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Computaional Modelling of Ti_{50-x}Pt₅₀Zr_x SMAs

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Abstract content
   (Max 300 words)
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Shape memory alloys (SMAs) are unique metals that can remember their previous shape after being deformed and can return to their previous form when heated above certain temperatures. SMAs exhibits two unique properties arising from a solid-to-solid, diffusionless phase transformation namely the shape memory effect and superelastisity. The stability of the Ti_{50-x}Pt₅₀Zr_x ternary is investigated using the supercell approach. The supercell approach, embedded in VASP was used to partially substitute Ti with Zr atoms on the cubic Ti₅₀Pt₅₀ to form Ti_{50-x}Pt₅₀Zr_x. We found that the lattice parameters were reproduced and agree with the available experimental values. The calculated heats of formation predict that the Zr_{18.25}Ti_{31.25}Pt<sub is the most stable structure whereas Zr₂₅Ti₂₅Pt₅₀ is the least stable. The mechanical properties in terms of elastic constant at 0K were found to be consistent with the calculated heats of formation. LAMMPS code was successfully used to determine the mechanical and temperature dependence of the Ti_{50-x}Pt₅₀Zr_x ternaries at various temperature range.

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

Hasani Chauke
hr.chauke@ul.ac.za
University of Limpopo

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Primary author: Mr MASHAMAITE, Mordecai (University of Limpopo)

Co-authors: Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo); Ms MAHLANGU, Rosinah (University of Limpopo)

Presenter: Mr MASHAMAITE, Mordecai (University of Limpopo)

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