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## First-principle study of $\text{Ti}_{50-x}\text{Pt}_{50}\text{Zr}_x$ High temperature shape memory alloys

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**Abstract content** (Max 300 words) [http://events.saip.org.za/getFile.py/?target=\\_blank](http://events.saip.org.za/getFile.py/?target=_blank) **Formatting** **Special chars**

Shape memory alloys (SMAs) exhibits two unique properties namely the shape memory effect and superelasticity which occur as a results of face transformation. These properties enable the metals to remember their previous shape after being deformed when heated above certain temperatures. The effect of ternary addition Zr on B2 TiPt SMAs has been investigated using density functional theory. The supercell approach embedded in VASP code was used to partially substitute Ti with Zr atom on the cubic TiPt to form TiPt(Zr). Their structural, mechanical properties and temperature dependence have been calculated. It was found that the shear modulus for  $\text{Zr}_{6.25}\text{Ti}_{43.75}\text{Pt}_{50}$  and  $\text{Zr}_{18.25}\text{Ti}_{31.25}\text{Pt}_{50}$  is negative suggesting mechanical instability, while a positive shear modulus is observed for  $\text{Zr}_{25}\text{Ti}_{25}\text{Pt}_{50}$  (mechanical stability). The phonon dispersions for the  $\text{Zr}_{6.25}\text{Ti}_{43.75}\text{Pt}_{50}$ ,  $\text{Zr}_{18.25}\text{Ti}_{31.25}\text{Pt}_{50}$  and  $\text{Zr}_{25}\text{Ti}_{25}\text{Pt}_{50}$  shape memory alloys were calculated and the phonon dispersion curves revealed a softening of modes along high symmetry directions M, R and  $\Gamma$ . This is due to  $C_{44}$  being  $> C'$ , which corresponds to branches in the negative direction. Furthermore, LAMMPS code was used to determine the lattice expansion of the  $\text{Ti}_{50-x}\text{Pt}_{50}\text{Zr}_x$  ternaries at various temperature range. It was observed that as Zr content is increased with increased temperature, the structure remains cubic below 900K. However, at temperature above 900K, the lattice parameter are different ( $a \neq b \neq c$ ) suggesting a possible transformation from a cubic to triclinic phase.

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Yes

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MSc

**Main supervisor (name and email) and his / her institution**

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