Exploring the role of H-induced stress fields and H-H interactions in hydrogen embrittlement by atomistic simulations

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Established theories of hydrogen embrittlement (HE) can partially describe this phenomenon by taking specific features of hydrogen-metal interactions into account. It is generally known that H atoms decrease the formation energies of defects such as free surfaces and dislocations, leading to enhanced decohesion and enhanced localized plasticity, respectively. In this talk, we will focus on two other aspects. First, we discuss the decisive role of the H-H interaction in the accumulation of sufficient hydrogen atoms at the critical regions in the metal. The attractive H-H interaction is a prerequisite for the accumulation of H atoms at the critical regions despite the low concentration of H in the bulk. As a descriptive example, the feasibility of the formation of the nano-hydrides around the dislocations in FeCr20 alloy is demonstrated using the ab initio simulations. The presence of these nano-hydrides explains the significant reduction in the pop-in loads in the H-charged samples.

The second aspect of interest is the stress field of the H atoms. Since the H atoms occupy interstitial sites in the host metals, they increase the local stress field. This effect intensifies, if a large number of H atoms is attracted to defects such as grain boundaries (GBs) and is essential for the explanation of nano-void formation in H-charged polycrystalline nickel. Extensive experimental observations indicate the presence of nano-voids and the increase of the free volume along the grain boundaries in hydrogen-charged nickel. We explain this effect by molecular dynamics (MD) simulations and theoretical considerations. They show that the barrier for cross-slip of screw dislocations considerably decreases due to the H-induced stress field in the nanometer-sized regions around GBs. The enhanced cross slip of dislocations facilitates the formation of jogs at specific loading rates. These jogs can emit vacancies during the jog-drag process.