Contribution ID: **78** Type: **Oral Presentation**

Computational modelling of binary titanium-based shape memory alloys

Tuesday, 26 June 2018 12:40 (20 minutes)

Ab initio density functional theory approach was employed to investigate the structural properties, elastic constant and phonon dispersion of B2 binary TiPt, TiCo, TiNi and TiZr shape memory alloys. We employed the plane-wave pseudopotential method within generalized gradient approximation parameterized by Perdew, Burke and Enzerhof using VASP code. These alloys have the ability to remember their shapes after deformation, and this is due to their shape memory effect and super elasticity properties. We found that the lattice parameters are in good agreement with the experimental results within 2%. Furthermore, the TiCo system is more stable B2 and displayed higher transformation temperature. The Pugh's ratio clearly indicates that TiPt, TiCo and TiNi binary alloys are ductile (B/G>1.75) while TiZr alloy are brittle (B/G<1.75). Phonon dispersion curves shows that TiCo is vibrational stable and there are acoustic modes observed at the gamma directions while TiPt and TiNi are not due to the existence of imaginary frequencies observed along M high symmetry direction, in agreement with the literature.

Please confirm that you
have carefully read the
abstract submission instructions
under the menu item
"Call for Abstracts"
(Yes / No)

yes

Consideration for
student awards
Choose one option
from those below.
N/A
Hons
MSc
PhD

MSc

Supervisor details
If not a student, type N/A.
Student abstract submision
requires supervisor permission:
please give their name,
 institution and email address.

R. Modiba, CSIR rmahlangu1@csir.co.za, H.R. Chauke, UL hasani.chauke@ul.ac.za and P.E. Ngoepe phuti.ngoepe@ul.ac.za

Primary author: Mr BALOYI, Mphamela Enos (UL)

Co-authors: Prof. CHAUKE, Hasani (UL); Prof. NGOEPE, Phuti (UL); Dr MODIBA, Rosinah (CSIR)

Presenter: Mr BALOYI, Mphamela Enos (UL)

Session Classification: Physics of Condensed Matter and Materials

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