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Temperature dependance of Pt, Pd, Ru and Ag on FeAl systems

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The Fe-Al based systems have recently attracted a lot of attention in various industries for future development of steels due to their excellent resistance to oxidation at high temperatures. These systems suffer from limited room temperature ductility and a sharp drop in strength above 600^{<0>0</0>;}C. The FeAl alloys are regarded as promising material for construction and steel coating especially for high temperature applications in aggressive and corrosive environment. They create wide prospects for applications such as in industries, aerospace, automotive parts and steel-IT coating components. In our previous work, attempts have been made on ternary alloying of FeAl systems, and it was reported that Pt and Ru showed improvement on the structural stability. The current study used a combination of ab-initio and molecular dynamics employing virtual crystal approximation (VCA) and DMol to investigate the influence of ternary addition of Pt, Pd, Ru and Ag and their temperature effect. Heats of formation, density of states and elastic constants were calculated to describe the structural, thermodynamic and mechanical stability of these systems. It will also be shown that addition of Pt, Ru, Pd and Ag may significantly enhance the ductility of the FeAl-X ternary systems at high temperature.

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