UNIVERSITI TEKNOLOGI MARA

SYNTHESISE AND CHARACTERISATION OF PULVERIZED TITANIUM NIOBIUM ALLOY FOR POTENTIAL BIOMEDICAL APPLICATION

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ABSTRACT

Biomaterials is a rising field of research that focuses on introducing bioinert materials as a substitution or an aid in the human bone healing process. Ongoing investigation in finding suitable materials for implant application is endless. Among the types of biomaterials, metal-based were favoured due to their excellent strength and being biocompatible with human body fluids. Metal-based materials such as stainless steel, Ti, and cobalt chrome have been used extensively in biomedical applications owing to their unique properties, such as high strength and corrosion resistance. Some do not produce toxic substances that may be harmful to the human body. In recent advancements, Ti alloys have become the primary candidate for bone replacement due to their ability to closely mimic the human bone requirement. Ti6Al4V has been used considerably in biomedical applications, but the toxicity of vanadium is always a serious concern. One of the alloying elements of Ti that have been researched extensively is Nb. Nb has been introduced as a non-toxic element that creates the beta phases and potentially to lower Young's modulus of Ti metal. However, the beta phase in Ti alloys is metastable, which strongly influence the mechanical properties. Even though it is an excellent strategy to reduce Young's modulus, the fundamental question on these metastable phases is unknown theoretically and experimentally. Hence the objectives of this study are to simulate the concentration Nb elements for Ti-Nb alloys, synthesise and prepare the Ti-Nb alloys, determine Young's modulus of Ti-Nb alloys, and characterise the Ti-Nb alloys of Y-shaped bio-plate. The methods of achieving the objectives are to use the first principle study with density functional theory (DFT) via CASTEP© computer code with pseudopotential calculations, and to synthesize all Ti-Nb alloys via conventional powder metallurgy method with elemental powder metals as the primary materials. The process consisted of mixing, compacting, and sintering, and preparing alloys into bars for the compressive test to determine Young's modulus of alloys. Finally, the preparing the alloys into Y-shaped plates. The results show that the optimisation of the Ti-Nb crystal structure using DFT calculation provided an atomic bonding analysis and predicted Young's modulus of Ti-Nb alloys. Alloying with Nb showed random and disordered atomic arrangements and a strong *d-d* hybridization, which provided phase stability to the Ti alloys. The Young's modulus at the fully beta phase was approximately 82 GPa. The as-sintered sample showed reducing volume shrinkage from 28% to 17%, an average relative density of 90.7% relative density, and 9.3% mean porosity. At 40 wt% Nb, the alpha phase dissipated, and only the beta phase existed. The impurities level for all as-sintered samples was sufficiently low due to mixing without the PCA or binders, although the initial powders exhibit slightly higher oxygen (O) levels. The hardness value obtained for 40 wt% Nb in this research study is lower than other literature but still higher than bone hardness with HV=143.6±19. The value obtained from the compression test is yield strength, $\sigma_{0.2}$=413.99 MPa, Young's modulus, E=18.09±1.39 GPa and compressive strain, ε=25.23±5.17% for 40 wt% Nb composition. Preparing the exact composition of Nb (40 wt%) into a Y-shaped fracture plate revealed that the major fraction beta phase was observed with a slightly higher hardness value HV=195.57±11.87. The hardness value may be due to the higher compaction pressure during the powder pressing process. This finding is beneficial for the potential alloy as bone replacement with a very stable beta phase of Ti-Nb alloys.

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