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Microstructural and mechanical properties of Ti-Mo alloys designed by the cluster plus glue atom model for biomedical application

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Abstract

β-type titanium alloys are acquiring research interest in orthopaedic applications because of their exceptional properties such as moderate strength, good biocompatibility and corrosion resistance, high ductility and low elastic modulus. The study aims at designing a series of binary Ti-Mo alloys (Ti-8.71 Mo, Ti-10.02 Mo, Ti-11.78 Mo and Ti-15.05 Mo (wt%)) using the cluster plus glue atom model to design the compositions. The prediction methods such as the molybdenum equivalence, the average electron ratio and the d-electron methods were used to predict the stability of the β phase. Microstructural evolution and phases of the designed alloys were characterized using the optical microscopy (OM), scanning electron microscopy (SEM), electron backscatter diffractometry (EBSD) and X-ray diffractometry (XRD), while the microhardness and tensile properties were measured using the Vickers hardness tester and tensile testing machine. The microstructure of the cast Ti-Mo alloys comprised primarily the β phase and secondary orthorhombic martensitic α″ and athermal omega (ω) phases. Their elastic moduli (96.8–70.5 GPa) decreased with the amount of Ti in the glue side and were found to be lower than the commercially available 316 L stainless steel, Co-Cr and Ti6Al4V alloys. The microhardness values of the as-cast Ti-Mo alloys decreased as the amount of Ti in the glue side decreased in the cluster formula. The tensile strength of the as-cast alloys ranges from 796.76 to 593.48 MPa with Ti-8.71 wt% Mo alloy showing the highest tensile strength owing to the amount of Ti in the glue side. The yield strength of all the designed alloys decreased as the amount of Ti atoms placed in the glue side decreased. The elongation at fracture ranged between 0.28 and 0.71%, indicating that all the designed alloys fractured in a brittle manner. The elastic admissible strain of the designed alloys (Ti-15.05 wt% Mo) was significantly higher than the conventional orthopaedic implant materials (CP-Ti, Ti6Al4V) indicating that this study is promising for the development of excellent biomedical materials.