Hydrogen-surface interaction from first-principles calculations and its implication to hydrogen embrittlement mechanisms of titanium

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Abstract Hydrogen embrittlement (HE) caused by the interaction between hydrogen and crack tip is the key factors for the stress corrosion crack (SCC) of titanium alloys utilized in marine environment. In the present work, the interactions between hydrogen and the fresh surface of crack tip in titanium, including the adsorption, desorption, diffusion of hydrogen atom near the surface, are investigated systematically by using a first-principles method. The surface energy of titanium with H adsorption is calculated. We show that H atoms are prone to adsorb on the surface of titanium and then accumulate beneath the surface whereas both desorption of H atoms to form H_2 and diffusion of H atom into bulk cost energy. The surface energy decreases with increasing coverage of H, which reduces the fracture work of titanium. The H-induced reduction of the fracture work at the crack tip is expected to accelerate the crack propagation. The accumulation of H beneath the surface facilitates the formation of hydride ahead the crack tip which is critical for the hydride induced embrittlement. The H_2 pressure mechanism is not supposed to be responsible for the HE of titanium because the desorption of H atoms from the surface to form H_2 is energetically unfavorable.

Keywords Hydrogen embrittlement; Titanium alloy; Surface energy; First-principles calculations.

Reference

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