Discerning the duality of H in Mg: H-induced damage and ductility

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Abstract Prone H reduction is considered an important factor in the poor corrosion resistance of Mg and its alloys, while the reduced H simultaneously impacts their mechanical properties whose mechanism is still unclear. It can be experimentally found that the elongation of Mg charged with atomic H is 2.76% greater than that in air. To reveal the underlying physics, multi-scale modeling combining first-principle calculation, molecular dynamic/static (MD/MS) simulation, and crystal plasticity finite element method (CPFEM) is first employed to elaborate the influence of H on Mg at different length scales. The first-principle results show that the Prism-I $\{10\bar{1}0\}$ exhibits the most corrosive nature with an effective H adsorption density that reaches 18 nm-2 and its diffusion barrier is only 0.156 eV H-1. Conversely, the Basal {0001} has the best surficial H resistance. After H infiltration into the Mg matrix, the generalized stacking fault energies of most twining planes decrease by 2.26% ~18.49%. Especially for the Basal {0001}, the H not only lowers its stacking fault energy to -7.13 J/m^2, but also impedes its cleavage cracking along $[10\bar{1}0]$ according to the MD/MS simulation. The presence of H within the grains induces early initiation of stacking fault and elevates the critical stress at the crack tips. The CPFEM modeling reveals that the difference in twining growth is concentrated within 4% strain. The H addition promotes the twining of Mg, however, following 4% strain, the relative activity of planes in the Mg/Mg-H models is consistent.

Keywords Magnesium; Hydrogen-induced ductility; Cracking; Twining; Multi-scale calculation.

Reference

[1] Yucheng Ji, F. Shuang, Zhiyang Ni, Chenyang Yao, Xiao Li, Xiaoqian Fu, Zhanghua Chen, Xiaogang Li, Chaofang Dong*. Discerning the duality of H in Mg: H-induced damage and ductility, International Journal of Plasticity. 181 (2024) 104084.