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Effect of Ta, Hf and V on Structure and Stability of Ti50Pt50 shape memory alloys

First principle density functional theory approach was employed to study the effect of Ta addition on the TiPt shape memory alloys (SMAs). SMAs have the ability to remember their shapes after deformation, and this is due to their shape memory effect and super elasticity properties. These alloys have the capability to operate as high temperature shape memory alloys considering that they possess a reversible martensitic transformation. All the calculations in this study are carried out at the Centre for High Performance Computing (CHPC), employing VASP code embedded in Material design MedeA platform. We employed the generalized gradient approximation parameterized by Perdew, Burke and Enzerhof using the supercell approach. The equilibrium lattice parameters, elastic properties and the phonon dispersions were calculated to investigate the stability of the Ti50Pt50-XMX. We have found that the calculated heats of formation predicted the 6.25 at.% V, Ta and Hf as the stable structures. Interestingly, the vanadium, tantalum and hafnium addition was found to stabilise the TiPt with all the Cij's being positive. The predicted phonon dispersion curves revealed that increasing the V, Ta and Hf content in the system stabilizes the structure.

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