

Modeling of a Crack-induced Hydride Formation at a Grain Boundary in Metals

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Crack-induced hydride formation can occur in specific metallic structures, reducing their mechanical properties and facilitating failure. Grain boundaries are observed to be preferential sites for hydride formation. We present a phase-field approach describing the kinetics of crack-induced hydride formation at a grain boundary, by using the Allen–Cahn formulation and including the increase in grain boundary energy. Hydride development is found to occur at the crack tip and in the grain boundary. These regions seemingly evolve independently, except when the crack is very close to or lies in the grain boundary.

INTRODUCTION

Hydrogen-rich environments are commonly seen as threats to metallic structures in operation. The interaction hydrogen/matter can lead to the reduction of the mechanical performance or even the derogation of the function of a component (ASM International, 2002). In specific metals such as titanium and zirconium alloys, this interaction can result in the formation of brittle phases within the bulk, affecting the material properties. One hydrogen-induced degradation process involving hydride formation is the so-called delayed hydride cracking (DHC), for which crack propagation is delayed and occurs stepwisely as brittle hydride phases form in the crack-tip vicinity (Puls, 2012). In fact, the stress is known to be a vector for hydrogen diffusion in metallic materials. Hydrogen migrates toward high hydrostatic stress regions, where the concentration can exceed the solubility limit, which can itself be reduced by the presence of tensile stress. Thus, hydrides possibly form in tensile stress regions such as areas in proximity of a crack tip, as observed in Shih et al. (1988). Additionally, grain boundaries have been found to be preferential sites for hydride formation in polycrystals (Coleman, 2003; Liu et al., 2018). When a crack lies near and in a grain boundary (GB), hydride formation might be promoted by the combination of the two aforementioned situations. The phase-field theory based on a smooth interface formulation is suited, in terms of simplicity and computational efficiency, to study microstructure evolution and second-phase precipitation (Provatas and Elder, 2010). This approach has been used in numerous applications (Chen, 2002; Moelans et al., 2008) and has been successfully employed to study defect-induced hydride formation (Massih, 2011; Bjerken and Massih, 2014; Nigro et al., 2018). In this paper, a phase-field method is used to investigate hydride precipitation in the presence of an opening crack lying near and in a GB. To this end, and to minimize the computational cost, linear elastic fracture mechanics (LEFM) is utilized to model the implicit presence of the crack near and perpendicular to the interface between two grains. The solid solution is assumed to be

isotropic and elastic. Possible plastic effects are disregarded. During phase transformation, a volume change connected to the lattice misfit between hydride and solid solution has been observed to occur (Banerjee and Arunachalam, 1981). This type of dilatational effects is taken into account in the model. Moreover, the bulk energy density, also known as the Landau potential, is written such that the energy barrier level in the GB can be controlled. In this paper, the evaluation of the model potentialities is made by focusing on the effects of the crack-tip/GB distance and the magnitude of the energy barrier in the GB on hydride formation. The results are presented for a titanium alloy for which we consider an α/α crystal interface.

MODEL DESCRIPTION

In this study, the considered domain is an infinite plate, which is divided into two semi-infinite regions, as presented in Fig. 1. Regions 1 and 2 can represent two different grains of the same phase, α , and are supposed to contain the same content of hydrogen. To model the phase evolution, the present approach employs a dimensionless non-conserved phase-field variable $\eta_i = (\eta_1, \eta_2)$. This two-component field function depends on time t and space, defined in a cylindrical coordinate system (r, θ, z) or a Cartesian one $(x, y, z) = (r \cos \theta, r \sin \theta, z)$. The first component of the phase-field variable represents the microstructural state of the material making the distinction between matrix and hydride: $\eta_1 = -1$ indicates the matrix, $\eta_1 = 1$ refers to the hydride phase, and the intermediate values are associated with the matrix/hydride interface. The second component of the phase-field variable is used to distinguish the different matrix regions so that $\eta_2 = 1$ represents region 1 and $\eta_2 = -1$ refers to region 2. The separation line between the matrix regions is a smooth interface, which corresponds to values of η_2 taken in $]-1, 1[$.

In this model, the second-phase precipitation is driven by a kinetic equation, based on an energy minimization scheme, also known as the Allen–Cahn equation, which can be expressed as (Allen and Cahn, 1979)

$$\frac{\partial \eta_i}{\partial t} = -\Gamma_{ij} \frac{\delta F}{\delta \eta_j} \quad (1)$$

where Γ_{ij} is a diagonal matrix referred to as the mobility tensor and is multiplied by the functional derivative of the total free energy F of the system with respect to the phase-field variable.

Received February 28, 2020; updated and further revised manuscript received by the editors April 9, 2020. The original version (prior to the final updated and revised manuscript) was presented at the Twentieth International Ocean and Polar Engineering Conference (ISOPE-2019), Honolulu, Hawaii, June 16–21, 2019.

KEY WORDS: Hydrogen embrittlement, phase transformation, phase-field method, Allen–Cahn formulation, hydride precipitation, mode I crack, grain boundary.