Two-way coupled modeling of dislocation substructure sensitive crystal plasticity and hydrogen diffusion at the crack tip of FCC single crystals

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Abstract

Dislocation substructure-sensitive crystal plasticity (DSS-CP) modeling accounts for the evolution of mesoscale structures using dislocation-based parameters informed by experiments and computation at various lower length scales. To a first-order approximation, DSS-CP model parameters are affected by hydrogen (H) concentration, accounting for both H-dependent yield strength and strain hardening rate. This H-affected DSS-CP model is two-way coupled with H-diffusion to explore both effects of plastic deformation on H-diffusion and effects of H on yield strength and strain hardening in the DSS-CP model. Crack tip simulations are performed for face-centered cubic (FCC) metals under monotonic loading conditions with and without H. Enhanced maximum plastic deformation in the vicinity of the crack tip (i.e., localization or intensification of plastic strain) and crack tip opening displacement (CTOD) are predicted in the presence of H, consistent with experimental observations. In spite of increased initial strength due to H, subsequent reduction of the rate of strain hardening in the presence of H is shown to enhance localization of crack tip plasticity. Furthermore, this modeling framework predicts that higher H-diffusivity (leading to a larger H-affected zone) will enhance the crack tip plasticity, making use of the two-way coupling algorithm implemented in this work. On the other hand, we find that the H-sensitivity of crack tip strain localization response, based only on modification of model parameters, is too weak to explain typical experimental observations. This points to the need to develop more advanced DSS-CP constitutive relations that consider highly complex dislocation interactions with point defects.

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