Towards modeling hydrogen embrittlement of ferritic steels: a phase-field/gradient-damage model

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Abstract

Recently published experimental studies by Neeraj et al. (2012) show the presence of nanoscale voids on fracture surfaces of ferritic steels in the presence of hydrogen. A potential hydrogen embrittlement mechanism proposed by Li et al. (2015) in connection with these experiments, is that plastic deformation leads to production of vacancies due to dislocation multiplication interactions, which in the presence of hydrogen are stabilized as hydrogen-vacancy complexes which can agglomerate and grow in size to nucleate nanovoids, which in turn serve as precursors to final fracture. In addition to the nanoscale voids observed by Neeraj et al. (2012), the recent experimental studies of Martin et al. (2011a,b) show that the fracture surfaces in steels also show *quasi-cleavage* features; quasi-cleavage is a common feature of hydrogen-induced fracture surfaces, which is cleavage-like but not along any known cleavage plane, or grain boundaries.

Based on these recent experimental obervations, and guided by the hydrogen embrittlement mechanism suggested by Li et al. (2015), we have formulated a continuum theory for the diffusion of hydrogen coupled with the elastic-viscoplastic response of metals, together with an accounting for microscopic effects due to trapping of hydrogen in hydrogen-vacancy complexes, culminating in eventual fracture. We postulate that when the hydrogen which is trapped in hydrogen-vacancy complexes reach a critical concentration, then there is a change in mechanism of inelastic deformation from standard plastic flow by dislocation glide to plastic flow by a quasi-cleavage type mechanism — a change in mechanism which is reminiscent of a transition between "shear-yielding" and "crazing" in amorphous polymers. We have formulated a criterion for this change in mechanism together with an attendant dilatant craze-plasticity flow rule, and a corresponding craze strain based fracture criterion to model hydrogen embrittlement of ferritic steels.

Our theory introduces an equivalent craze strain ϵ^c as a measure of the history of crazing in the material. An increase in the craze strain will result in the formation of localized dilational craze bands. Eventually when the craze strain exceeds a critical value, $\epsilon^c_{\rm cr}$, the process of "break-down" of the crazed material will start. In order to model the final fracturing process we introduce an *order-parameter* $\varphi(\mathbf{X},t) \in [0,1]$, which evolves ($\dot\varphi > 0$) when ϵ^c exceeds $\epsilon^c_{\rm cr}$. In a monotonic deformation process when ϵ^c reaches $\epsilon^c_{\rm cr}$ the material has crazed to a critical level, and the order parameter has a value $\varphi = 0$. The process of craze break-down starts as ϵ^c exceeds $\epsilon^c_{\rm cr}$, and φ increases. When $\varphi = 1$ at some material point, then that point is fractured; values of φ between zero and one correspond to partially-fractured material. With the aim of *regularizing* the strain-softening behavior during craze break-down, and to obtain mesh-objective results in finite element simulations, we follow recent phase-field theories of fracture in ductile materials (cf., e.g., Miehe et al., 2015b, 2016) and develop a fracture theory which depends not only on φ but also its gradient $\nabla\varphi$, which is considered to be a measure of the spatial inhomogeneity of the damage during the craze break-down fracture process.

We have numerically implemented our coupled diffusion-deformation-failure theory in a finite element program, and we present representative numerical examples which show the ability of the simulation capability to qualitatively replicate the failure due to hydrogen embrittlement in some technically relevant geometries.

References

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