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Thermodynamic surface stability of Pd doped on the ordered FeAl (011) alloy: A first-principles study

The Fe-Al phase has variable compositions and temperatures; it is dominated by two ordered phases, respectively β2 and DO3, each of which has a wide compositional stability range. FeAl alloys have a good specific modulus, strength-to-weight ratio, and corrosion resistance to oxidation and other forms of corrosion. Because of these properties, FeAl alloy is an appealing contender for high-temperature applications in harsh conditions. They contain elements that are cost effective and readily available, such as Ni, Fe, and Al. Theoretical studies of solids and surfaces of FeAl have grown in prominence over the last 30 years especially with the use of powerful simulation softwares such as DFT have become more accessible for improved structural properties. The alloy composition and the environment that the steel is exposed to are the primary factors that influence corrosion in PGM doped stainless-steels. In stainless-steels, corrosion happens where the oxide film is breached. We have employed ab-initio approach to predict the interaction of Pd on the β2 FeAl (011) stable surface within the Metadise code. We observed that the (011) plane is the most stable surface resulting in the lowest surface energy, followed by (111) plane and lastly (001) least stable. The difference between these active slip directions affects the ductility of intermetallics significantly. It is expected that Pd doping enhanced surface stability from the Fe- and Fe/Al- termination on (001), (011) and (111) plane, respectively, formed a well-adherent protective oxide layer to enhance the hardness and ductility for steel-It component coating.
Keywords: Surface stability, (011) surface plane, FeAl-Y ternary systems.

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