

## Microstructure and mechanical properties of Ti-Mo-Nb alloys designed using the cluster-plus-glue-atom model for orthopedic applications

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*The International Journal of Advanced Manufacturing Technology* volume 115, pages 3053–3064 (2021)

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### **ABSTRACT:**

The aim of this study is to investigate the effect of niobium on the microstructure and mechanical properties of Ti-Mo-Nb alloys, which include Ti-11.1Mo-10.8Nb (TMN1), Ti-10.2Mo-19.5Nb (TMN2), and Ti-9.2Mo-26.7Nb (TMN3) alloys designed using the cluster-plus-glue-atom model. The molybdenum equivalence, average electron concentration ratio, and d-electron method approaches were used to predict the stability of the  $\beta$  phase. Microstructural analysis was performed using x-ray diffraction, optical microscopy, and electron backscatter diffraction, while the microhardness tests, tensile tests, and bend tests were also conducted. The microstructure of the TMN alloys comprised primarily the  $\beta$  phase and secondary martensitic  $\alpha''$  and athermal  $\omega_{\text{ath}}$  phases. Their elastic moduli of the TMN alloys were far greater than those of the common orthopedic implant materials. The alloys showed superior tensile strengths, bend strengths, and microhardness due to the solid solution effect of both Mo and Nb and the precipitation hardening of the  $\omega_{\text{ath}}$ . Brittle fracture resulting from the existence of the  $\omega_{\text{ath}}$  phase in the alloys was also observed. The designed metastable TMN alloys designed using a synergic combination of the approaches of the cluster-plus-glue-atom model and the  $\beta$ -phase predicting tools can be promising candidates for orthopedic applications.

