ROLE OF DEFECT INTERACTIONS DURING HYDROGEN EMBRITTLEMENT IN IRON: A MULTISCALE PERSPECTIVE

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Hydrogen embrittlement (HE) is a phenomenon that affects both the physical and chemical properties of several intrinsically ductile metals. Consequently, understanding the mechanisms behind HE has been of particular interest in both experimental and modeling research. Discrepancies between experimental observations and modeling results have led to various proposals for HE mechanisms. Therefore, in this work we systematically examined the effect of hydrogen on two fundamental HE mechanisms in iron, namely, adsorption induced dislocation emission (AIDE) and hydrogen-enhanced decohesion (HED). In this work, we used density functional theory, atomistic simulations, and continuum Rice-Thompson criterion to systematically investigate: a) the incipient event ahead of a crack tip in single crystals subjected to mode-I loading conditions; b) the cohesive strength of grain boundaries; and c) the energy barrier for a slip transmission across the grain boundary. We observed that the presence of hydrogen 1) reduces the stress intensity factor required for both the dislocation nucleation and the cleavage response for different crack orientations, and 2) increases the energy barrier for slip transmission. Most importantly it was found that the AIDE and HED mechanisms are acting together to cause HE.