Contribution ID: **111** Type: **Oral Presentation**

Effect of Hf and Cu on the cubic B2 TiPt shape memory alloys

Thursday, 28 June 2018 12:20 (20 minutes)

Computational modelling approach has been used to investigate the effect of hafnium and copper on the B2 TiPt shape memory alloys. The calculations were performed using the CASTEP code embedded in materials studio. Cubic B2 TiPt is known to be thermodynamically unstable at 0 K as compared to the B19 orthorhombic phase with it having the highest heats of formations and soft modes in the lowest frequency. Moreover, the C′ of the structure was previously found to be negative as compared to the commercialised B2 NiTi which is positive. With the recent increasing demand on shape memory alloys that can be used at high temperatures in aerospace and automobiles, TiPt is found to be one of the promising alloys with the transformation temperature of 1300 K. These alloys are known to remember their original shape when a certain temperature or pressure is exerted on them upon cooling. In order to enhance the elastic properties of the B2 TiPt alloy, Hf and Cu elements are substituted in the TiPt to form ternary and quaternary alloys. The stability of these structures are investigated with respect to their heats of formation, elastic constants and density of states. Interestingly, the addition of these elements increases the C′ of the structures with all the elastic constants being positive for the hafnium addition.

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

n/a

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

n/a

Primary author: Dr MODIBA, Rosinah (CSIR)

Presenter: Dr MODIBA, Rosinah (CSIR)

Session Classification: Physics of Condensed Matter and Materials

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