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Ground state phase stability simulation of Fe-X-Al alloys (X= Pd and Ag)

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Transition-metal alloys, such as iron-aluminides are significant because of their impact on the industrial sector, such as excellent unique corrosion properties and resistance to high-temperature oxidation, which outperform Ni-based superalloys. Due to their extraordinary resistance to oxidation at high temperatures, Fe-Al based materials have recently received a lot of attention as a potential steel substitute. Previous research has shown that increasing the Al concentration reduces the density of materials and, as a result, improves the protective oxide layer at high temperatures. However, these systems are easily influenced by environmental effects and limited by their tendency for low-temperature fracture and decreased ductility. In this study, DFT was employed to investigate the thermodynamic ground state structural energies at varied concentrations for better yield strength of these materials to improve the application for stainless steel-IT superior protection with the addition of a third element Pd and Ag. The Universal Cluster Expansion (UNCLE) code was employed to predict new phases and stability of Fe-X-Al alloys. The ground state phase diagrams were predicted for Fe1-x-Pdx-Al and Fe1-x-Agx-Al systems. The Fe-Pt-Al indicated miscible constituent; in particular, the FePtAl₂ and FeAgAl₂ composition due to their lowest energy predicted by the enthalpy of formation. The enthalpy of formation (DHf) clearly indicates that Ag-doping with DHf of -0.222 eV/atom is the most stable system with the lowest energy, followed by Pd-doping with DHf of -0.110 eV/atom. Fe-Pd-Al and Fe-Ag-Al systems indicated miscible constituent behaviour due to negative enthalpy of formation, in particular the FePtAl₂ and FeAgAl₂ composition indicated thermodynamic stability. These results are in agreement with elastic properties, phonon dispersion curve and X-Ray diffraction pattern, implying a condition of stability.

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yes

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

PhD

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