



Contribution ID: 544

Type: **Poster Presentation**

## First-Principles Study of Thermodynamic and Dynamic Stability of Ru-Cr Alloys

*Tuesday, 9 July 2013 17:40 (1 hour)*

### Abstract content <br> &nbsp; (Max 300 words)

Planewave pseudopotential calculations were conducted to predict the thermodynamic stability of five different phases, L12, A15, DO<sub>3</sub>, DO<sub>3</sub>C and tP16 of Ru<sub>3</sub>Cr and RuCr<sub>3</sub> alloys. The heats of formation of all studied compositions and phases of Ru-Cr are positive. We have investigated the dynamic stability at 0 GPa for RuCr<sub>3</sub> A15 phase, which was found to be dynamically stable.

### Apply to be<br> considered for a student <br> &nbsp; award (Yes / No)?

No

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

No

**Primary author:** Dr TIBANE, Malebo (University of South Africa)

**Co-author:** Prof. NGOEPE, Phuti (University of Limpopo)

**Presenter:** Dr TIBANE, Malebo (University of South Africa)

**Session Classification:** Poster1

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