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Phase stability of Fe-Pt-Al alloys: A Cluster expansion approach

Alloy-based Fe-Al intermetallic are important for high-temperature applications and are corrosion resistant to oxygen. This is due to a well-adherent protective oxide layer that forms on the surface of the metal interface. These alloys are a major driver as a component for better infrastructure, industrial coating and the improvement of automotive parts. The automotive industry is a major user in demand to increase vehicle performance, weight reduction, cost dependability and fuel efficiency. They do, however, have limited ductility at ambient temperature and suffer rapid loss in strength over 873 K. 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 application for stainless steel-IT superior protection with the addition of a third element (Pt). We employed Universal Cluster Expansion (UNCLE) code and Monte Carlo (MC) technique embedded in MedeA to investigate phase stability of Fe-Al alloys. These sets of calculations were performed at CHPC using 48 core processors and, 5 priority with 12 atoms. The Fe-Pt-Al system demonstrated condition of thermodynamic stability due to the predicted structural energies of the system indicating negative enthalpy of formation. The predicted structures on the ground state line indicate that the shear moduli (C'>0) and B/G ratio > 1.75 which implies condition of stability. Thus, these systems have shown to be promising candidates to improve the strength and ductility of these materials at high-temperatures, to resist oxygen or water permeating through to create corrosion-resistant conditions.
Keywords: Phase stability, Fe-Al, Coating, UNCLE, MC.

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