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Exploring the effect of hydrogen adsorption on Fe2SiCr surface

Fe-Cr-based alloys are ideal for fusion reactor structural components because of their reduced activation and swelling, corrosion resistance, and excellent hardening or embrittlement properties in various radiation environments. However, Fe-Cr alloys have high hydrogen uptake capacity, and enhance hydrogen embrittlement can cause material degradation and premature failure, necessitating an understanding of the hydrogen interaction with this alloy surfaces. This paper investigates hydrogen adsorption on Fe2CrSi using first-principle calculations, considering three different adsorption sites: top, bridge and hollow sites to analyse hydrogen interactions with the surface. The current findings showed that the adsorption energy of the H atoms is thermodynamically stable, with E_ads < 0 for all adsorption sites. This suggests that H atoms spontaneously adsorb on the surface of Fe2CrSi (110). More importantly, the effect of van der Waals (vdW) forces and dispersion correction was investigated, it was found that all adsorption sites exhibit the most stable adsorption energies than standard density functional theory, with E_ads^(DFT-D)>E_ads^DFT. The adsorption energy strength of H at the top site was observed to follow the order of E_ads^Fe > E_ads^Cr >E_ads^Si. This means that the presence of Fe on the metal surface will expedite the formation of metal hydrides and hydrogen embrittlement, while the presence of Si on the metal surface will slow it down. Overall, the findings show that the Fe2CrSi surface, rich in Fe-Cr, may undergo metal hydride and HE formation during application, while an increase in Cr content may limit hydrogen embrittlement.

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