio that we obtained was (0.29), so the substance has ionic bonds [24].

We obtained the value of compressibility (0.0037 1/Gpa) and its convergence with the result reached by I.D. Muhammad (0.00350 1/Gpa) [1]. The average velocity of sound in the c-ZrO2 (4765.11 m/s) convergence with the result reached by Lei Jin (4184 m/s) [35]. Debye temperature of c-ZrO2 (645.34 k), also its convergence with the result reached by Yang (626.2 k) [36].

IV. Conclusions

After studying structural, electronic, and mechanical properties for c-ZrO2, we can conclude:

The results of the mechanical properties showed us that the compound is mechanically stable and conforms to the conditions of mechanical stability through elastic constants. The results of the study of the elastic properties of the material, specifically through the ductility property (B/G), showed that the material is ductile and not brittle, and through the Poison Ratio, the bonds that bind the atoms of the substance together are ionic bonds. The results of X-ray diffraction (XRD) showed that the two-component compound had multiple phases and showed us distinct diffraction peaks for some levels, which provided us with useful information for calculating the intermediate distances of the crystal levels. The results of the electronic properties of the energy beams and the energy gap showed us, through which it was found that (c-ZrO2) is an insulating material due to the large energy gap of the compound.

References

[1] I. D. Muhammad, M. Awang, and O. Mamat., Modelling the Elastic Constants of Cubic Zirconia Using Molecular Dynamics Simulations ., Adv. Mater. Res., 845(2014) 387–391 doi: 10.4028/www.scientific.net/AMR.845.387.

[2] J. Zhang, A. R. Oganov, X. Li, H. Dong, and Q. Zeng., Novel compounds in the Zr-O system, their crystal structures, and mechanical properties, Phys. Chem. Chem. Phys., (2015) doi: 10.1039/C5CP02252E.

[3] F. Qunbo, W. Fuchi, Z. Huiling, and Z. Feng, Study of ZrO 2 phase structure and electronic properties, Mol. Simul., 34(2008) 10–15,1099–1103, doi: 10.1080/08927020802101759.

[4] Y. Pan, Influence of Oxygen Vacancies on the Electronic and Optical Properties of Zirconium Dioxide from First-Principles Calculations, J. Electron. Mater., 48(8)(2019) 5154–5160, doi: 10.1007/s11664-019-07325-0.

[5] L. K. Dash, N. Vast, P. Baranek, M. Cheynet, and L. Reining, Electronic structure and electron energy-loss spectroscopy of ZrO 2 zirconia, Phys. Rev. B, 245116(2004) 1–17, doi: 10.1103/PhysRevB.70.245116.

[6] Z. Yang, L. Zhu, B. Lin, G. Zhang, C. Ni, and T. Sui, The grinding force modeling and experimental study of ZrO 2 ceramic materials in ultrasonic vibration-assisted grinding, Ceram. Int., 45(7)(2019) 8873–8889, doi: 10.1016/j.ceramint.2019.01.216.

[7] G. Fadda, G. Zanzotto, and L. Colombo, First-principles study of the effect of pressure on the five zirconia polymorphs . I. Structural, vibrational, and thermoelastic properties, Phys. Rev. B 82, 064105, (2010), doi: 10.1103/PhysRevB.82.064105.

[8] R. Terki, G. Bertrand, H. Aourag, and C. Coddet, Structural and electronic properties of zirconia phases: A FP-LAPW investigations, Mater. Sci. Semicond. Process., 9(6)(2006) 1006–1013, doi: 10.1016/j.mssp.2006.10.033.

[9] C. N. Mihai, L.L., Parlatescu, I., Gheorghe, C., Andreescu, C., Bechir, A., Pacurar, M., and Cumpata, In vitro study of the effectiveness to fractures of the aesthetic fixed restorations achieved from zirconium and alumina, Rev. Chim., 65(6)(2014) 725–729.

[10] S. R. Gul, M. Khan, and C. Tsai, Electronic Band Structure Variations in the Ceria Doped Zirconia : A First Principles Study, Mater. 11(7)(2018) 1238, doi: 10.3390/ma11071238.

[11] Q. Liu, Z. Liu, and L. Feng, Elasticity, electronic structure, chemical bonding and optical properties of monoclinic ZrO 2 from first-principles, Phys. B Phys. Condens. Matter, 406(3)(2011) 345–350, doi: 10.1016/j.physb.2010.10.057.

[12] Najat Ahmed Dahham, A. Hamoud, and S. S. Ali, A study of structural, mechanical, thermodynamics and electronic properties of Zinc sulpphide (ZnS) composite by using (materials studio) software, M.SC thesis, University of Tikrit, (2018).

[13] V. K. Pecharsky and P. Y. Zavalij, FUNDAMENTALS OF POWDER DIFFRACTION AND STRUCTURAL CHARACTERIZATION OF MATERIALS., Ames, IA, U.S.A. Peter, Binghamton, NY U.S.A., (2005).

[14] M. G. Mulaudzi, AB INITIO STUDY OF STRUCTURAL STABILITY AND ELECTRONIC PROPERTIES OF ZrO2 xSx FOR $0 \leq x \leq 2$., M.SC thesis, Univ. LIMPOPO, (2015).

[15] G. P. Cousland, X. Y. Cui, A. E. Smith, A. P. J. Stampfl, and C. M. Stampfl, Mechanical properties of zirconia, doped and undoped yttria-stabilized cubic zirconia from first-principles, J. Phys. Chem. Solids, (2018), doi: 10.1016/j.jpcs.2018.06.003.

[16] J. Lienemann and J. G. Korvink,Electrostatic Beam Model, Univ. Freibg. IMTEK,Technische Fak. Albert Ludwig Univ. Georg. Kohler Allee 103, D-79 110 Freiburg, Ger., (2003).

[17] X. Luan and H. Qin, The Mechanical Properties and Elastic Anisotropies of Cubic Ni 3 Al from First Principles Calculations, Crystals, 8.8(2018) 307, doi: 10.3390/cryst8080307.

[18] J. Zhao, X. Song, and B. Liu, Standardized Compliance Matrices for General Anisotropic Materials and a Simple Measure of Anisotropy Degree Based on Shear-Extension, Int. J. Appl. Mech., 8.06(2016) 1650076, doi: 10.1142/S1758825116500769.

[19] G. Cousland, Investigation of material properties of yttria-stabilized zirconia using experimental techniques and first-principles calculations, M.SC, thesis, The Faculty of Science The University of Sydney, Australia Investigation, (2014).

[20] Dengg and Thomas., Computation of Temperature-Dependent Elastic Constants within the Framework of Density-Functional Theory, PhD. THESIS, Karl-Franzens-Universität Graz,Austria, (2017) .

[21] W. Wang, Z. Liang, X. Han, J. Chen, C. Xue, and H. Zhao, Mechanical and Thermodynamic Properties of under High-Pressure Phase Transition : A First-Principles Study, J. Alloys Compd., (2014), doi: 10.1016/j.jallcom.2014.08.114.

[22] P. R. Rauta, P. Manivasakan, V. Rajendran, B. B. Sahu, B. K. Panda, and P. Mohapatra., Phase transformation of ZrO 2 nanoparticles produced from zircon, Phase Transitions, 85(2012) 1–2,13–26, doi: 10.1080/01411594.2011.619698.

[23] G. KATZ, X-Ray Diffraction Powder Pattern of Metastable Cubic ZrO2, J. Am. Ceram. Soc., 54(10) (1971)531–531, doi: 10.1111/j.1151-2916.1971.tb12197.x.

[24] N. A. Dahham, A. Hamoud, and K. Abdullah, A study of structural, mechanical and electronic properties of Barium Orthotitanate (Ba2Tio4) composite using materials studio software, M.sc. Thesis, University of Tikrit, (2017).

[25] C. J. Howard, R. J. Hill, and B. E. Reichert., Structures of ZrO2 polymorphs at room temperature by high-resolution neutron powder diffraction., Acta Crystallogr. Sect. B, 44(2)(1988) 116–120, doi: 10.1107/S0108768187010279.

[26] B. T. Wang, P. Zhang, H. Y. Liu, W. D. Li, and P. Zhang, First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium, J. Appl. Phys., 109(6)(2011) doi: 10.1063/1.3556753.

[27] R. H. French, S. J. Glass, F. S. Ohuchi, Y. Xu, and W. Y. Ching, Experimental and theoretical determination of the electronic structure and optical properties of three phases of ZrO2, Phys. Rev. B, 49(8)(1994).

[28] J. E. Medvedeva and A. J. Freeman., Screened-exchange Determination of the Electronic Properties of Monoclinic, Tetragonal and Cubic Zirconia, Phys. Rev. B, 76(2)(2007) 35115, doi: 10.1103/PhysRevB.76.235115.

[29] H. M. Kandil, J. D. Greiner, and J. F. Smith, Single-Crystal Elastic Constants of Yttria-Stabilized Zirconia in the Range 20 to 700 ° C, J. Am. Ceram. Soc. 67.5(1984) 341–346.

[30] Y. Yang, X. Fan, C. Liu, and R. Ran, First-principles study of structural and electronic properties of cubic phase of ZrO2 and HfO2, Phys. B Phys. Condens. Matter, (2013) doi: 10.1016/j.physb.2013.10.037.

[31] J. Robertson, K. Xiong, and S. J. Clark, Band structure of functional oxides by screened exchange and the weighted density approximation., phys. stat. sol., 2070(9)(2006) 2054–2070, doi: 10.1002/pssb.200666802.

[32] F. ZANDIEHNADEM, R. A. MURRAY, and W. Y. CHING, ELECTRONIC STRUCTURES OF THREE PHASES OF ZIRCONIUM OXIDE, Phys. B, 150(1988) 19–24.

[33] A. Van De Walle and G. Ceder, Correcting overbinding in local-density-approximation calculations, Phys. Rev. B, 59(23)(1999).

[34] Z. Liang et al., Author 's Accepted Manuscript Structural, Mechanical and Thermodynamic Properties of ZrO 2 Polymorphs by First-Principles Calculation,Phys. B Phys. Condens. Matter, (2017) doi: 10.1016/j.physb.2017.01.025.

[35] L. Jin, Q. Yu, A. Rauf, and C. Zhou, Elastic, electronic and thermal properties of YSZ from first principles, Solid State Sci., 14(1)(2012) 106–110, doi: 10.1016/j.solidstatesciences.2011.11.003.

[36] J. Yang, M. Shahid, C. Wan, F. Jing, and W. Pan, Anisotropy in elasticity, sound velocities and minimum thermal conductivity of zirconia from first-principles calculations, J. Eur. Ceram. Soc., (2016) doi: 10.1016/j.jeurceramsoc.2016.08.034.