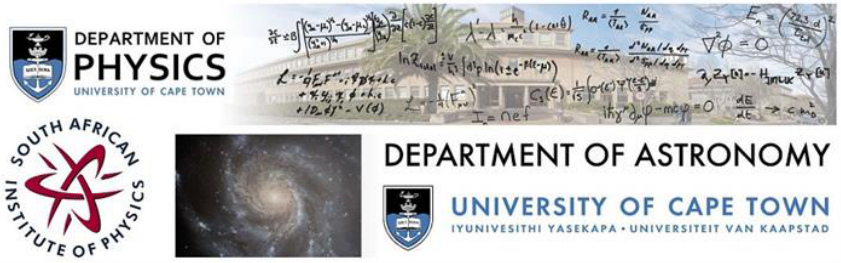

Contribution ID: **365** Type: **Poster Presentation**

High temperature and phase transformation studies of Pt₃Al compounds

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
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Platinum group alloys, particularly the Pt₃Al alloys are of importance in high temperature environment, such as aerospace and gas turbine. The Pt₃Al exist in four phases that is L1₂, DOc, DOc′ and tP16; the L1₂ is stable at high temperatures (HT) and transforms to tetragonal phases at low temperature (LT). In particular, the cubic L1₂ Pt₃Al is ductile but unstable, while the lower temperature (LT) phase which has the tetragonal lattice DOc′ is stable but brittle. However, the tetragonal tP16 is observed to be the ground-state structure at lower temperature. In this study, the relative phase transformation behaviour from L1₂ to tP16 and DOc′ has been investigated using Molecular Dynamics within the LAMMPS code. The calculated X-ray diffraction (XRD) pattern reveals a transformation trend from L1₂ to DOc′ and L1₂ to tP16 between 400K and 1300K. The observed L1₂ to DOc′ XRD peaks vanishes above 800K, while the L1₂ to tP16 peaks are observed above 1000K. This confirms that the DOc′ and L1₂ are stable below 800K and above 1000k, respectively. The L1₂ to tP16 transformation showed distinct XRD peaks above 800 K. The L1₂ XRD pattern are consistent with the experimental results, and also confirms that the tP16 phase is stable below 1000K.

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Main supervisor (name and email)
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Session Classification: Poster Session (1)

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