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Physical Properties of New A Type Titanium Alloys TI $_{0.95}$X$_{0.05}$(X=Mo, Cr and Tc) for Implant Materials from Computational Study

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Abstract

In this work, using the density functional theory (DFT) implemented in the thermo-pw and CASTEP code, we have performed a computational study of the structural, electronic, elastic and mechanical properties of the α phase of $Ti_{0.95}X_{0.05}$binary alloys (*X* = Mo, Cr and Tc). The exchange and correlation functional in the generalized gradient approximation (GGA) proposed by Perdew-Burke-Ernzerhof were used. Due to it has been successfully applied in various doped materials; we have used a virtual crystal approximation (VCA) to replace the 0.05 of Ti atom with a X atom. Our findings for the electronic properties explain the nature of metallic structures. In addition, our results of the elastic properties prove the stable nature of the pure and doped compound. The mechanicals results, which include both bulk modulus, shear modulus and Poisson's ratio, which are in excellent agreement with the available theoretical and experimental results. Moreover, our results for Young's modulus were found to be 109, 114 and 85 GPa for both $Ti_{0.95}$-$_{0.05}$Mo, $Ti_{0.95}$-$_{0.05}$Cr and $Ti_{0.95}$-$_{0.05}$Tc respectively to be a competitive candidate for the α-Ti pure alloy.Furthermore, all alloys studied demonstrate the required ductile mechanical behaviour of biomaterials. Calculated phonon spectrum, as well as their density of states at equilibrium, of these compounds, in the hexagonal phase along the main directions of high symmetry of the first Brillouin zone, are presented and discussed. We hope that this study will help as a predictive guide for relevant experimental applications that can benefit from the properties of available biomaterials.

Keywords: Ti–0.05X, Elastic Properties, Young's Modulus, Stiffness, CASTEP

Introduction

The science of biomaterials is one of the most interesting fields, it allows to determine the relations that exist between the structures and the properties of materials. Due to the increasing life span of the population, biomaterials are used in the biomedical field as medical implants and dental alloys. Among these biomaterials are titanium alloys, which have a number of highly desirable properties due to their biocompatibility, low modulus of elasticity and corrosion resistance [1-5]. Titanium (Ti) was considered a rare metal but today it is one of the important metals in industry, this element was discovered at the end of the 18th century and its first industrial production began in 1948, so it is a very recent transition metal [6,7]. In recent years, the major challenge for scientists is to invent new materials that meet all the criteria for biomedical applications with a Young's modulus close to that of human cortical bone [8-10]. Biomaterials that have a higher modulus of elasticity than human bone cause a flexible gap between the implant and the bone, which leads to bone resorption after implantation [11]. To overcome these challenges, research is aimed at developing new implantable biomaterials. Titanium can be alloyed with a variety of elements to modify and improve its properties, the materials used for the manufacture of dental prostheses and medical implants are pure titanium (Cp-Ti) (α-type titanium alloy) and Ti-6Al-4V (α+β-type titanium alloy) [12]. These were chosen because of their properties of corrosion resistance, mechanical strength and biocompatibility. However, the elements of the Ti-6Al-4V alloys cause some cancer and Alzheimer's diseases due to the toxicity of Vanadium (V) and Aluminum (Al). Therefore, many efforts are currently devoted to the development of new binary, non-toxic, low modulus α-titanium alloys [13,14]. Through the use of niobium as an alloying element in novel Ti alloys for orthopedic and dental devices is widely recognized, due to their higher biocompatibility and osseointegration properties as compared to conventional Ti-6Al-4V alloys [15]. In addition, other research on Ti-Nb alloy showed that when the concentration of Nb was less than 15 wt%, the Ti alloys were composed of α martensites and when Nb exceeds 30 wt%, there are β phases in the alloy [16]. Another study exploring the influence of low Nb content (0-25%) on the mechanical and biological properties of Ti-xNb alloys (x=5,10,15,20 and 25%) with the use of commercially pure grade 2 titanium (cp-Ti) as a control, the results showed that all Ti-xNb alloys included Ti(α+β) alloy phases such that the β-phase increases with increasing amount of Nb in the alloy as well as reducing E (69-87 GPa) [17]. In addition to a study on the effect of Ta on the properties of titanium alloys, their results showed that the elastic modulus curve of Ti-Ta alloys varies with the concentration of Ta, when the contents is 30 and 70% the elastic modulus is the lowest 69 and 70 GPa respectively [18]. Calculations are made on the alloy $Ti_{0.98}X_{0.02}$ (X= Ag, Cd, Co, Cr, Cu, Fe, Mn, Mo, Nb, Ni, Pd, Rh, Ru, Tc and Zn) on the stability mechanism of β-titanium, the results showed that the addition of small amounts of X is beneficial to the thermodynamic stability of β-titanium, but the tetragonal shear moduli of $Ti_{0.98}X_{0.02}$ are negative which indicates that β-titanium doped with low concentrations of X is elastically unstable in the ground state [19]. The elastic constants are calculated by first principles methods, and the calculated values are different with the experimental values with an accuracy of 10%, the elastic constants such as a bulk modulus are reproduced well by these calculations, and it is expected as an effective method to show how to develop a new stable material with a controlled Young's modulus [20]. In this research, DFT simulations were performed to systematically study the α-titanium doping of the binary system $Ti_{0.95}X_{0.05}$with three metal elements X (X=Mo, Cr and Tc). We performed first principal calculations and calculation of their structural, electronic, elastic properties. The mechanical properties such bulk, shear and Young's modulus were estimated from the elastic constants calculated by the method introduced by Voigt-Reuss-Hill. From the calculated results, we discuss a guideline for the realization of new materials with low modulus of elasticity, due to the possibility of making them experimentally realized materials used in various applications, especially biomedical. The following part of the paper is organized in this way, a brief description on the calculation methodology which is given in section 2 or the results and discussion part of the work is presented in section 3 and at the end the conclusions of the study in section 4.

Theoretical Methodology

In order to study the binary α-titanium alloy $Ti_{0.95}X_{0.05}$, we cared out the first-principles calculations within the framework of density functional theory (DFT) [21]. The structural, electronic and elastic properties were calculated using the thermo-pw package implemented in the Quantum Espresso code which is an integrated suite of open-source computer codes for electronic structure calculations and material modeling at the nanoscale based on DFT, plane waves and pseudo potentials [22]. In our calculations, we applied the generalized gradient approximation (GGA) method of the Perdew-Burk-Ernzhof function (PBE) [23] for the correlation exchange energy [24]. We em-

ployed the pseudo-potential (Pseudodojo) [25], which produces highly transferable norm-conserving pseudo-potentials, and for Brillouin zone (BZ) sampling we applied Monkhorst-pack k-point [26]. Before beginning the calculations, we must select the correct values for two crucial convergence test parameters: the kinetic energy 'cut-off energy' Ecut, which determines the size of the wave in the base plane used in the calculation, and the number of k-points taken into account in the integration through the first Brillouin zone. The values determined for Ecut=720 eV and k-point (nkpt 12×12×10) that give the best possible convergence of the total energy and they are then used to calculate the total energy for various pressures. In terms of material doping, we employed a virtual crystal approximation (VCA) [27] to substitute a portion of Ti with a 5% concentration of three distinct materials (Cr, Mo, and Tc). In terms of calculation, the VCA approach is significantly easier and less expensive than the supercells method utilized in crystalline structures. It also enables the investigation of mixed type crystals while conserving the initial material's unit cell. In the solid-state calculations, the Kohn-Sham equation is solved by the iterative diagonalization scheme to speed up the convergence [28]. The elastic constants were calculated by the stress-strain approach implemented in the thermo-pw package. As a result, we were able to confirm our findings and compare them to existing experimental and theoretical data on the calculated properties of α-Titanium.

Results and Discussion

Structural Properties

Before we can calculate the different properties of doped α-Ti, we need to optimize and relax the structure in order to minimize energy and eliminate the Hellmann-Feynman forces acting on the atoms. In all there are three degrees of freedom, the parameters of the cell a and c, and the general atomic positions. The α-Ti and $Ti_{0.95}X_{0.05}$alloy has a hexagonal P6_3/mmc crystal structure (Figure 1).

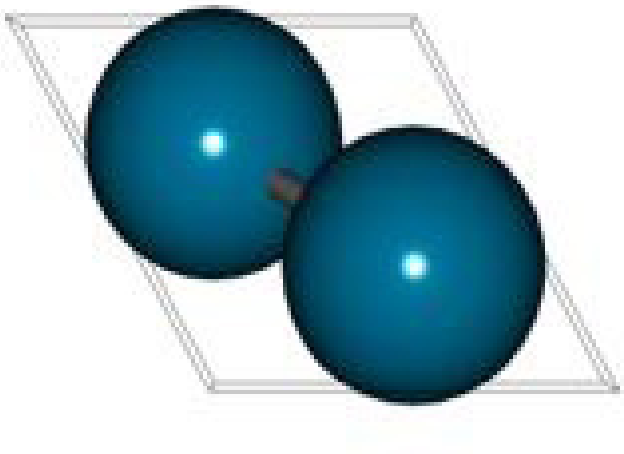

Figure 1: Crystal structures of alpha-Ti

In order to study its structural properties such as lattice constants (a, b, c) and bulk modulus $B_0$and their derivatives B', we fitted the variation of the total energy as a function of volume using the Murnaghan equation of state [29] which is given by the following expression:

$$E(V) = E_0 + \frac{B_0}{B'(B'-1)}\left[V\left(\frac{V_0}{V}\right)^{B'} - V_0\right] + \frac{B_0}{B'}(V - V_0) \quad (1)$$

With $V = V_0\left(1 + \frac{B'P}{B_0}\right)^{\frac{-1}{B'}}$

Where E_0, B_0, V_0 and $B'$are respectively: the total energy per unit cell, the modulus of compressibility and the volume at static equilibrium and the first derivative of (B_0) with respect to pressure. In addition, we used the BFGS algorithm [20] to optimize the structure with the THERMO-PW code The calculated parameters are given in Table 1 with previous theoretical and experimental data. The optimized lattice parameters are (a=2.933, c=4.651) for α -Ti, (a=2.922, c=4.67) for $Ti_{0.95}Mo_{0.05}$, (a=2.905, c=4.64) for $Ti_{0.95}Cr_{0.05}$ and (a=2.909, c=4.637) for $Ti_{0.95}Tc_{0.05}$.

From this table, it is evident that the value of the calculated lattice constants for the α -Ti phase is in excellent agree-

Table 1: Calculated lattice parameters (a and c) (Å), mass modulus (GPa) and its derivative and energy (Ry) compared with available theoretical and experimental data

Materials	a (Å)	c (Å)	c/a	B(GPa)	B'	E(Ry)
α -Ti						
present.	2.933	4.651	1.586	107.7	3.921	-237.407
Exp.	2.950 [7]	4.683 [7]	1.583[30]	110.02[30]	3.59[30]	
Ref.	2.93 [31]	4.65 [31]				
Others.	2.946 [20]	4.666 [20]				
	2.95 [32]	4.683 [32]				
	2.957 [33]	4.685[33]	1.585[33]			
$Ti_{0.95}Mo_{0.05}$	2.922	4.67	1.597	118.9	3.614	-232.54
$Ti_{0.95}Cr_{0.05}$	2.905	4.64	1.592	118.3	3.738	-235.348
$Ti_{0.95}Tc_{0.05}$	2.909	4.637	1.590	115.8	4.067	-241.67

ment with the experimental values [30- 32] and other theoretical values [7, 20 and 33]. The calculated total energies for compounds (α -Ti and $Ti_{0.95}X_{0.05}$) are plotted as a function of volume in figure 2 (a, b, c and d).Concerning the bulk modulus and its derivative, we find a good agreement between our calculated values and the available theoretical values [31] with a deviation of 2.6% and 1.8% respectively. For doped compounds, our calculation is predictive, as to our knowledge there are no previous calculations for the various properties.

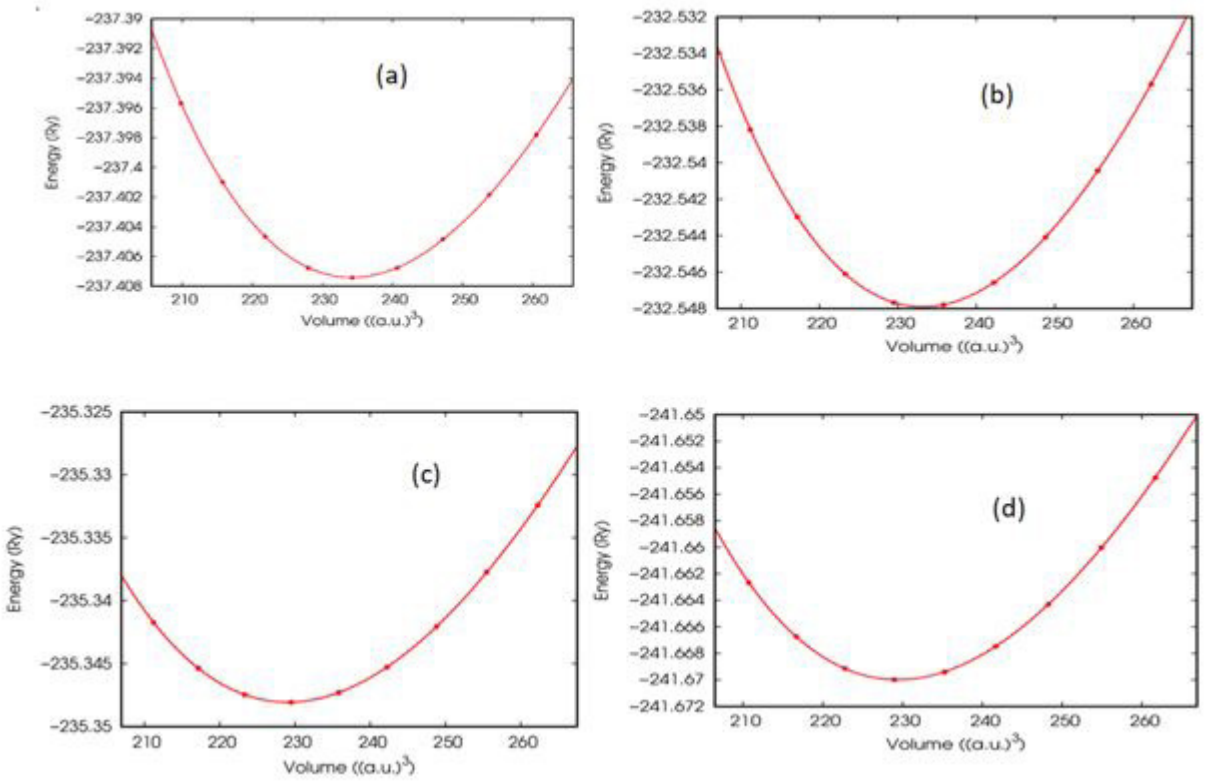

Figure 2: Calculated total energy as a function of unit cell volume for (a) alpha-Ti (b)$Ti_{0.95}Mo_{0.05}$(c) $Ti_{0.95}Cr_{0.05}$, and (d) $Ti_{0.95}Tc_{0.05}$

Electronic Properties

The electronic structure which includes the electron density, the structure of the energy bands and the density of total and partial electronic states were calculated by the FT-PW method. The main goal is to know the nature of the bonds between atoms. The electronic band structures calculated with the (GGA-PBE) approximation of the compounds α-Ti, $Ti_{0,95}Mo_{0,05}$, $Ti_{0.95}Cr_{0.05}$ and $Ti_{0.95}Tc_{0.05}$ are presented in Figure 3 (a, b, c and d) respectively.The computed band structure of alpha Ti and its doped compounds, as shown in Fig. 3, indicates the metallic property respect to the position of valence band maxima (VBM) at the gamma point and conduction band minima (CBM) at the X high symmetry, with 0 eV. Our GGA-PBE-calculated values are consistent with other theoretical and experimental results.

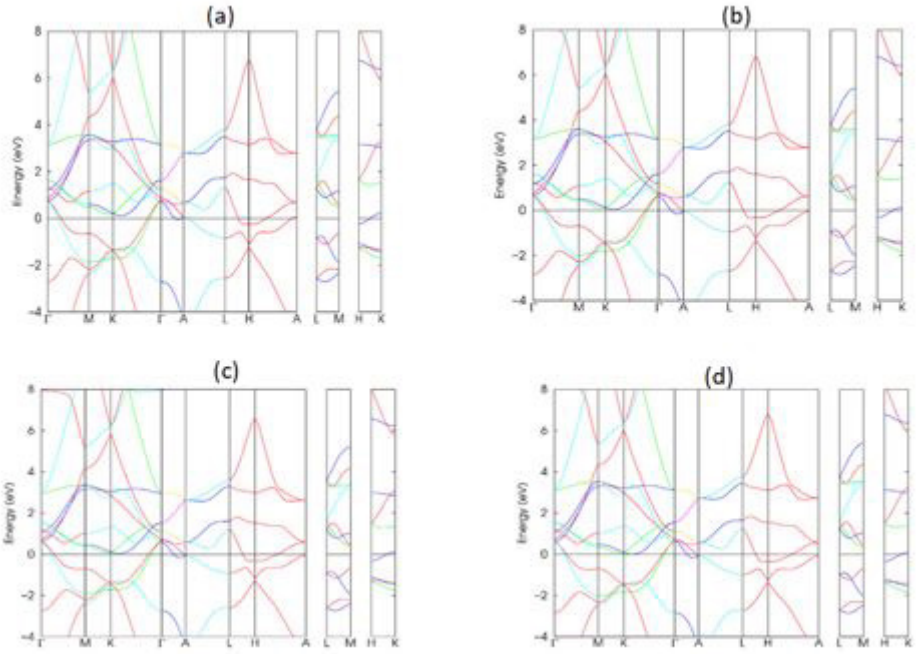

Figure 3: Calculated band structure for (a) alpha-Ti, (b)$Ti_{0.95}Mo_{0.05}$(c) $Ti_{0.95}Cr_{0.05}$, and (d) $Ti_{0.95}Tc_{0.05}$

Further, to better understand the electronic structure of these compounds, we have calculated total (TDOS) and partial (PDOS) density of states for all the investigated compounds and represented the same in figure 4 (a, b, c and d) within the energy interval from (– 10 to 25) eV.The density of states correlates with the chemical bond between Ti and X atoms and can provide insight into the range of solubility between $Ti_{0.95}Mo_{0.05}$ and $Ti_{0.95}Cr_{0.05}$ and $Ti_{0.95}Tc_{0.05}$ compounds. Figure 3, for all the compositions studied with the PW-VCA code (intentionally we have hidden the contributions of electrons from the Ti and X layer), highlights several characteristics:(i) the energy region of -12 to -2 eV is characterized by the strong hybridization of the d-type electrons of metals with the d-type electrons of Ti, which is at the origin of the covalent bond of these materials [11]. These orbitals move towards high energies with increasing atomic fraction y of Ti-X. They are characterized by two peaks, which are initially found at -5 and -7 eV for $Ti_{0,95}Tc_{0,05}$and gradually shift to reach -5 and -6 eV for $Ti_{0.95}Cr_{0.05}$ and -5 and -7 for $Ti_{0.95}Mo_{0.05}$. (ii) the energy region of -5 to 5.5eV shows the energy states represented mainly by the d-type orbitals of (Ti_yX_{1-y}) and a small contribution of the p-type orbits of Cr, Tc, and Mo. This region changes significantly by increasing the concentration y of Ti_yX_{1-y}.

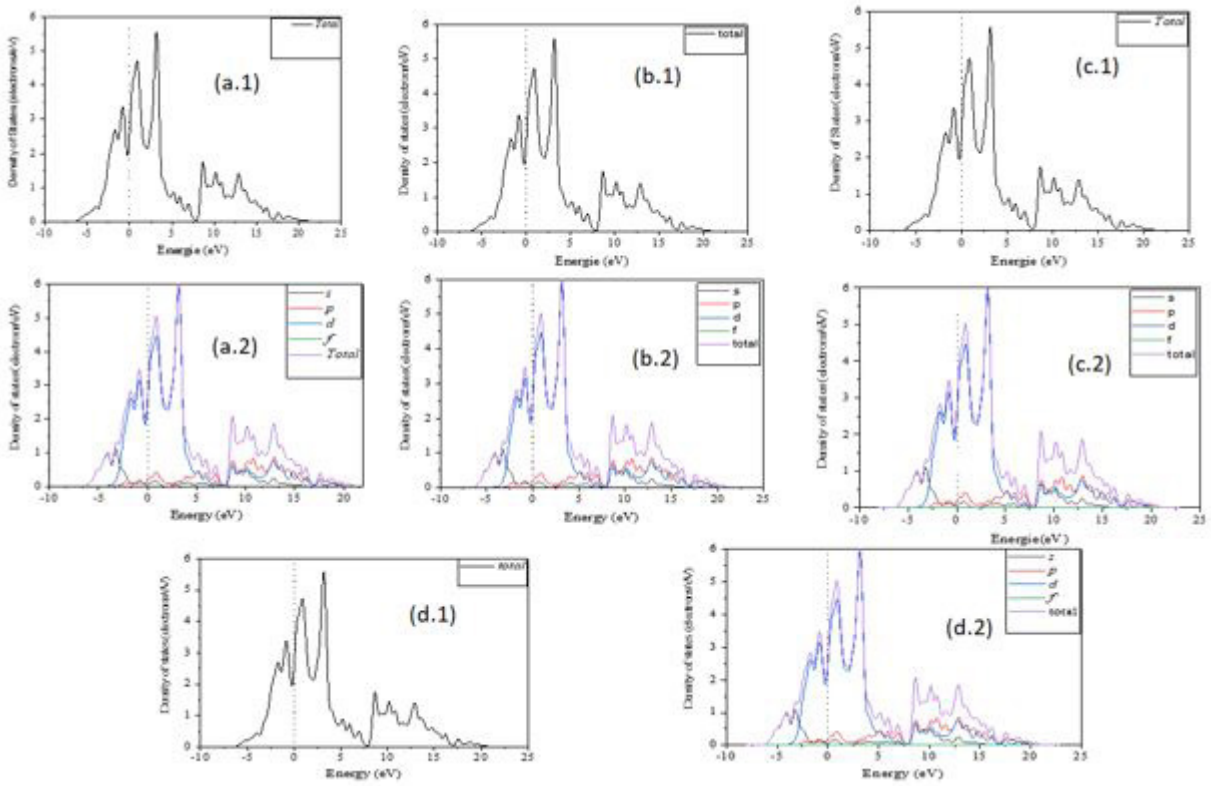

Figure 4. Calculated density of state total and partial for (a) alpha-Ti, (b)$Ti_{0.95}Mo_{0.05}$ (c) $Ti_{0.95}Cr_{0.05}$, and (d) $Ti_{0.95}Tc_{0.05}$

Elastic and Mechanical Properties

The elastic properties of materials are very important because they provide information on the fundamental properties of the solid state [34] such as mechanical stability, strength and ductility of the material. It is thus a question of determining the elastic constants Cij which connect the constraint to the deformation and to extract the mechanical and physical properties of materials. The elastic constants can make us fully understand the stability of α-titanium doping with a small amount of the transition metal X (Mo, Cr, Tc). In this section, we estimate the elastic constants of Ti-X binary systems to study their mechanical stabilities in the ground state. The Voigt-Reuss-Hill (VRH) technique [35] is a valid scheme for the elastic constants of polycrystalline materials, despite the fact that the elastic constants are normally obtained from total energy and represent the elastic characteristics of a single crystal. During the calculations, we used the values of the Voigt-Reuss-Hill approximation to acquire the right values of the elastic constants. For hexagonal crystals, five independent elastic constants namely C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. The elastic constants calculated for the α-Ti and $Ti_{0,95}X_{0,05}$ alloys are presented in the table 2 with the former theoretical studies of refs. [20, 30, 36, 37] and experimental data of refs [38, 39].Furthermore, these constants (C_{11}, C_{12}, C_{13}, C_{33} and C_{44}) must meet the traditional Born stability requirements for hexagonal crystals [40], which are written as follows:

$C_{44}>0$, $C_{11}>C_{12}$ and $(C_{11}+2C_{12})\,C_{33}-2C_{13}^{2}>0$ (2)

The results of table 2 shows that the elastic constants of α-Ti and Ti-X alloys comply with the stability requirements described earlier. As a result, the acquired values for the current calculated elastic stiffness constants and the existence of mechanical stability character of theinvestigated alloys are within the range of previously reported experimental work on α-Ti alloys [38,39], as shown in Table 2.

Table 2: A comparison for the elastic stiffness constants of α-Ti and $Ti_{0.95}X_{0.05}$alloys

Materials	C_{11}**(GPa)**	C_{12}**(GPa)**	C_{13}**(GPa)**	C_{33}**(GPa)**	C_{44}**(GPa)**
α -Ti (Present)	193.2	57.3	71.4	189.6	46.3
Others	175 [30]	89 [30]	84 [30]	192 [30]	45 [30]
	171.6 [20]	86.8 [20]	72.6 [20]	190.6 [20]	41.1 [20]
	172.2 [36]	70.6 [36]	76.3 [36]	179.0 [36]	29.4 [36]
	174 [37]	95 [37]	72 [37]	188 [37]	58 [37]
	176.1[38]	86.9[38]	68.3[38]	190.5[38]	50.8 [38]
	162.4[39]	92.0[39]	69.0[39]	180.7[39]	46.7[39]
$Ti_{0.95}Mo_{0.05}$	187.7	83.1	79.7	211.5	32.7
$Ti_{0.95}Cr_{0.05}$	186.8	82.3	79.6	209.4	31.8
$Ti_{0.95}Tc_{0.05}$	168.1	96.09	83.3	187.1	24.4

These constants are used to calculate other mechanical properties such as the Bulk modulus (B), Shear modulus (G), the Young modulus (E) and the Poisson's ration (V) which are presented in Table 3. From the values of the calculated elastic constants, we estimated the elastic wave velocities of Ti-X along the principal directions ([100], [110] and [111]) by solving the Christoffel equation [16].

Table 3: The mechanical properties of α-Ti and $Ti_{0.95}X_{0.05}$alloy

Materials	**B(GPa)**	**G(GPa)**	**E(GPa)**	**B/G**	**v**
This work	107.7	55.4	141.9	1.94	0.280
Others	107.7 [36]	40.5 [36]	105 [7]	2.65 [36]	0.332 [36]
			108.2 [36]		
	107.3[43]	43.4 [43]	114.6[43]	2.47[43]	0.363[43]
$Ti_{0.95}Mo_{0.05}$	118.9	46.5	116.01	2.55	0.337
$Ti_{0.95}Cr_{0.05}$	118.3	42.5	114.09	2.78	0.339
$Ti_{0.95}Tc_{0.05}$	115.8	31.7	87.3	3.65	0.369

The calculated longitudinal wave (V_G) and the two elastic wave strain rates ((V_P), and V_B) in the directions [100], [110] and [111] at zero pressure for $Ti_{0.95}Mo_{0.05}$, $Ti_{0.95}Cr_{0.05}$ and $Ti_{0.95}Tc_{0.05}$are listed in Table 4. From these values, we can calculate Debye temperature to be 392.13, 396.77 and 336.92 K 392.13, 396.77 and 336.92 K, respectively. In addition, Young's modulus, bulk modulus, and shear modulus all refer to a material's ability to resist uniaxial tension, volume transformation, and plastic deformation, respectively [41]. The Young modulus (E) and the Poisson's ratio (v) are then calculated from B and G as follows:

$$E = \frac{9BG}{3B+G} \text{and } v = \frac{3B-2G}{2(3B+G)} \quad (3)$$

Table 4. Other mechanical properties of α-Ti and $Ti_{0.95}X_{0.05}$alloy

Materials	V_P(m/s)	V_B(m/s)	V_G(m/s)	Ť de debye (K̊)
α -Ti	6323.38	4857.96	3505.56	448.30
$Ti_{0.95}Mo_{0.05}$	6087.18	4964.72	3050.23	392.13
$Ti_{0.95}Cr_{0.05}$	6142.61	5017.79	3068.39	396.77
$Ti_{0.95}Tc_{0.05}$	5701.60	4852.63	2592.32	336.32

The B/G ratio shows the ductility of the materials. The ductile/brittle behavior of the materials is significant in terms of applications. If the value of this ratio (B/G) is higher than 1.75, it indicates a favorable ductility [42]. The results obtained indicate that the B/G values for the studied alloys are higher than the critical value (1.75), which confirms the ductility of these alloys. To advance our research, we estimated the Young's modulus (E), Bulk modulus (B), shear modulus (G) and Poisson's ratio (^{V}) of pure α-Ti alloy and compared it to the most current experimental data of ref [43]. As indicated in the table 3, the derived values are in good agreement with the experimental values in ref [43]. We have also calculated these elastic constants (E, B, G and v) for Ti-X alloys, we obtained the values of a Young's modulus equal to 116.1 GPa,114.9 GPa and 87.3 GPa for $Ti_{0.95}Mo_{0.05}$, $Ti_{0.95}Cr_{0.05}$ and $Ti_{0.95}Tc_{0.05}$ respectively. From this perspective, we can conclude that these alloys present good mechanical behaviors. However, a low modulus of elasticity (E) is one of the most important features of a good biomaterial. From the results obtained on Ti-X alloy, it can be seen that the addition of small amounts of transition metals Mo, Cr and Tc plays a very important role in reducing the value of Young's modulus, which makes these alloys capable of being applied in biomaterials.

Phonon Dispersion

The PHONOPY package [44] was used to evaluate the phonon spectra, by adopting a 2×2×2 supercell with atomic displacement amplitude of 0.02 bohr, in order to calculate the properties of the phonons, using the functional density disturbance theory (DFPT) [45], with a linear response method, can be obtained using a harmonic approximation, is usually called the dynamic matrix, which determines the equation of motion for such a wave vector q in reciprocal space [46]:

$$D_{ij}(\mu\upsilon,q) = \frac{1}{\sqrt{m_\mu m_\upsilon}} N_0^{-1} \sum_{MN} \Phi_{ij}(M_\mu, N_\upsilon) e^{iq.[R(N_\upsilon)-R(M_\mu)]} \quad (4)$$

Where m mass,N_0number of atoms, R position vector, (M, N) index of lattice points, (μ,υ) the index of atom in unit cell and $\Phi_{ij}(M,N)$ the force constant matrices can be calculated from finite displacement calculation:

$$\Phi_{ij}(M_\mu, N_\upsilon) = \frac{\partial^2 V}{\partial u_i(M_\mu)\partial u_j(N_\upsilon)} \simeq -\frac{F_i(M_\mu)}{U_j(N_\upsilon)} \quad (5)$$

Where $U_j(N_\upsilon)$displacement of atom N_υ and $F_i(M_\mu)$ force on atomM_μ.

Calculated phonon spectrum, as well as their density of states at equilibrium, of the compounds α-Ti and $Ti_{0.95}X_{0.05}$ (X = Mo, Cr and Tc), in the hexagonal phase along the main directions of high symmetry of the first Brillouin zone, are presented in Figure 5 (a, b, c and d). Considering that the tetragonal primitive cell of our compounds contains two atoms, their full spectrum of phonons consists of 6 normal modes of vibration including 3 acoustic branches and 3 optical branches. The acoustic phonon seems to have lower frequencies and moves in the unit cell in almost the same phase. It does have 2 transverse acoustic modes and 1 longitudinal acoustic mode (LA) with a significant phonon phase velocity (TA). As a result, acoustic phonons have a significant impact on thermal conductivity, making a bigger phonon phase velocity and a lengthy phonon relaxation time-critical. The optical phonon seems to have a higher frequency than the acoustic phonon, and the vibration directions of one atom and its neighboring atom are in opposite directions. As a result, compared to acoustic phonon modes, it has a smaller phonon band velocity and a wider energy spectrum. It combines with photons in particular. The dipole moment is caused by out-of-plane motion. As a result, optical phonon causes the structure's IR and Raman active characteristics. It is clear that the crystal structure considered is dynamically stable over the entire Brillouin zone for the α-Ti, However, there exist imaginary modes (negative frequencies) at the Γ point for the compounds $Ti_{0.95}X_{0.05}$ (X = Mo, Cr and Tc), whose phonon dispersion curves are shown below zero frequency, indicating unstable modes. This unstablemode

of vibration at the Γ point governs the nature of the phase transition. According to Figures 5a, b, c and d, the values of the optical frequencies are of the order of 120 cm^{-1}, 90 cm^{-1} at the point Γ for α-Ti and Ti0.95 X0.05 (X = Mo, Cr and Tc) respectively, as we can observe no splitting is observed between the longitudinal optical mode (LO) and the transverse optical mode (TO) at point Γ as well as at point Afor our compounds.In addition, the values of the maximum frequency of the optical modes LO = 270 cm^{-1}, located at point H for α-Ti and LO = 230 cm^{-1} at point K for Ti0.95 X0.05 (X = Mo, Cr and Tc). We compared the phonon dispersion results to the experimental results of inelastic neutron scattering measurements [47]. Other theoretical predictions in ref [48, 49] appear to be more accurate. We note an overall agreement between our results with other theorical and experimental results.

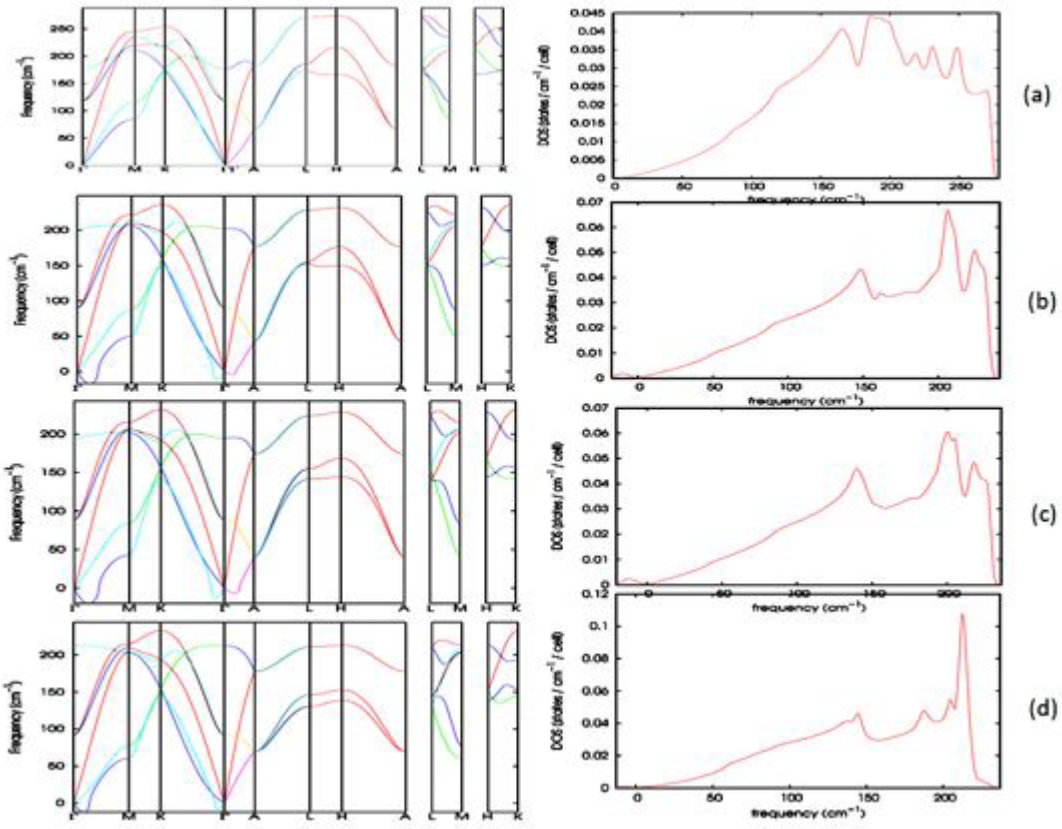

Figure 5: Phonons dispersion results and phonon DOS for (a) alpha-Ti, (b)$Ti_{0.95}Mo_{0.05}$(c) $Ti_{0.95}Cr_{0.05}$, and (d) $Ti_{0.95}Tc_{0.05}$

Conclusion

In this paper, the first principles study is used to calculate the structural, electronic, elastic, mechanical and, phonon dispersion of the compounds $Ti_{0.95}Mo_{0.05}$, $Ti_{0.95}Cr_{0.05}$, and $Ti_{0.95}Tc_{0.05}$. Elastic constants and mechanical stability conditions are fulfilled for all deformed compounds. The properties of the phonon also prove the possibility of thermodynamic stability of the compounds. Our results for a pure compound for most properties are in good agreement with the previously available results. For $Ti_{0.95}Mo_{0.05}$, $Ti_{0.95}Cr_{0.05}$, and $Ti_{0.95}Tc_{0.05}$, we found Young's modulus values of 116.1 GPa, 114.9 GPa, and 87.3 GPa, respectively. From this standpoint, we deduce that certain alloys have good mechanical properties. However, one of the most significant features of a good biomaterial is a low modulus of elasticity (E). The mechanical parameters obtained can help biomedical applications, especially dental implants, because they have a very low modulus of elasticity.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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