Contribution ID: **324** Type: **Poster Presentation**

The structural and elastic properties of Ti₅₀Pt_{50-x}Co_x ternaries using solid solution method employed in CASTEP

Thursday, 12 July 2012 17:30 (2 hours)

Abstract content
   (Max 300 words)

There is a growing demand of shape memory alloys that can be applied at high temperatures and TiPt was found to be one of the potential alloys since the transformation occurs at temperatures more than 1000◦C. Since Pt is expensive, in this work we replace some of the Pt by Co using the solid solution method. The Ti₅₀Pt_{50-x}Co_x ternaries were determined using the visual crystal approximation (VCA). The structures were optimized and the equilibrium lattice parameters and their formation energy were calculated. The lattice parameters were found to be decreasing minimally with an increase in the Co and the structures become mechanically unstable with respect to the formation of energy. The elastic properties and the density of states were also calculated.

Apply to be
 consider for a student
   award (Yes / No)?

No

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

Prof P.E Ngoepe, University of Limpopo

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

Primary authors: Prof. NGOEPE, PE (University of Limpopo); Ms MAHLANGU, Rosinah (University of Limpopo)

Co-authors: Dr CHAUKE, HR (University of Limpopo); Mr PHASHA, MJ (CSIR)

Presenter: Ms MAHLANGU, Rosinah (University of Limpopo)

Session Classification: Poster Session

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