Theoretical and computational framework for the prediction of fracture energy in brittle and ductile materials in presence of hydrogen

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ABSTRACT

In presence of hydrogen, most of materials experience significant degradation of their mechanical properties which is commonly known as hydrogen embrittlement (HE). These detrimental effects are reported in terms of reduction in ductility, strength and toughness. As a result, HE may cause premature catastrophic failures such that materials fail at loading levels much lower than the hydrogen free case. Two mechanisms have been suggested in the literature to explain HE, namely, hydrogen induced decohesion (HID) and hydrogen enhanced local plasticity (HELP). In HID mechanism, hydrogen accumulates at a crack tip and reduces the atomic bond strength and hence the energy required to fracture. In HELP mechanism, hydrogen accelerates the dislocation mobility by reducing the elastic interaction energy between dislocations, i.e. known as elastic shielding effect, which results in material softening. Hence, we are interested in investigating HE effects on crack initiation. In particular, we aim to develop mechanistic models to explain and predict the loss in loading capacity of cracked solids.

In this work, theoretical and computational investigations of fracture deriving force and fracture toughness in presence of hydrogen are presented. The fracture zone is assumed to be concentrated in a narrow zone directly ahead of the crack tip. The objective is to predict crack initiation in two classes of materials; brittle and ductile materials, and to investigate the effect of different material parameters on the crack initiation. The fracture deriving force and fracture toughness were determined using the path-independent integral for fracture of solids under combined chemical and mechanical loadings that is introduced by Haftbaradaran and Qu (2014). We concentrated initially in studying brittle fracture. The bulk material is assumed to be isotropic elastic and a traction-separation model is proposed to model the fracture process. More specifically, a simple traction-separation law of a constant traction without damage development is adopted. A double cantilever beam specimen (DCB) subjected to a shear force is then investigated. We obtained expressions for the fracture deriving force and fracture toughness by evaluating the *J*-integral in chosen contours in the far field and surrounding the fracture zone. The critical load is then obtained by invoking the path independence of the J-integral using these contours. We determined that the presence of hydrogen introduces an additional fracture driving force that can be expressed in terms of an increase in the total compliance of the system. In the second part of the study, we investigated the effect of hydrogen in elastic-plastic materials in which the plastic deformation at the crack tip is limited to small scale yielding. We developed the form of fracture toughness for the cases of plane stress and strain conditions for small scale yielding. Further, we extended the study on the DCB specimen and used the finite element method to determine the fracture toughness and the plastic work. The result shows that the reduction of the cohesive strength due to HID reduces the total work of fracture significantly and may lead to a transition to brittle failure.

REFERENCES

[1] H Haftbaradaran and J Qu, "A path-independent integral for fracture of solids under combined electrochemical and mechanical loadings." *Journal of the Mechanics and Physics of Solids*, **71**, 1-14 (2014).