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# High temperature and phase transformation studies of Pt<sub>3</sub>Al compounds

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## Abstract content <br>   (Max 300 words)<br><a href="http://events.saip.org.za/getFile.py/a target="_blank">Formatting &<br>Special chars</a>

Platinum group alloys, particularly the Pt<sub>3</sub>Al alloys are of importance in high temperature environment, such as aerospace and gas turbine. The Pt<sub>3</sub>Al exist in four phases that is L1<sub>2</sub>, DOc, DOc′ and tP16; the L1<sub>2</sub> is stable at high temperatures (HT) and transforms to tetragonal phases at low temperature (LT). In particular, the cubic L1<sub>2</sub> Pt<sub>3</sub>Al 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 L1<sub>2</sub> 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 L1<sub>2</sub> to DOc′ and L1<sub>2</sub> to tP16 between 400K and 1300K. The observed L1<sub>2</sub> to DOc′ XRD peaks vanishes above 800K, while the L1<sub>2</sub> to tP16 peaks are observed above 1000K. This confirms that the DOc′ and L1<sub>2</sub> are stable below 800K and above 1000k, respectively. The L1<sub>2</sub> to tP16 transformation showed distinct XRD peaks above 800 K. The L1<sub>2</sub> XRD pattern are consistent with the experimental results, and also confirms that the tP16 phase is stable below 1000K.

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

yes

## Level for award<br> (Hons, MSc, <br>   PhD, N/A)?

MSc

## Main supervisor (name and email)<br>and his / her institution

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

NO

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No

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