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Computational modelling of Ti50Pd50-xCux (0≤x≤25) high temperature shape memory alloys

Ti50Pd50 system is considered as one of the potential high temperature shape memory alloy (HTSMA) due to their high martensitic transformation temperature at 823 K. Previous studies showed that this alloy is unstable displaying a negative shear modulus (C′) at 0 K. In order to improve the properties, partial substitution of Pd with Cu are being investigated. The equilibrium lattice parameters, elastic properties and the phonon dispersion curves were calculated using first-principle calculations within the generalized gradient approximation based on density functional theory. The independent elastic constants result revealed that stability is attained at above 25 at. % Cu (Ti50Pd25Cu25). The calculated moduli confirm that alloying with Cu effectively increases hardness and ductility in Ti50Pd50 systems. Partial substitution of Pd with Cu was found more effective in enhancing mechanical properties. Furthermore, the addition of Cu may enhance the martensitic transformation temperature of the Ti50Pd50 alloy. These findings can have important implications for future materials design in aerospace industries.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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