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Effects of hydrogen on steady, ductile crack growth: Computational studies

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ABSTRACT

This paper describes studies of the near tip fields and the effects on void growth rates for a steadily advancing crack through a ductile metal in the presence of hydrogen, under plane-strain and quasi-static conditions. The computational model determines directly the deformation history of a steadily propagating crack without the need for a priori (transient) analysis that considers blunting of the pre-existing stationary crack and subsequent growth through the associated initial plastic zone. The present approach enables straightforward investigation over a range of geometric constraint configurations encountered in test specimens and structural components by application of a far field $K_I - T$ loading. The ductile crack propagation simulated in these studies represents that observed in a high-solubility model material, where the diffusion rate can sustain equilibrium of the hydrogen concentration ahead of the steadily propagating crack tip. The constitutive model accounts for the influence of hydrogen on the elastic-plastic regimes of material response at the continuum level, e.g. hydrogen-induced material softening. The model reflects the amount of hydrogen in the material under stress and the intensity of hydrogeninduced softening in the material. The hydrogen influenced, crack front fields serve as input to an exponential-based characterization of void growth rates which provides qualitative estimates for the impact of hydrogen on tearing resistance curves. The analyses suggest significantly higher void growth rates exist in a hydrogen-charged material than in a hydrogen free material, with a corresponding reduction in tearing resistance in the presence of hydrogen regardless of the level of imposed constraint.

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1. Introduction

The rising interest in hydrogen as a fuel motivates new concerns for the design and maintenance of facilities employed in the manufacture, transport, and storage of hydrogen. Structural metals exhibit mechanical properties that often differ in hydrogen charged and hydrogen free conditions, e.g. the detrimental effect of hydrogen on the resistance to the propagation of crack-like defects (Robinson and Stoltz, 1981). Well-understood methodologies of defect assessment appropriate for hydrogen free metals will likely require modifications in the presence of hydrogen to reflect metallurgical scale effects. For example, the conventional view of fracture behavior in ductile metals at engineering scales neglects complex interactions that may develop between the mechanical fields and materials in the presence of hydrogen. A key component of defect assessment strategies thus requires an understanding of the engineering behavior and failure mechanisms of hydrogen charged metals.

Ductile crack propagation occurs in metals most often by the growth of micro-voids ahead of the crack tip that coalesce to form

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new crack surfaces. High triaxiality levels and large plastic strains accelerate void growth (Rice and Tracey, 1969) and lead to the onset of void coalescence. Hydrogen facilitates plastic deformation by increasing dislocation velocities which leads to a local flow stress reduction that influences both the local triaxiality and plastic strain in a complex manner. Changes in the local triaxiality and plastic strain in the presence of hydrogen impact void growth rates at the metallurgical scale and the resistance to macroscopic crack extension at the engineering scale. Studies that describe crack propagation in ductile metals enriched by hydrogen may examine, for example: cyclic fatigue growth, growth emerging from a plastically deforming-blunting crack tip, crack advancement under a sustained load, or slow stable tearing under increased load. The present study focuses on steady crack extension outside the region of material influenced by initial blunting of the pre-existing stationary crack when the tearing resistance approaches a constant value. Such steady-state growth conditions at constant front loading, and where the diffusion rate can sustain equilibrium of the hydrogen concentration ahead of the propagating crack tip, represent the classical Stage II regime of sustained load crack growth (Wei et al., 1984).

Various numerical studies examine the characteristics of a steadily propagating crack in an elastic-plastic material based

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Nomenclature

- ctotal concentration of hydrogen in atoms per solvent
atomcLNILS concentration of hydrogen in atoms per solvent
- atom *c*_T trap site concentration of hydrogen in atoms per solvent atom

c_L^0	initial NILS concentration of hydrogen in atoms per sol-
-	vent atom in stress-free lattice
c_T^0	initial trap site concentration of hydrogen in atoms per
-	solvent atom in stress-free lattice
J	J-integral value applied remotely
K _I	stress intensity factor applied remotely
Т	elastic T-stress

on a small-scale yielding (SSY) formulation first suggested by Dean and Hutchinson (1980). Their method integrates the steady-state constitutive relations along planes parallel to an advancing crack tip. Freund and Douglas (1982) extend this method to rapidly propagating cracks including inertial forces and, using a critical strain-characteristic distance criterion, generate toughness vs. crack velocity curves in good agreement with experimental results. By imposing positive and negative *T*-stress conditions in the SSY framework, Varias and Shih (1993) determine that key values of stress field ahead of an advancing crack decrease with non-zero values of the remotely imposed T-stress. Landis et al. (2000) incorporate a rate dependent, cohesive zone ahead of a propagating crack in an elastic-viscoplastic material; their computations indicate that the steady-state toughness may increase or decrease with increasing crack tip velocity. For cracks propagating within a weld, Niordson (2001) employs a cohesive zone model and finds that thinner welds lead to higher values of crack driving force and that crack propagation slightly outside of the weld metal generates lower driving forces. Ferracin et al. (2003) extend the steady-state formulation to include finite rotation effects, while retaining small deformation kinematics, to determine the cohesive zone properties of an adhesive bonding two sheets of metal that deform plastically. In a key finding that simplifies models for steady-growth, the asymptotic analyses of Reid and Drugan (1993) demonstrate that the size of the blunting region for propagating cracks remains significantly smaller than for a stationary crack, thereby minimizing the need to incorporate finite deformation effects.

The hydrogen enhanced, localized plasticity mechanism (HELP) represents a viable model for hydrogen-induced material degradation (Beachem, 1972; Birnbaum and Sofronis, 1994). Over a range of temperatures and strain rates, hydrogen decreases the barriers to dislocation motion (Shih et al., 1988; Sirois et al., 1992; Sirois and Birnbaum, 1992). Both experimental observations (Sirois et al., 1992; Sirois and Birnbaum, 1992; Robertson, 2001) and theoretical calculations (Birnbaum and Sofronis, 1994; Sofronis, 1995; Sofronis and Birnbaum, 1995) support this interpretation. Thus, the amount of plastic deformation increases within regions of hydrogen accumulation, and, consequently, the fracture event becomes a highly localized process of ductile rupture—not an embrittlement (Birnbaum et al., 1997).

Sofronis et al. (2001) argue that a critical question remains unresolved: how hydrogen-induced material softening at the microscale promotes shear localization at the macroscale with concomitant ductile fracture. Clearly, hydrogen-induced softening promotes inhomogeneous plastic deformation (Birnbaum et al., 1997), but the mechanistic means by which hydrogen pro-

$\overline{arepsilon}^p$	equivalent plastic strain
θ_L	hydrogen occupancy at NILS
θ_T	hydrogen occupancy at trap sites
σ_0	initial yield stress of hydrogen free material
σ_e	Von Mises stress
σ_m	mean stress ($\sigma_{kk}/3$)
σ_y	post-yield flow stress
ξ	intensity of hydrogen-induced softening parameter
ζ	measure of ductile void growth
■ref	calculated values of variable . when $T/\sigma_0 = 0, \ c_I^0 = 0$
HÉLP	hydrogen enhanced, localized plasticity
NILS	normal interstitial lattice sites

motes localization of plastic flow remains unclear. Finite element simulations indicate complex interactions of the localized material response and geometric constraint in hydrogen-charged materials. Taha and Sofronis (2001) calculate the hydrogen concentrations ahead of a stationary, blunting crack under SSY conditions and in a four-point bend specimen for a non-softening material in the presence of hydrogen. For softening materials, Sofronis et al. (2001) predict the conditions for development of shear bands in the presence of hydrogen. Liang et al. (2004) study the influence of material softening, the level of imposed constraint via the T-stress, and the concentration of initial hydrogen on the void growth rates ahead of a stationary, blunting crack. As predicted in a SSY analysis by Ahn et al. (2007a,b), propagating cracks in a hydrogen-charged material exhibit reduced fracture toughness and tearing resistance during the early stages of crack extension within the initial blunting field. The present work extends the efforts of Ahn et al. (2007a,b) to represent larger amounts of ductile crack extension when steadystate conditions prevail also in a hydrogen-charged material, with the hydrogen concentration in equilibrium. When the crack-tip velocity, material properties and loading preclude the equilibrium of hydrogen concentration adopted for the present analyses, the interaction effects must be included as in the work of Dadfarnia et al. (2009) for austenitic steels in which hydrogen diffusion is extremely slow. From experimental work, Wei and colleagues (1984) conclude that hydrogen diffuses very rapidly through systems such as ferritic steels and that steady crack growth approaching 1 mm/s is sustainable without diffusion limitation. Hence, the assumption of equilibrium conditions for hydrogen ahead of a steadily propagating tip is a valid one for systems in which hydrogen diffuses fast.

This paper begins with a description of the computational model for steady-state crack growth in SSY conditions and the material constitutive model that reflects hydrogen-induced softening. The following section describes key features of the near tip fields ahead of a steadily propagating crack as influenced by the hydrogen-induced initial reduction of the yield stress, the initial hydrogen concentration in the stress-free material, and the imposed constraint modeled through the T-stress. These crack tip fields drive a simple, damage parameter for void growth as described in the next section to examine the influence of hydrogen on crack growth resistance. The final section summarizes the major results and conclusions of the present study. Two appendices present additional details for the steady-state formulation and the constitutive implementation of the effect of hydrogen on the plastic deformation in the material.

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