UNIVERSITI TEKNOLOGI MARA

FIRST PRINCIPLES STUDY ON STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF TITANIUM-BASED ALLOYS FOR BIOIMPLANT APPLICATIONS

NUR AISYAH BINTIAB MALIK MARWAN

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ABSTRACT

Titanium (Ti) alloys, particularly known as vanadium-free titanium alloys, have become the focus of research due to their outstanding and potential properties in biomedical applications. Due to the less compatibility of a-type Ti alloys, P-type Ti alloys have been marked as valuable materials in the current research due to their lower modulus, and they can satisfy most of other requirements for an ideal metallic biomaterial. Hence, the aim of this work is to focus on developing a novel or new material of P-type Ti alloys as an alternative material for orthopaedic human bone. Furthermore, the study of concentration dependence for binary and ternary Ti alloys is required to alter certain properties to reach a good requirement value. This present systematic study has been completed by observing the structural, electronic and mechanical properties of a and P phases of Ti, binary Ti and ternary Ti alloys systems. The calculation was performed using first-principles calculations based on Density Functional Theory (DFT). The geometrical optimisation of Ti alloys shows that GGA-PBE functional has a close agreement in lattice parameters for a and P phases. The phase stability of pure Ti gives a stable structure in the a phase due to the lower energy obtained. The higher peak in DOS for both a and P phases shows that the titanium materials undergo metallic behaviour. The metallic bonding is expected to reduce the elastic performance of titanium. The analysis results of the mechanical properties of both Ti phases show that the P phase has a lower modulus compared to the a phase. However, the P phase Ti is mechanically unstable due to the negative value of Young's modulus (-52.9 GPa). Hence, the alloys are required to stabilise the unstable structure of Ti. The study continues with the investigation of binary Ti_{i_n}-X_n alloys and ternary Ti alloys system by usingthe P phase. The transition metals (TMs) of niobium (Nb), molybdenum (Mo), manganese (Mn) and rhenium (Re) were used as alloy products to enhance the properties performance of Ti alloys. The calculations are systematically studied at various concentrations to attain ideal and optimum results for Young's modulus that can reach human bone's elasticity (30 GPa). This work predicts that the ideal binary Ti alloys lie at range n = 0.250 (at %) with the elastic of 14.1 GPa. The ternary Ti alloys showing the optimum value of Young's modulus were obtained at Tio.5-Mno.25-Nbo.25 by 32 GPa, Tio.563-Mno.25-Moo.i87 by 35.85 GPa and Ti_{0}.69-Mn_{0}.25-Reo.o6 by 36.21 GPa. Hence, the modification of Ti by adding an alloy has lowered the modulus and can improve the mechanical properties of Ti for bioimplant applications. Therefore, the calculation of these novel alloys could provide new findings to assist experimentalists in manufacturing the low modulus value of Ti alloys that closely meet the biomedical demand and hence extensively contribute to bio-friendly technology.

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