First-principles analysis of the stability and hydrogen adsorption properties of the α-Ti/α2-Ti3Al interface towards clarified hydrogen embrittlement mechanism of titanium alloys

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Abstract First-principles calculations were employed to investigate the adsorption and diffusion energy of hydrogen (H) in the Ti/Ti_3Al binary system, along with the evolution of the interfacial stability induced by the presence of H. The penetration energy barrier indicates that H can more easily penetrate the substrate through the Ti/Ti_3Al interface. The formation energy of H increases with distance from the interface and the Ti/Ti_3Al interface acts as a sink for trapping hydrogen interstitials. When all interstitial sites are completely occupied by H, the cleavage energy along the interface decreases from 1.935 to 1.094 J/m^2, suggesting that H doping significantly reduces the strength of the Ti-Ti_3Al (01-10) interface. When the area density of H-doping at the interface exceeds 0.37 atoms/$Å^2$, the α-Ti lattice expands. Consistent with experimental observations, this triggers atomic migration and the generation of Ti-hydrides. Further analysis of the atomic structure and Bader charge transfers indicate that the interaction of Ti and H can alter the localized electronic structure of Al, leading to a weakened interface due to loss of interface bond strength. In summary, the theoretical calculations have provided new insights into possible hydrogen embrittlement (HE) mechanism in titanium alloys.

Keywords *Titanium, corrosion, hydrogen-embrittlement, HE, DFT*

Reference

[1] S Chen, M Liu*, C Leygraf, F Huang, L Fan, L Ma*, Y Jin*. First-principles analysis of the stability and hydrogen adsorption properties of the α-Ti/α2-Ti3Al interface towards clarified hydrogen embrittlement mechanism of titanium alloys. International Journal of Hydrogen Energy, 2024, 72: 338-348.