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The elastic properties and martensitic transformation behaviour of $\text{Ti}_{50}\text{Pt}_{50-x}\text{Co}_x$ shape memory alloy HASANI CHAUKE, ROSINAH MAHLANGU, PHUTI NGOEPE, University of Limpopo — Ti-based shape memory alloys (SMAs) such as PdTi, AuTi and PtTi are important in the design for high temperature alloys due to their high martensitic transformation (M_s) of above 673 K. PtTi is the most attractive for the development of high temperature shape memory alloys (HTSMAs) since it has the highest M_s of about 1273 K. Above 1273 K The crystal structure is the ordered cubic B2 phase, and transforms to an orthorhombic B19 phase at lower temperature. The supercell approach method was used to investigate the effect of partial substitution of Pt with Co on the TiPt potential shape memory alloy. The first-principles calculations were carried out within the generalized gradient approximation to determine the stability of the $\text{Ti}_{50}\text{Pt}_{50-x}\text{Co}_x$ for $x=6.25, 18.75$ and 25 . We found that the calculated heats of formation and density of states predicted the 6.25 at.% Co to be the most stable structures compared. The elastic properties and the phonon dispersion results suggest that the partial substitution of Pt with Co increases the M_s of TiPt with the softening of the ' shear moduli.

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