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Prediction of diffusion assisted hydrogen embrittlement failure in high strength martensitic steels

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ABSTRACT

A stress assisted hydrogen diffusion transport model, a dislocation-density-based multiple-slip crystalline plasticity formulation, and an overlapping fracture method were used to investigate hydrogen diffusion and embrittlement in lath martensitic steels with distributions of $M_{23}C_6$ carbide precipitates. The formulation accounts for variant morphologies based on orientation relationships (ORs) that are uniquely inherent to lath martensitic microstructures. The interrelated effects of martensitic block and packet boundaries and carbide precipitates on hydrogen diffusion, hydrogen assisted crack nucleation and growth, are analyzed to characterize the competition between cleavage fracture and hydrogen diffusion assisted fracture along preferential microstructural fracture planes. Stresses along the three cleavage planes and the six hydrogen embrittlement fracture planes are monitored, such that crack nucleation and growth can nucleate along energetically favorable planes. High pressure gradients result in the accumulation of hydrogen, which embrittles martensite, and results in crack nucleation and growth along {110} planes. Cleavage fracture occurs along {100} planes when there is no significant hydrogen diffusion. The predictions indicate that hydrogen diffusion can suppress the emission and accumulation of dislocation density, and lead to fracture with low plastic strains.

1. Introduction

Hydrogen diffusion in metals and alloys results in embrittlement and fracture due to introduction of hydrogen, which can be due to electrochemistry, diffusion, or external loading conditions (Lynch, 2012; Olden et al., 2008b). Hydrogen embrittlement can be generalized as a three-step sequential process: (1) the introduction of hydrogen into metals, through processes, such as electrochemical charging or gaseous absorption; (2) the transportation of hydrogen atoms through crystalline lattice; (3) the nucleation and growth of hydrogen assisted cracks (Eliaz et al., 2002; Serebrinsky et al., 2004). Several embrittlement mechanisms have been proposed, which include hydride formation and fracture (Lufrano et al., 1996), hydrogen enhanced decohesion (HEDE) (Oriani and Josephic, 1977, 1974), and hydrogen enhanced local plasticity (HELP) (Birnbaum and Sofronis, 1994; Martin et al., 2011).

High strength martensitic steels are extremely susceptible to hydrogen embrittlement, even at very low hydrogen concentrations (Lee et al., 2010; Lee and Gangloff, 2007; Nagao et al., 2012; Ramamurthy and Atrens, 2013). The effects of

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hydrogen concentration on embrittlement in martensitic steels have been investigated using quasi-static and creep tests, which indicate that hydrogen can decrease tensile strength in a power law manner (Kim et al., 2009; Wang et al., 2007, 2005). Microstructural characteristics, such as grain size, carbide precipitates, and retained austenite, can also significantly affect the susceptibility of martensitic steels to hydrogen diffusion and embrittlement due to interfacial effects, such as dislocation-density interactions and interfacial stress mismatches (Craig and Krauss, 1980; Fuchigami et al., 2006; Kim et al., 1986). Hydrogen diffusion assisted microstructural fracture in lath martensitic steel occurs on {110} glide planes (Kim and Morris, 1983; Shibata et al., 2012), which is different from the cleavage planes of {100} (Guo et al., 2004; Randle and Davies, 2005; Morris, 2011).

Finite element models for hydrogen diffusion have been used to investigate the effects of hydrostatic stress on hydrogen distribution ahead of a stationary crack tip (Krom et al., 1999; Sofronis and McMeeking, 1989; Taha and Sofronis, 2001). Hydrogen assisted crack growth in high strength steels was investigated by the use of a hydrogen dependent cohesive zone model (Serebrinsky et al., 2004) and it was coupled to a stress-assisted hydrogen diffusion model, but this approach did not account for the crystalline structure and the inherent anisotropy of martensitic steels. Rimoli and Ortiz (2010) coupled a cohesive zone model and grain boundary diffusion to crystal plasticity to investigate intergranular hydrogen diffusion and embrittlement. However, the critical martensitic characteristics, such as ORs, morphologies, parent austenite orientations, initial dislocation densities, retained austenite, carbide precipitates, and crack growth along specific crystallographic planes were not accounted for in that investigation.

To address these issues, we have adapted a stress-assisted hydrogen diffusion model (Serebrinsky et al., 2004) and a dislocation-density based multiple-slip crystalline plasticity formulation (Wu et al., 2013; Shanthraj and Zikry, 2012; Zikry and Kao, 1996) to investigate hydrogen diffusion and embrittlement in lath martensitic steels. In this framework, we account for variant morphologies and ORs that are uniquely inherent to lath martensitic microstructures. A dislocation-density GB interaction scheme that is representative of the resistance to dislocation transmission across martensitic block and packet boundaries has been incorporated into the dislocation-density based crystalline plasticity formulation. A fracture method based on the overlapping element method of Wu and Zikry (2014) and Hansbo and Hansbo (2004), is also used to generate failure surfaces along hydrogen assisted microstructural fracture planes {110} as a function of hydrogen concentration and diffusion, carbide precipitate interfaces, dislocation-density evolution, and martensitic block orientations. The formulation is then used to investigate the effects of martensitic block and packet boundaries and carbide precipitates on hydrogen diffusion and embrittlement, and to understand and predict how hydrogen diffusion affects dislocation-density evolution and subsequent martensitic embrittlement.

This paper is organized as follows: the dislocation-density based crystalline plasticity formulation, the derivation of the dislocation-density GB interaction and the stress assisted hydrogen diffusion model are presented in Section 2, the microstructure-based failure criterion, and the numerical implementation of overlapping element method for fracture are outlined in Section 3, the results are presented and discussed in Section 4, and a summary of the results and conclusions are given in Section 5.

2. Constitutive formulation

In this section, only a brief outline of the multiple-slip crystal plasticity rate-dependent constitutive formulation and the evolution equations for the mobile and immobile dislocation-densities, which are coupled to the constitutive formulation, are presented. A detailed presentation is given by Shanthraj and Zikry (2011).

2.1. Multiple-slip dislocation-density based crystal plasticity formulation

The dislocation-density based crystal plasticity constitutive framework used in this study is based on a formulation developed by Zikry (1994), Shanthraj and Zikry (2012), and Ziaei and Zikry (2015), and a brief outline will be presented here. It is assumed that the velocity gradient is decomposed into a symmetric deformation rate tensor D_{ij} and an anti-symmetric spin tensor W_{ij} (Asaro and Rice, 1977). The tensors D_{ij} and W_{ij} are then additively decomposed into elastic and inelastic components as

$$D_{ij} = D_{ij}^{*} + D_{ij}^{p}, \quad W_{ij} = W_{ij}^{*} + W_{ij}^{p}, \tag{1 a-b}$$

The superscript * denotes the elastic part, and the superscript p denotes the plastic part. W_{ij}^{*} includes the rigid body spin. The inelastic parts are defined in terms of the crystallographic slip-rates as

$$D_{ij}^{p} = \sum_{\alpha} P_{ij}^{(\alpha)}\dot{\gamma}^{(\alpha)}, \text{ and } W_{ij}^{p} = \sum_{\alpha} \omega_{ij}^{(\alpha)}\dot{\gamma}^{(\alpha)} \tag{2 a-b}$$

where α is summed over all slip-systems, and $P_{ij}^{(\alpha)}$ and $\omega_{ij}^{(\alpha)}$ are the symmetric and anti-symmetric parts of the Schmid tensor in the current configuration respectively.

A power law relation can characterize the rate-dependent constitutive description on each slip system as