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The Structural, Electronic and Mechanical Properties of α and β Phases in Titanium Using Density Functional Theory

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ABSTRACT

In this paper, the structural, electronic and mechanical properties of α and β phases in titanium (Ti) with the space group of $P6_3/mmc$ and Im3m were computed by using first-principles calculations through density functional theory (DFT) method. The Cambridge Serial Total Energy Package (CASTEP) code that is based on the Density Functional Theory (DFT), which uses a total energy plane-wave pseudopotential method, is carried out the calculation of the properties. The accuracy of the model was confirmed by comparing the data with other previous theoretical and experimental studies in the literature. Using the computational method, we obtain that GGA-PBE functional has close agreement in lattice parameters and volume for α and β phases. The phase stability of Ti gives stable structure in α phases due to the lower energy obtained. The higher peak in DOS of β phase shows that the β-Ti undergoes metallic characterized bond and α-Ti phase undergoes strong hybridization of covalent atom. Analyzing the mechanical constant of both phases of Ti, the elastic constants (C_{ij}) for α and β phases Ti are calculated together with their related bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's ratio (B/G) and Poisson's ratio (ν) in order to explore the mechanical behaviour of Ti. The result suggests that β phase for Ti shows that it is mechanically stable for biomedical application due to the lower value of E.

Keywords: Biomedical, Density Functional Theory, Electronic Properties, First Principles, Mechanical Properties, Structural Properties, Titanium.

1. INTRODUCTION

Over the previous decade, titanium (Ti) was introduced into global industries and also known as biomaterials due to its excellent properties such as non-toxicity, high corrosion resistance and good biocompatibility towards human bones. Essentially, Ti also broadly used in lots of field such as aerospace [1], automotive field, power generation, engineering scope, petrochemical, dental, bone implantation, biomedical and medical industries [2-6] due to its enticing and compatible properties mainly correspond to low density, good mechanical properties, high strength element and corrosion resistance [3, 7-9]. The most frequent compound that has been used widely is titanium dioxide, which gives good contribution in photocatalyst [10]. In biomedical application, a lot of biomaterials such as ceramics, polymers and even metals have been considered. However, ceramics are rigid, hard and brittle solids without exception with low mechanical, tensile and shear strength under fatigue loading [11],

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whereas polymers are easily affected by changes in temperature, environment and position and has low mechanical properties hence susceptible to mechanical fracture [12].

Many of the materials used today in the clinical environment were not originally designed for application to biomaterials. In crude terms, they became biomaterials when they were implanted in the human body in a variety of forms and found to work by series of trial and error experimentation. Apparently, there were also other materials that did not match and fit causing pain and distress to patients at least and needless misery and death at worst. Host tissue should be biocompatible with the materials used in medical procedures. To produce good biomaterials which are recognized and assimilates by the body, the implants must have high degree in biocompatibility, high strength and high corrosion resistance [13-14]. Due to that consequence, metallic materials such as Ti are marks as a crucial sector in rehabilitation of failed hard tissue in biomedical and the rate of growth in market has emerged every day from the previous decades [13, 15].

Ti is an element with remarkable characteristics [16]. By following the phase diagram of Ti, it may undergoes transition phases based on the effect of changes in temperature, pressure or both of them. Numerous studies stated that Ti metal shows a series of allotropic phase transformations from a low temperature (at ambient temperature) closed-packed hexagonal crystal structure (HCP) of the form $P6_3/mmc$ known as α phase, having c/a ratio of ~1.58 with the unit cell parameters are a = 2.946 Å and c = 4.666 Å [17,7] to a high temperature (1155 K/882 ℃) body-centered cubic crystal structure (BCC) called β phase with space group of *Im3m* and the unit cell parameter is a = 3.264 Å [4, 7, 18-19]. At ambient temperature with high pressure, Ti undergoes ω phase. It should be noticed that this phase also referred to as the hexagonal phase. The stable phases that has been considered for Ti is α and β phases [17]. Sun et al. [18] reported the structural, electronic and mechanical properties of Ti alloy and their phase such as α"(orthorhombic), ω (hexagonal) and β (cubic) phases using DFT while Li et al. [20] have successfully reported relative stability and lattice parameters of α", α and β phases in binary Ti alloys by using exact muffin-tin orbitals (EMTO) basis sets. Presently, the cubic structure of Ti in β phase was investigated widely compare to other phases due to its excellent mechanical properties [7-8,21]. However, among the theoretical and experimental studies, not many studies have been focused on comparison between structural, electronic and mechanical properties of pure material of Ti in both α and β phases (at their ambient temperature) in term of biomedical applications.

Hence, the aim of this present work is to investigate and provide details comparison on metal Ti between α and β phases in order to identify and achieve a good properties in biomaterial (Ti) for future biomedical applications. The systematic investigations of the crystal structure and their properties of both phases of Ti are desirable and helpful for the rational design of future works related to Ti and Ti-alloys. The first principles method was employed to predict accurately the lattice constant and the properties. These present results are carried out by using Cambridge Serial Total Energy Package (CASTEP) code that is based on the Density Functional Theory (DFT) and are expected to be useful for other research which concerning Ti material. This work assimilates recent characterization of α phase and β phase of Ti development techniques such as calculation model on structural, electronic and mechanical structure methods (DFT calculation). The crucial factors to express are the mechanical properties and determining strength of the material's elastic constant.

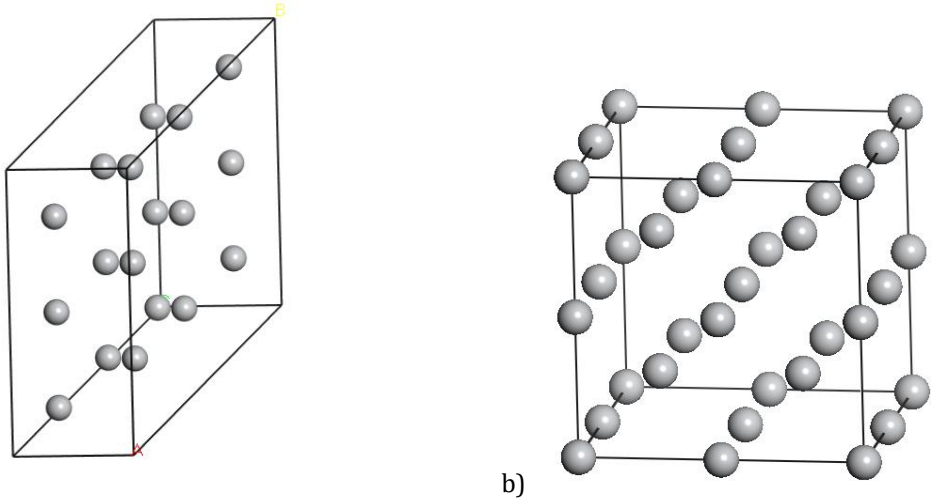
2. COMPUTATIONAL METHOD

The first-principles calculations in this work were performed based on density functional theory (DFT) using exchange-correlation functional of three functional which is local density

approximation (LDA), generalized gradient approximation with Perdew –Burke – Ernzerhof (GGA-PBE) and gradient approximation with Perdew –Burke – Ernzerhof for solid (GGA-PBEsol) within Cambridge Serial Total Energy Package (CASTEP) computer code [22-25]. The pseudopotential and plane-wave basis set were used for the conventional cell calculations. The structures of α and β phases titanium are illustrated in Figure 1. The structures of α-Ti (*P6₃/mmc*) and β-Ti (*Im3m*) has been set in supercell structures. Table 1 indicated the reported values of the space group, basis vectors and atoms coordination of the structures respectively. The atomic positions are (0.33, 0.66, 0.25) for α-Ti and (0,0,0) for β-Ti respectively. All the calculations are performed on the basis of the optimized lattice structure to get the structural properties (lattice parameters, volume, bond length and phase stability), electronic properties (band structures and density of state) and mechanical properties (elastic's constant, bulk modulus, shear modulus, Young's modulus and Poisson's ratio). The bulk modulus, shear modulus and Young's modulus were calculated by formula of Voigt-Reuss-Hill approximation (VRH). All the calculations were carried out within ultrasoft pseudopotential. All forces on atoms were converged to less than 0.03 eV $Å^{-1}$, the energy at 1.0e-5 eV/atom, the maximum ionic displacement was set to 0.001 Å and the total stress tensor was decreased to the 0.05 GPa. The electron wave functions were expanded and converged in a standard plane wave basis set with kinetic energy cutoff of 320 eV and the calculations were performed using Monkhorst-Pack *k*-points meshes of 4×4×4 with ultrasoft pseudopotential scheme.

Table 1 Space groups, basis vectors and basic atoms coordinates for α-Ti and β-Ti phases

Phase	α phase	β phase
Space group	*P6₃/mmc* (No. 194)	*Im3m* (No. 229)
Basis vectors	α = β = 90°;γ =120°	α = β = γ = 90°
Basis atoms	(1/3, 2/3, 1/4);(2/3, 1/3, 1/4)	(0,0,0)



a) b)

Figure 1. The crystal structures of (a) α-Ti and (b) β-Ti.

3. RESULTS AND DISCUSSION

3.1. Structural Properties

The crystal structures α-Ti and β-Ti phases were firstly undergoes optimization to verify the equilibrium lattice constants for α-Ti and β-Ti respectively. The lattice parameters and volumes

within the functional of LDA, GGA-PBE and GGA-PBEsol from the full structural optimization are listed in Table 2 along with the other theoretical and experimental works for comparison. The results indicated that the functional from GGA-PBE provides the best agreement with the experimental data. Lattice constant of α-Ti phase has underestimated for a by 0.271% while lattice b has overestimated by 0.598% and underestimated in lattice volume by 0.816% respectively. Lattice constant and volume of β-Ti phase has underestimated by 0.276% and 0.834% when compared to experimental result. When compared with LDA-CAPZ, the result of lattice and volume for α-Ti phase demonstrated the relative deviation of +2.406%, +2.988% and +6.800% together with relative deviation of β-Ti phase which are +2.543% with +7.420% respectively. Whereas, lattice a and b for functional GGA-PBEsol indicated overestimated by 1.017%, 1.878% and 3.042% for α-Ti phase. On the other hand, our result for β-Ti phase also overestimated by 1.011% and 2.991% for lattice a and volume. Hence, our results indicate good agreement with other studies with small error less than 10%. Thus, the calculation methods in this work are equitable to be achieved. The bond length for each α-Ti and β-Ti between each atom are 2.887 Å and 2.835 Å. It is shown that β phase has shorter bond length and may give stronger interaction between the atoms. The phase stability of the α-Ti and β-Ti phase can be determined by cohesive energy, E_{coh} whereby $f.u$ is formula unit for Ti and $E\,\alpha/\beta$ is energy of α-Ti and β-Ti phase [20]:

$$E_{coh} = \frac{Total\ energy\ of\ E\ \alpha/\beta}{f.u} - E\,\alpha/\beta \quad (1)$$

The lower value of E_{coh} will shows that the phase is more stable. The fits to the calculated total energy as a function of the volume for the different phases are shown in Figure 2. The graph presented in Figure 2 stated that α phase has lower value in energy with -126.1 eV while β phase reported -109.4 eV. The α phase implies has more degenerated in energy as compared to β phase [20]. According to Li et al [20], the lower value of phases might be due to the finite temperature effect. As the present calculations were performed at 0 K, the expectation of α phase for Ti to be stable in structure as compared to β phase are acceptable by taking into account the effect of temperature. Hence, the theoretical total energy in respect of volume for different phases of Ti shows that α phase has stable phase as compared to β phase.

Table 2 Lattice parameters (a and c) and volume (V) of α-Ti and β-Ti. Previous theoretical and experimental data also included for comparison

Phases	Method	Space group	a (Å)	c (Å)	V (Å^3)
α Ti	LDA-CAPZ	*P6$_3$/mmc*	2.880 (+2.406%)	4.544 (+2.988%)	37.69 (+6.800%)
	GGA-PBE		2.959 (-0.271%)	4.656 (+0.598%)	40.77 (-0.816%)
	GGA-PBEsol		2.921 (+1.017%)	4.596 (+1.878%)	39.21 (+3.042%)
	Theory [26]		2.920	4.600	39.22
	Experiment [7]		2.946	4.666	40.44
	Experiment[27]		2.951	4.684	40.79
β Ti	LDA-CAPZ	*Im3m*	3.181 (+2.543%)	-	32.19 (+7.420%)
	GGA-PBE		3.273 (-0.276%)	-	35.06 (-0.834%)
	GGA-PBEsol		3.231 (+1.011%)	-	33.73 (+2.991%)
	Theory [21]		3.258	-	34.58
	Theory [28]		3.247	-	34.23
	Experiment [7]		3.264	-	34.77

(+) overestimate; (-) underestimate

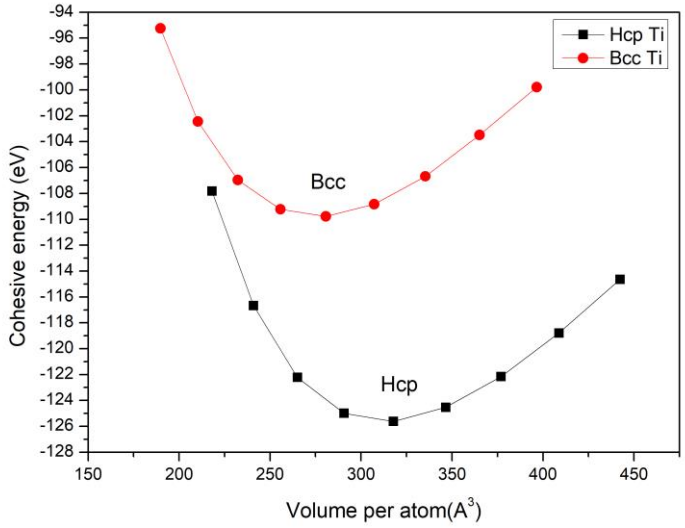


Figure 2. The total energy as a function of volume for α (HCP) and β (BCC) phases of Ti.

3.2. Electronic Properties

The electronic structures of α-Ti and β-Ti phases were investigated in this work in order to interpret more understanding influencing phase stability of Ti and their phases. At DFT within GGA-PBE, we used CASTEP simulation software to measure the band structure of both phases of pure Ti. Figure 3 displays the band structure of α-Ti and β-Ti phases respectively. Both band structures were calculated at first Brillouin zone along high-symmetry points $\mathrm{G} \rightarrow F \rightarrow Q \rightarrow Z \rightarrow \mathrm{G}$. The Fermi energy level represented by a dash black line and set at 0 eV on the energy scale. The band structures of both phases emphasize a gapless result at Fermi level, valence band and conduction band. In order to elucidate the nature of the electronic properties of Ti, the total correlation between electrons occupied orbital is illustrated by density of states (DOS) as shown in Figure 3. The Fermi level that located in the bonding region of the spectrum curves indicated that the DOS at Fermi level of β-Ti illustrated high peak with higher value of 37.7 states per eV and atom whereby shows that the β phase has metallic characterized. Whereas a pseudogap is seen towards the α phase around the Fermi level. The formation of pseudogap reveals strong hybridization between the electronic states of the atoms, indicating a covalent bonding between the atoms in α phase of Ti. The DOS of α phase separates two peaks of which the peak are shows at valence band (lower than Fermi level) and another peak at conduction band (higher than Fermi level). The peak at valence band indicated to the bonding states of the atoms and the conduction band indicated to anti-bonding states. The DOS at Fermi level of α phase of Ti differ to β phase by 21.3 states per eV and atom which suggest that α phase is more stable than β phase. These results may cause by the stronger covalent bond in the α phase than β phase that do behaves as metallic material [20].

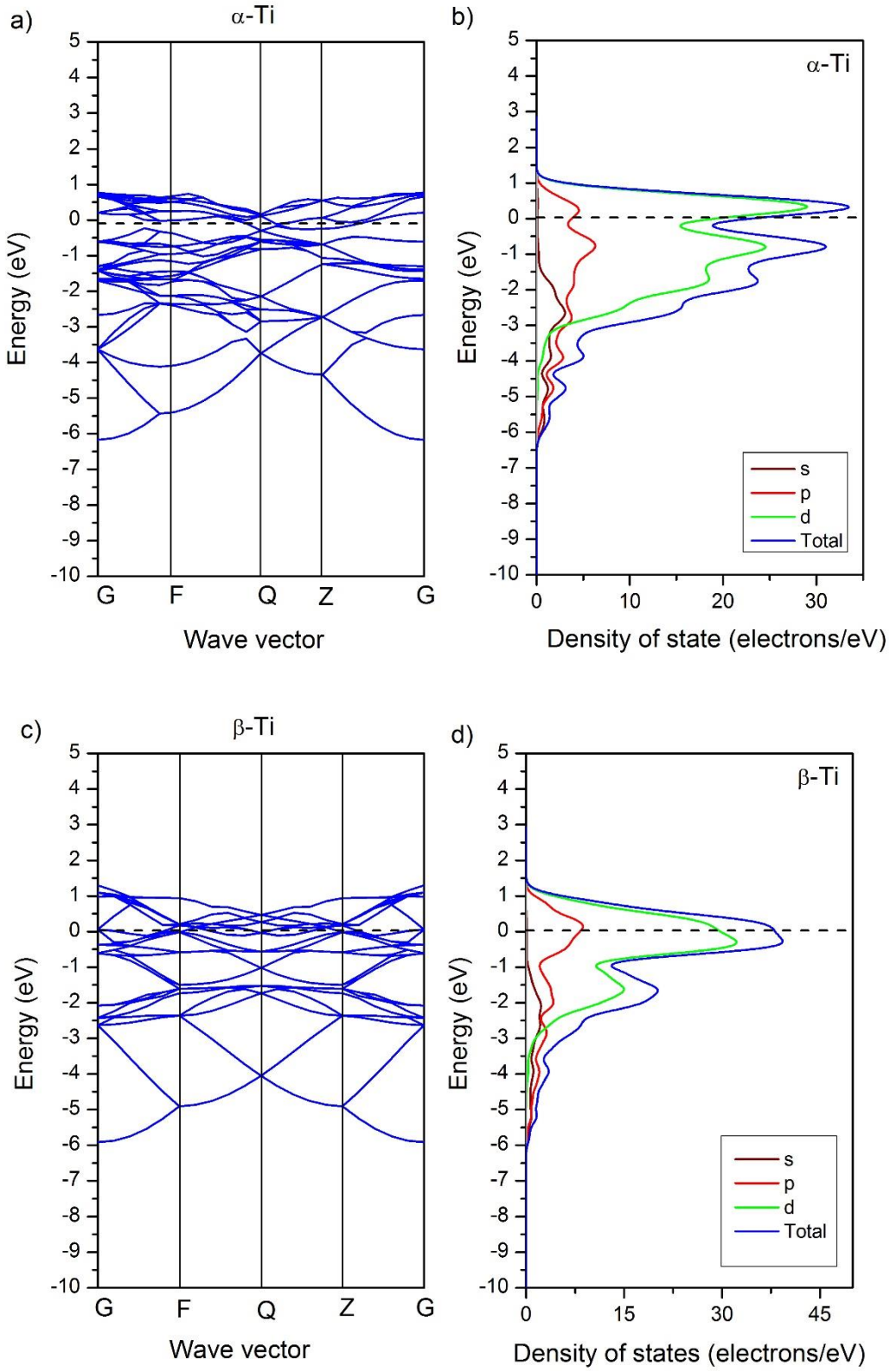


Figure 3. (a) Band structure of α-Ti and (b) DOS of α-Ti and (c) Band structure of β -Ti and (d) DOS of β-Ti.

3.3 Mechanical Properties

The elastic moduli C_{ij} plays an important role in application of crystal phase. The elastic moduli depend mainly with the crystal structure to external forces and it is said to present the bond strength between the atoms [29]. This relationship possess calculation on bulk modulus B, shear modulus G, Young's modulus E and Poisson's ratio ν. The crystal structure of Ti has been studied widely in order to predict a new material as proposed. Presently, the structures of Ti in α and β phase are investigated due to their excellent characteristic. In order to calculate the elastic constants of the α phase structure (hexagonal closed packed) the nonzero strain mode of ε_{33}, ε_{11} and ε_{23} must be consider. As for β phase structure (cubic), ε_{11} and ε_{23} is used. Sun et al. [18], have successfully reported the elastic constant for cubic structure comes with three elastic constants (C_{11}, C_{12} and C_{44}) whereby C_{11} represents the linear compressive resistance along x and z direction. C_{12} and C_{44} indicated Poisson effect and shear resistance in [001] direction. The criteria require of mechanical stability for each crystal structure are;

$$
\begin{aligned}
&C_{44} > 0 \\
&C_{12} + 2C_{11} > 0 \\
&C_{11} - |C_{12}| > 0 \\
&C_{ii} > 0 \qquad (i = 1\text{-}6), \\
&C_{22} C_{33} - C_{23}^{2} > 0 \\
&2C_{12} C_{13} C_{23} - C_{12}^{2} C_{33} - C_{13}^{2} C_{22} > 0 \\
&C_{44} > 0 \\
&(C_{11} + C_{12}) C_{33} - 2C_{13}^{2} > 0 \\
&C_{11} - |C_{12}| > 0
\end{aligned}
\tag{2}
$$

Thus, the calculated elastic properties are satisfied and may represent mechanically stable structure with the above criteria. As for bulk modulus B, shear modulus G, Young's modulus E can be estimated by using Voigt-Reuss-Hill (VRH) approximation as shown in following equations;

$$B = \frac{1}{2}(B_V + B_R) \tag{3}$$

$$G = \frac{1}{2}(G_V + G_R) \tag{4}$$

$$E = \frac{9B.G}{3B+G} \tag{5}$$

$$\nu = \frac{3B-2G}{2\,(3B+G)} \tag{6}$$

whereby B_V, B_R and B are the bulk moduli calculated by VRH approximation respectively. G_V, G_R and G represent shear moduli and E and ν indicated Young's moduli and Poisson's effect [24]. The elastic constants and B, G, E and ν of both phases are presented in Table 3 and Table 4. The computed elastic constant for α and β phases for Ti shows the result has good agreement with the previous experimental and theoretical studies. The results of both phases are consistent with other first-principles calculations. The intrinsic hardness of the material is correlated are determined by bulk modulus B and shear modulus G. As for Young's modulus E provides a calculation of the stiffness of the solid. Concerning biomedical application, the E, Young's modulus was investigated in order to interpret the good properties of Ti biomaterials. Based on the results obtain, the α phase Ti gives higher value in B, G and E whereby indicate that β phase has lower mechanical properties than α phase. As for E for α phase give 133.5 GPa while -52.9 GPa for β phase. The result of β phase Ti may give a good mechanical compatibility of the implant with the human body which mark as an important issue in the selection of implant materials. The Pugh's modulus ratio (B/G) for both phases of Ti indicated 2.256 for α phase Ti and -6.275 for β phase Ti. The Poisson's ratio ν of α phase are about 0.306, which seems less high in position as compared with β phase. Both Pugh's modulus ratio and Poisson's ratio

exhibit ductile behavior of material as it indicated lower value from the critical value of ductile-brittle transition ratio for Ti material [30].

Table 3 Elastic constants (GPa) of α-Ti and β-Ti

Phase	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
α	187.1	87.8	70.6	203.5	45.9
	171.6 [a]	86.6 [a]	72.6 [a]	190.6 [a]	41.1 [a]
	162.4 [b]	92.0 [b]	69.0 [b]	180.7 [b]	46.7 [b]
β	82.6	115.9	-	-	39.8
	87.8 [a]	112.2 [a]	-	-	39.8 [a]
	90.2 [c]	113.1 [c]	-	-	40.8 [c]

[a] Reference [7]
[b] Reference (Exp) [7]
[c] Reference [21]

Table 4 Bulk modulus (B), shear modulus (G), Young's modulus (E), Pugh's modulus ratio ($^{B}/_{G}$) and Poisson's ratio (ν) for α-Ti and β-Ti

Phase	B (GPa)	G (GPa)	E (GPa)	$^{B}/_{G}$	ν	Ref
α	115.1	51.0	133.5	2.256	0.306	This work
	-	-	92.8	-	-	[31]
β	104.8	-16.7	-52.9	-6.275	0.577	This work
	108	-12.9	-40.4	-8.372	-	[26]
	105	-15	-46	-7.0	-	[21]
	104	-19	-60	-5.473	-	[7]

4. CONCLUSION

In this paper, first-principles investigations have been carried out on the structural, electronic and mechanical properties of α and β phase for Ti. The structural, electronic and mechanical properties are calculated using GGA-PBE after being optimized using three functional which are LDA-CAPZ, GGA-PBE and GGA-PBEsol correspond to the result of the lowest value and percentage different as compared from experimental and theoretical value. The structural properties such as lattice parameter and volume are listed on table given. The result indicated the reasonable agreement with other first principle calculation and other experimental data. The analysis of the band structures and densities of states (DOS) can be concluded that Ti exhibit stronger hybridization of covalent bond for α phase and metallic bond for β phase referring to the peak of DOS. As for mechanical properties, the results show the good agreement on the elastic constant with other previous data reported. The mechanical properties are estimated from the calculated elastic constants. Born criteria for α and β phase for Ti are satisfied, the β phase for Ti suggesting that it is mechanically stable for biomedical application due to the lower value of E. Pugh's ratio and Poisson ratio predict that Ti material for both phases should be characterized as ductile material.

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