HYDROGEN EMBRITTLEMENT IN STEELS AND HIGH ENTROPY ALLOYS

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Abstract

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 quantitatively predicts a critical room-temperature H concentration above which an alloy is embrittled. Using first-principles DFT to compute the relevant alloy properties including H absorption, 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 and why SS316L is more resistant than the HEAs CoCrFeNi and CoCrFeMnNi. The theory thus opens a path toward computationally-guided discovery of embrittlement-resistant alloys, although limitations and challenges are discussed.

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