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Alloying on β2-ordered FeAl with Ru and Ir for ductility enhancement: A cluster expansion and MD approach

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Intermetallic iron aluminides alloys of Fe3Al and β2-ordered cubic FeAl structure amongst other various compounds of transition metals and aluminium compositions have been of interest to researchers for application in different industries to increase corrosion-resistance for high temperature application steel coating. The FeAl compound exists between 35-50 % of aluminum concentrations. This alloy possesses far much better oxidation and corrosion resistance and hardness qualities than the Fe3Al. Their long-range-ordered superlattices, which minimizes dislocation and diffusion at increased temperatures make them desirable for high temperature applications. We have employed the cluster expansion (CE) technique to construct the stability phase diagrams of Fe-Ru/Ir-Al ternary systems for stable compositions identification, Monte Carlo (MC) to determine the temperature needed to stabilize the system and ab-initio approach to predict the mechanical and dynamical properties using LAMMPS code. The cluster expansion results showed that the Fe1-XRuXAl ternary alloy has no thermodynamically stable compositions due to positive enthalpies of formation values, while the Fe1-XIrXAl alloy has values that are marginally above 0 eV. It was observed that the Fe1-XIrXAl system has three thermodynamic stable structures; the stability of the system increases with Ir concentration until the Fe:Ir reaches an equiatomic composition and began to decrease. Hence, FeIr2Al3 system was found to the most thermodynamically stable composition. Our findings showed that doping the β2-FeAl with Ru and Ir significantly enhanced the hardness and ductility for high-temperature application for steel-It component coating.

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Yes

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