Contribution ID: **173** Type: **Poster Presentation**

Alloy simulation of iron aluminides intermetallics

Thursday, 11 July 2019 15:00 (2 hours)

The Fe-rich part of the Fe-Al phase diagram has offered an overview regarding its capability as a replacement of steel in the application of intermetallic compounds. They are of excellent application in the energy sector, boilers, pipes and automotive parts. These compounds possess good mechanical properties, low density as well as accessibility of raw material. Thermodynamic stability phase diagrams were calculated and elaborated in order to improve the understanding of the corrosion mechanism. We employed VASP code to determine the thermodynamic and electronic properties from their equilibrium lattice constants on each system. In terms of the system stability, there exists correlation between the calculated shear modulus (C′) and Gibbs energy as well as the XRD pattern which corresponds to the FeAl bcc ordered compound. It was found that the addition of Pd, Pt and Ag enhances the stability at various (FeXAlXM)X compositions. The results obtained indicated that Pt substitution stabilised the system more, followed by Pd wherelse Ag showed to be the least in terms of stability.

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yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

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Session Classification: Poster Session 2

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