PREDICTING HYDROGEN EMBRITTLEMENT IN STEELS AND HIGH ENTROPY ALLOYS

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In spite of considerable experimental study, the mechanisms and understanding of Hydrogen embrittlement in metals remain open. No approaches are able to predict embrittlement conditions in austenitic steels without fitted inputs. New experiments on fcc high entropy alloys, such as CoCrFeMnNi, present an additional paradox, absorbing more H than Ni or austenitic 304 stainless steel (SS304) but being more-resistant to embrittlement. Here, a new theory of embrittlement in fcc metals is presented based on the role of H in driving an intrinsic ductile-to-brittle transition at a sharp crack tip. Hydrogen at the crack tip reduces the decohesion energy and prevents dislocation emission/blunting, and both are needed for embrittlement. The theory predicts a critical room-temperature H concentration above which an alloy is embrittled in terms of the dependence of both surface energy and unstable stacking fault energy on (segregated) H concentration and the distribution of H absorption energies in the bulk multicomponent alloy. Using first-principles DFT to compute the H-dependence of the relevant alloy properties, good agreement with available experiments for the transition concentration is found for the alloys SS304, SS316L, CoCrNi, CoNiV, CoCrFeNi and CoCrFeMnNi. The theory rationalizes why CoNiV is the most-resistant alloy, why SS316L is more resistant than the HEAs CoCrFeNi and CoCrFeMnNi, and why SS304 at a given concentration is embrittled at 300K but not at 400K. The theory thus opens a path toward computationally-guided discovery of embrittlement-resistant alloys, although limitations and challenges are discussed.