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Ti-Pt-Nb high temperature shape memory alloys towards industrial applications: A cluster expansion screening

Shape memory alloys (SMAs) possess two unique properties, superelasticity and shape memory effect. These properties are a result of phase transformation. The SMAs have received great attention owing to their excellent mechanical properties, biocompatibility, corrosion resistance, and their ability to transform close to room temperature. High-temperature shape memory alloys (HTSMAs) are a specific type of shape memory alloys that deliver shape recovery above 373 K by adding elements, such as Au, Pt, Pd and Hf binary NiTi materials. These alloys are expected to be used in applications such as aerospace and automotive. TiPt has a higher martensitic transformation above 1200 K, which makes it a good candidate for HTMSAs. It displays a martensitic transformation from an austenite B2 to a martensite B19 structure. However, TiPt exhibits negative shear tetragonal modulus (C′ = -32GPa). The addition of the third element is expected to stabilize the TiPt binary. In this study cluster expansion was utilized to predict ground state structures containing three (3) element Ti-Pt-Nb. The cluster expansion method generated 45 new Ti-Pt-Nb structures and these were ranked as stable and meta-stable structures based on their formation energies. Among the 6 predicted structures, the Ti4Nb2Pt2 alloy was selected around 50:50 on Platinum (Pt)-rich sites since it is the most stable structure on the ground state line. The supercell approach in MedeA (VASP) was used to create large supercells (64 atoms). The structures were evaluated on the CHPC cluster, using 48 cores to study the phase stability and mechanical properties of Ti-Pt-Nb alloys. The Ti4Nb2Pt2 alloy was studied further by determining the structural, thermodynamic and mechanical properties using first-principle density functional theory. The materials have similar properties as tetragonal Nb doped TiPt. The mechanical properties of these compounds revealed that they are ductile in nature and mechanically stable. Furthermore, the phonon dispersion curves showed the vibrational stability of the Ti4Nb2Pt2 alloy. This work suggests that the introduction of Nb stabilises the TiPt SMAs making them potential candidates for high temperature applications.

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