Atomistic Insights into Interfacial Reactions of FeCr₂O₄ Oxide Films in High-Temperature Water

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Interfacial reactions of FeCr₂O₄ oxide films in high-temperature pure water, oxygenated water and hydrogenated water have been investigated by means of ab initio molecular dynamics simulation based on the Born-Oppenheimer scheme. The simulation results show that the surface configuration of FeCr₂O₄ (100) is stable in high-temperature pure water, and the charge transfer of each layer in the oxide film is not significant before and after the film is immersed in water. Dissolved oxygen molecule dissociates spontaneously in high-temperature oxygenated water, and the Cr atoms in the surface layer of the oxide film tend to dissolve in water because of interactions among hydroxyl, oxygen and H₂O molecule. However, dissolved hydrogen molecule does not dissociate in high-temperature hydrogenated water during simulation.

Keywords: Oxide film; High-temperature water; Interfacial reaction; Ab initio molecular dynamics

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