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A multiscale study of hydrogen embrittlement of metals: Revisiting the hydrogen enhanced local plasticity (HELP) mechanism JOHANN VON PEZOLD, JÖRG NEUGEBAUER, Max Planck Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — The embrittlement of metals by H is a long-standing problem, whose underlying mechanisms are still largely unclear. Here we consider the atomistic basis of the HELP mechanism, which asserts that H mobilises dislocations by shielding elastic dislocation-dislocation interactions. Using a combination of density-functional theory calculations, semiempirical EAM potentials and an effective lattice gas Hamiltonian we determine the interaction of H with the strain field around edge dislocations in Ni. Our results reveal an attractive, but short ranged interaction between H interstitials, which leads above a critical concentration to the formation of a precursor hydride phase. The increased lattice parameter of this hydride phase induces significant misfit stress, but localises the dislocation stress field due to a localisation of the dislocation strain field. For H concentrations of up to 0.25 at. %, the stress localisation is found to dominate and thus effectively shields the stress field of the dislocation, pointing towards a novel atomistic basis for the HELP mechanism.

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