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Mechanical investigation of (Ti2NbPt)2 HTSMAs from binary phase diagram

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High temperature shape memory alloys (HTSMAs) are smart materials with unique ther-momechanical characteristics that can regain their original shape after deformation. HTSMAs have been used in a wide range of industrial applications, thus include actuators in automobiles, aviation parts in aerospace and biomedical equipment. Ti-based alloys such as NiTiPd, NiTiPd and NiTiFe have lower martensitic transformations (MT) around 700 K, which limits their performance for higher temperature usage. TiPt has a higher MT of about 1300 K, which has the potential to be used for higher temperature applications. Furthermore, TiPt exhibits negative C′ = -32 GPa. The addition of a third element such as Nb is expected to stabilize and improve the mechanical behavior of TiPt alloy. In this study, first principles calculations were used to explore the structural stability and mechanical properties of (Ti₂NbPt)₂ HTSMAs. It was found that the lattice parameters, density and volume decrease with Nb addition, enhancing the structural stability of the alloy. It was also found that (Ti₂NbPt)₂ alloy is thermodynamically stable due to the negative heats of formation (-0.361 eV/atom). The elastic constants (Cij), Bulk (B), Shear (G) and Young (E) moduli were found positive suggesting mechanical stability. Furthermore, the phonon dispersion curves showed vibrational stability due to the absence of soft mode across the Brillion zone direction. The Nb alloy addition can stabilize TiPt for higher temperature applications.

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