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First-Principles Calculations and Thermo-Calc Study of the Elastic and Thermodynamic Properties of Ti-Nb-ZR-Ta Alloy for Biomedical Applications

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Abstract : High alloyed beta (β) phase-stabilized titanium alloys are known to have a low elastic modulus comparable to that of the human bone (≈30 GPa). The β phase in titanium alloys exhibits an elastic Young's modulus of about 60-80 GPa, which is nearly half that of α-phase (100-120 GPa). In this work, a theoretical investigation of structural stability and thermodynamic stability, as well as the elastic properties of a quaternary Ti-Nb-Ta-Zr alloy, will be presented with an attempt to lower Young's modulus. The structural stability and elastic properties of the alloy were evaluated using the first-principles approach within the density functional theory (DFT) framework implemented in the CASTEP code. The elastic properties include bulk modulus B, elastic Young's modulus E, shear modulus c′ and Poisson's ratio v. Thermodynamic stability, as well as the fraction of β phase in the alloy, was evaluated using the Thermo-Calc software package. Thermodynamic properties such as Gibbs free energy (Δ?º?) and enthalpy of formation will be presented in addition to phase proportion diagrams. The stoichiometric compositions of the alloy is Ti-Nbx-Ta5-Zr5 (x = 5, 10, 20, 30, 40 at.%). An optimum alloy composition must satisfy the Born stability criteria and also possess low elastic Young's modulus. In addition, the alloy must be thermodynamically stable, i.e., Δ?º? < 0.

Keywords : elastic modulus, phase proportion diagram, thermo-calc, titanium alloys
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