Contribution ID: **106** Type: **Poster**

Ab-initio calculations of FeAl-X (X=Pd, Ag) intermetallic compounds

Iron-aluminides based alloys have created a great amount of interest due to their ability as candidates for applications in the energy sector, such as boilers, pipes, stainless Steel Coatings, automobile and aero-space industry in substitution of superalloys.
Thus, we used first-principles density functional theory to investigate the stability of FeAl and ternary FeAl-X alloys. Alloying with these precious metals increases the hardness and oxidation properties slightly. Employed virtual crystal approximation and supercell approaches to model various atomic compositions at $0 \leq x \leq 50$ for Pd and Ag.
The FeAl composition is the most favorable since it denotes a positive shear moduli, showing condition of stability. Addition of Pd and Ag was found to significantly improve the ductility of FeAl-X compound, respectively. Furthermore, their heats of formation were used to identify the most and least stable within the various concentrations, Density of states were used to describe the behavior of each phase near the Fermi level. This will allow more precise predictions on the materials behavior than experiments can handle.

Presenter Biography

I am a third year student doing masters in computational modelling studies of FeAl-X (X = Pt, Pd, Ru, Ag) at university of Limpopo.

Primary author: Ms MKHONTO, Christine (University of Limpopo)

Co-authors: Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Ms MKHONTO, Christine (University of Limpopo)

Session Classification: Poster session

Track Classification: Materials Science