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Coupling diffusion and mechanics modeling for hydrogen embrittlement (HE)

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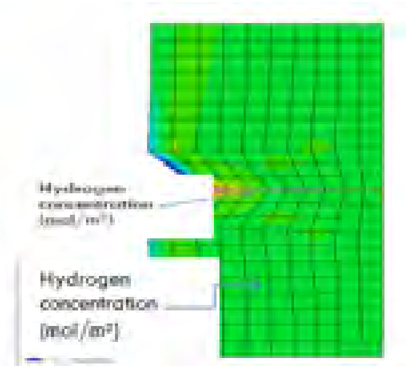
This work deals with modeling HE mechanisms in high strength steels. The aim is to elucidate two failure mechanisms in the presence of hydrogen: Hydrogen induced local plasticity (HELP) and hydrogen induced decohesion (HID). The HELP theory suggests that hydrogen, in contrast to the usual understanding of embrittlement, enhances the dislocation mobility and promotes slip localization, resulting in localized plastic failure. Furthermore, hydrogen reduces the bonding energy between atoms leading to decohesion. The HID mechanism might explain the brittle intergranular fracture surface observed in high strength steels. Experimental evidence of the occurrence of HELP versus HID or, more probably, their synergetic effect, is still an unresolved issue. Hydrogen atoms can accumulate, either within the matrix or at interfaces (i.e., between particles and the surrounding matrix, or grain boundaries) affecting the mechanical response of the material. We construct a finite element model in order to simulate the mechanical behavior of the matrix and interface coupled with hydrogen transport. We also include simple kinetic models of the flux of atoms into (and out of) an interface. We combine this understanding with micromechanical models of the interaction of dislocations with particles and with empirical models of the effect of hydrogen on interface decohesion and plastic deformation to provide a set of coupled constitutive equations for hydrogen transport and mechanical behavior. With this modeling framework, we aim to identify and explore the conditions under which HELP or HID or both mechanisms are activated. In particular, we model the failure of high strength steels which contain a distribution of nano-scale particles. We simulate the response in hydrogen and hydrogen-free environments and identify the conditions under which hydrogen can lead to: (1) a quasi-brittle macroscopic response through localization of plastic deformation facilitated by decohesion at the particle/matrix interface or (2) a brittle intergranular fracture process.



Biography

Olga Barrera is a Senior Research Associate at the University of Oxford. Her expertise is in the field of computational mechanics and computational material modeling. Her research focuses on solving a range of coupled diffusion mechanics problems focused on understanding the failure process of a number of material systems. She also has experience in applying the wide range of skills developed in the fields of materials modeling and computational solid mechanics to solve exciting and important problems in parallel disciplines such as biomechanics.

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