# First-principles predictions of structural, mechanical and electronic properties of βTiNb under high pressure

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## A R T I C L E   I N F O

## A B S T R A C T

Structural, mechanical and electronic properties of βTiNb alloy under high pressure have been investigated based on the density functional theory (DFT). The dependences of dimensionless volume ratio, elastic constants, bulk modulus, Young's modulus, shear modulus, ductile/brittle, anisotropy and Poisson's ratio on applied pressure are all calculated successfully. The results reveal that βTiNb alloy is mechanically stable under pressure below 23.45 GPa, and the pressure-induced phase transformation could occur beyond this critical value. Meanwhile, the applied pressure can effectively promote the mechanical properties of βTiNb alloy, including the resistances to volume change, elastic deformation and shear deformation, as well as the material ductility and metallicity. Furthermore, the calculated electronic structures testify that βTiNb alloy performs the metallicity and the higher pressure reduces the structural stability of unit cell.

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## 1. Introduction

As is known, Titanium alloys have been widely applied to the various industries especially to the biomedical engineering due to its exceptional properties with low density, high strength, excellent wear, corrosion resistance, and superior biocompatibility [1–3]. Currently, Ti-6Al-4V alloy is a major biomedical materials in biomedical applications of Ti alloys, while the elastic modulus of this alloy approximately reach up to 110 GPa with respect to human bone modulus of 30 GPa, thus, the modulus difference between metallic biomaterial implant and human bone is bound to result in 'stress shielding effect', and the toxic elements like Al and V would also be resorbed by human bone cell during long periods of use, which causes serious damage to human health and restricts the biomedical applications of Ti alloys [3–6]. For other βTi alloys doping nontoxic elements (Nb, Ta, Zr, Fe, Si and Mo etc.), however, the synthetic βTi alloys have become the main research hotspot in the biomedical applications, which depended on their many excellent properties including nontoxicity, good biocompatible, corrosion resistance, low elastic modulus, superelasticity and shape memory effect in these alloys [7–13].

Over the years, βTiNb alloy has attracted extensive attention as a new biomedical material, and plenty of researches have been conducted through calculating the electronic structure of alloys. Ikehata et al. [14] studied the polycrystalline Young's modulus of $Ti_{1-x}X_x$ (X = V, Nb, Ta, Mo and W) and $Zr_{1-x}X_x$ (X = Nb and Mo) binary alloys by utilizing first-principles

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calculations, indicating the Young's modulus of these binary alloys had the minimum values in the vicinity of $x = 0.25$ and their values were considerably affected by the valence electron number of alloys. Raabe et al. [15] put forward a new strategy for the theory-guided bottom up design of β-Ti alloys for biomedical applications using a quantum mechanical approach, and obtained nice results of ab initio simulations with respect to experiments for Ti−Nb and Ti−Mo binary alloys. Lazar et al. [16] presented a first-principles investigation of the structures and the dynamical stability of the austenite and martensite phases of $Ti_3Nb$ binary alloys, and calculated the phase-transition temperatures for $\beta \rightarrow \alpha''$ and $\beta \rightarrow \omega$ transitions. Meanwhile, Pathak et al. [17] investigated the structure of orthorhombic martensitic phase ($\alpha''$) using first-principles DFT for Ti−xNb ($x = 0 \sim 0.25$) binary alloys, and the results denoted that the higher Nb concentrations, the more unstable the $\alpha''$ phase in the alloy. Karre et al. [18] discussed the structures and Young's modulus of binary Ti−Nb and ternary Ti−Nb−Zr alloy systems using first-principles DFT, and proved that the additions of Nb in Ti and Zr in Ti−Nb increased the stability of the $\beta$-phase. Similarly, Zhang et al. [19] recently probed the phase stability and elastic property of binary Ti-xTM (TM = V, Cr, Nb, Mo) and ternary Ti-15TM-yAl alloys by using a first-principles method, and the similar results showed that the transition metal (TM) elements increased the elastic stability of the $\beta$ phase but decreased that of the $\alpha$ phase.

Based on the previous researches, although many superior properties of βTiNb alloy have been testified by lots of experiments and theories, the relevant investigations of the structural, mechanical and electronic properties for this alloy under high pressure have not been reported yet. In the present paper, however, we conduct a systematic study on the structural, mechanical and electronic properties of βTiNb alloy using the DFT, and calculate the relative parameters under high pressure in detail, including dimensionless volume ratio, elastic constants, bulk modulus, Young's modulus, shear modulus, ductile/ brittle, anisotropy and Poisson's ratio, as well as electronic structures. Furthermore, the computed results keep in good accordance with the experimental data and theoretical results, which can have a significant impact on designing and applying βTiNb alloy in the biomedical engineering or other industries.

## 2. Methodology

In the process of investigating the electronic structure, all calculations of electronic structure are accomplished by the Cambridge Serial Total Energy Package (CASTEP) Program [20–22], which is developed based on the plane-wave pseudopotential DFT [23,24]. The generalized gradient approximation (GGA) of Perdew−Burke−Eruzerhof (PBE) is chosen to describe the concrete formalism of exchange-correlation functional [25]. The electronic states of Ti ($3d^24s^2$) and Nb ($4d^45s^1$) are regarded as valence electrons, and the ion-electron interactions are determined by Vanderbilt-type ultrasoft pseudopotentials (USPP) [26]. Through the strict convergence test, the cutoff energy of the plane-wave basis set is defined as 400 eV and the $18 \times 18 \times 18$ Monkhorst−Pack $k$-point grid [27] is set for the Brillouin-zone sampling in all electronic calculations of βTiNb, which gets good convergent results of the total energy and lattice constants with respect to other parameters. The crystal structure of βTiNb belongs to the *Im-3m* space group with cubic crystal structure (see Fig. 1), and the structural geometry optimization has been implemented by applying the BFGS algorithm [28] for different equivalent hydrostatic pressures between −10 GPa and 30 GPa. Here, the total energies for self-consistent calculation are converged as $1.0 \times 10^{-5}$ eV/atom and the maximum force acting on the atom is under $3.0 \times 10^{-2}$ eV/Å. Meanwhile, the maximum stress for the convergence tolerance is controlled within the scope of $5.0 \times 10^{-2}$ GPa and the value of the maximum displacement between cycles is under $1.0 \times 10^{-3}$ Å. The self-consistent field tolerance is set as a rather small value with $1.0 \times 10^{-6}$ eV/atom for the purpose of obtaining a more precise solution of ground-state wave functions. The electronic minimization is carried out by using the density mixing method in the self-consistent calculation. These parameters are applied in all electronic structure calculations of this work.

## 3. Results and discussions

### 3.1. Structure properties and stability

For confirming the most stable crystal structure of βTiNb, the data of the total energy versus the primitive cell volume $V$ is computed and fitted to the Birch−Murnaghan equation of state (EOS) [29], where the volume $V$ changes from $0.9V_0$ to $1.1V_0$.
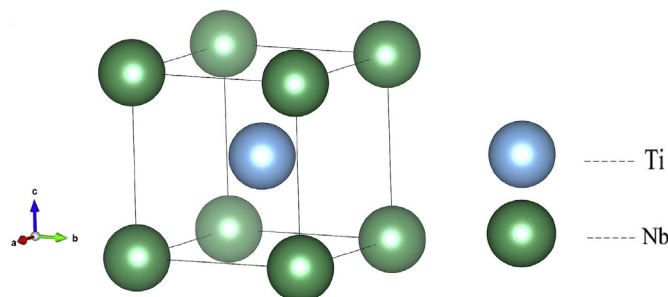


**Fig. 1.** The cubic crystal structure of βTiNb alloy with the lattice constant ($a_0 = 3.287$ Å).