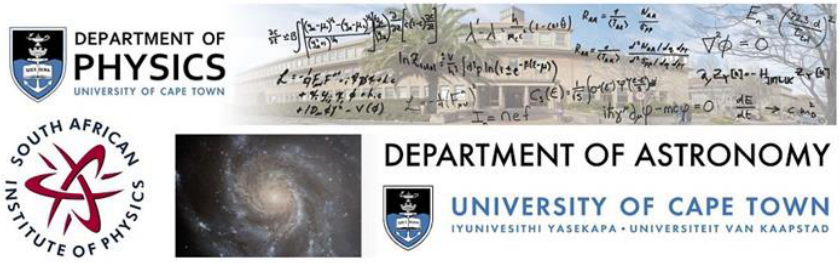

Contribution ID: **76** Type: **Poster Presentation**

First-principle study of Ti_{50-x}Pt₅₀Zr_x High temperature shape memory alloys

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
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Shape memory alloys (SMAs) exhibits two unique properties namely the shape memory effect and superelastisity 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 Zr_{6.25}Ti _{43.75}Pt₅₀ and Zr_{18.25}Ti_{31.25}Pt ₅₀ is negative suggesting mechanical instability, while a positive shear modulus is observed for Zr₂₅Ti₂₅Pt₅₀ (mechanical stability). The phonon dispersions for the Zr_{6.25}Ti_{43.75}Pt₅₀, Zr_{18.25}Ti_{31.25}Pt₅₀ and Zr₂₅Ti₂₅Pt₅₀ shape memory alloys were calculated and the phonon dispersion curves revealed a softening of modes along high symmetry directions M, R and Γ. This is due to C44 being > C', which corresponds to branches in the negative direction. Furthermore, LAMMPS code was used to determine the lattice expansion of the Ti_{50-x}Pt₅₀Zr_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≠b≠c) suggesting a possible transformation from a cubic to triclinic phase.

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Session Classification: Poster Session (1)

Track Classification: Track A - Division for Physics of Condensed Matter and Materials