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PII: S0022-5096(18)30358-2
DOI: https://doi.org/10.1016/j.jmps.2018.09.012
Reference: MPS 3443

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 30 April 2018
Revised date: 10 September 2018
Accepted date: 12 September 2018

Please cite this article as: Lallit Anand, Yunwei Mao, Brandon Talamini, On modeling fracture of ferritic steels due to hydrogen embrittlement, *Journal of the Mechanics and Physics of Solids* (2018), doi: https://doi.org/10.1016/j.jmps.2018.09.012

# On modeling fracture of ferritic steels due to hydrogen embrittlement

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## Abstract

Experimental studies in the literature show that the fracture of ferritic steels in the presence of hydrogen occurs primarily perpendicular to the direction of the maximum principal tensile stress, is transgranular in nature, and has fracture surfaces which show "quasi-cleavage" features. Such features are cleavage-like but not along any known cleavage plane or grain boundaries. While the precise micromechanisms which lead to a transition from regular plastic deformation of the steel to "quasi-brittle" fracture are at present unclear, in this paper we have formulated a continuum theory for the diffusion of hydrogen coupled with the elastic-viscoplastic response of metals, together with a simple model which leads to quasi-brittle fracture in the presence of hydrogen. We assume that when an internal variable $\varphi$ of the theory reaches a critical value $\varphi_{\rm cr}$, then the inelastic deformation transitions from (a) a volume-preserving plastic stretching which occurs in the direction of the stress deviator — as in standard Mises-type plasticity, to (b) a different form of inelastic stretching which occurs in the direction of the maximum principal stress, and which is dilational in nature. We call this latter form of inelastic deformation *craze inelasticity.* We view the strain produced due to crazing as a "quasi-brittle" form of inelastic deformation. We allow only a small amount of inelastic craze-strain before the process of craze-breakdown and fracture sets in. To model craze-breakdown we introduce a damage variable $\mathsf{d} \in [0,1]$; if $\mathsf{d}=0$ at a point then that point is intact, while if $\mathsf{d}=1$ at some point then that point is fractured. With the aim of "regularizing" the strain-softening behavior during craze-breakdown, and to avoid mesh-dependency related issues during finite element simulations, we develop a damage theory which depends not only on $\mathsf{d}$ but also its gradient $\nabla\mathsf{d}$, which is considered to be a measure of the spatial inhomogeneity of the damage during the craze-breakdown process. We have numerically implemented our coupled diffusion-deformation-damage theory in a finite element program, and we present representative numerical examples which show the ability of the simulation capability to qualitatively replicate the process of fracture due to hydrogen embrittlement in some technically relevant geometries.

Keywords: elastic-plastic deformation; hydrogen diffusion; hydrogen embrittlement; coupled theory; phase field fracture.

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