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Adsorption behavior of ternary Fe1-XYXAl alloy with H2O and O2

Iron aluminide is a metal alloy with unique properties, including high strength and temperature resistance, making it suitable for applications in aerospace and energy sectors. FeAl alloy has a good specific modulus, strength-to-weight ratio, and corrosion resistance to oxidation, sulfidation, and other forms of corrosion. These iron-aluminides showed a major embrittlement mechanism at room temperature, resulting in a loss of cohesive strength at their interfaces. Hence, the concept of surface is used to form a boundary as a protective layer on the outermost layer of a material through surface doping. This phenomenon influences factors such as adsorption and the formation of surface states. For high-temperature structural applications, such as high melting and disordering temperatures, high stiffness, low diffusivity, etc., also makes these alloys a challenge to process into useful developed materials. Hence, the need to improve the surface properties to enhance strength, adhesion, and durability through the development of new materials. The increasing availability of computational software programs with advantageous and improved methodologies, such as Metadise and VASP codes were was employed to evaluate surface properties. The alumina layer (Al2O3) formed on the metal's surface acts as a good barrier against oxygen penetration, delaying the production of other faster-growing oxides, which deteriorate the surface stability. The Eads/H2O showed higher surface energies compared to those of O2, which implies that Eads/O2 is more stable with the lowest surface energies compared to those of H2O. This is confirmed by literature that a protective Al2O3 oxide layer forms on the surface of the material, thus minimizing oxidation behaviour.

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