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## Computational modelling study on elastic properties and temperature variation in $\text{Ti}_{50}\text{Pt}_{50-x}\text{Cu}_x$ shape memory alloys

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Recently, there is a high demand of shape memory alloys that can be used at high temperatures. TiPt is found to be one of the promising alloys with the transformation temperature of 1300 K. Previous studies showed that the alloy is mechanically unstable with the negative  $C'$  modulus at 0 K. In order to enhance the mechanical properties of the alloy, a third element Cu was substituted in the TiPt. The stability of the structures with respect to their equilibrium lattice parameters and heats of formation were determined. It was found that increasing Cu content stabilizes the TiPt with a positive  $C'$  observed for 12.25 at.% Cu. Furthermore, we investigated the temperature dependence of the lattice parameters and Copper is found to be lowering the martensitic transformation temperature of the TiPt shape memory alloy.

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

no

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

n/a

Would you like to submit a short paper for the Conference Proceedings (Yes / No)?

no

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