Simulation of hydride-induced steady-state crack growth in metals – Part II: general near tip field

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Abstract Hydride-induced steady-state crack propagation in metals is investigated under conditions of constant temperature, plane strain, small-scale yielding and small-scale hydride precipitation, by taking into account the coupling of the operating physical processes. It is shown that the near-tip field depends on a normalized stress intensity factor, which incorporates both effects of the applied stress intensity factor and the crack velocity. According to Part I of the present study, when the normalized stress intensity factor tends to zero, the crack-tip field near the threshold stress intensity factor is produced, which is characterized by a constant hydrostatic stress in the hydride precipitation zone. As the value of the normalized stress intensity factor increases, the evolution of the near-tip field for crack propagation from stage-I to stage-II regime is produced: the actual size of the hydride precipitation zone decreases, the hydrostatic stress increases, deviating from the level of the plateau, and the near-tip field tends to that of a hydrogen-free metal. The near-tip field depends strongly on hydrogen concentration, far from the crack tip. The stage-II crack growth velocity is predicted and the experimentally observed effect of metal yield stress and temperature on crack velocity is confirmed.

Keywords Crack growth, Steady state, Hydrogen embrittlement, Hydride

1 Introduction

Hydrogen embrittlement in metals can be divided in two broad categories: (a) embrittlement with the precipitation of hydrides, as in the case of zirconium-, titanium-, niobium- and vanadium- alloys, (e.g. [3, 12, 15, 17]) and (b) embrittlement without hydride formation, observed, for example, in alloys of iron, nickel, aluminum and titanium (e.g. [14–16, 18]).

The objective of the present work, discussed in two parts, is the simulation of sub-critical crack growth, when hydrides form. Emphasis has been placed in the coupling of the operating physical processes, which as shown has very important consequences on the structure of the near-tip field. Indeed, hydride induced sub-critical crack growth generally results from the simultaneous operation of the interrelated processes of hydrogen diffusion, hydride precipitation, non-mechanical energy flow, material deformation and fracture (e.g. [21]). The diffusion of hydrogen is driven by the gradients of temperature and its chemical potential (e.g. [5]), which in addition depends on stress [9]. The terminal solid solubility of hydrogen, at which hydride precipitation occurs, increases with temperature but also depends on stress. The stress effect on hydride precipitation is a consequence of the different lattice dimensions and elastic properties of the hydride and the metal as well as of the volume occupied by hydrogen in solid solution [20]. The deformation of the material is also strongly affected by the volume changes, which are caused mainly by temperature variations and hydride precipitation.

The degradation of a metal, due to hydride precipitation ahead of a stationary crack, under constant temperature, was simulated by Lufrano et al. [10–11]. The coupling between hydrogen diffusion, hydride precipitation and elastic [11] as well as elastic-plastic [10] material deformation was taken into account. Varias and Massih [21–22] considered in addition non-mechanical energy flow and transient crack propagation. The bulk of the material was assumed to be elastic. However, non-linear effects were taken into account in defining the constitutive relations of the de-cohesion layer, which was used to simulate crack growth. Reviews and detailed references on previous developments can be found in the works by Lufrano et al. [11] and Varias and Massih [21].

The present study focuses on steady-state sub-critical crack growth, where no earlier publications have been made by considering the coupling of the operating physical processes. The general structure of the near-tip field is revealed for crack growth under plane strain, small-scale yielding, small-scale hydride-precipitation and constant temperature. In Part I [20] crack growth near hydrogen chemical equilibrium, i.e. near the threshold stress intensity factor, was presented. It was shown that hydride-induced propagation is associated with a near-tip field, which is completely different from...
that of a hydrogen-free metal (e.g. [6]). A peculiar characteristic of this field is a hydrostatic stress plateau, which dominates in an annulus of the hydride precipitation zone near the crack tip, i.e. ahead as well as behind the crack tip. The plateau was shown, analytically, to be a consequence of approaching hydrogen chemical equilibrium. The features of this field were used to predict the conditions, under which no hydride precipitation occurs ahead of the crack tip and therefore the sub-critical crack growth mechanism is suppressed. In the case of hydride precipitation near the crack tip, the threshold stress intensity factor was also predicted. The model was applied to single-phase zirconium alloys of different values of yield stress as well as at different temperatures. The theoretical predictions of the threshold stress intensity factor were found to be in excellent agreement with the experimental measurements.

In the second part, hydride-induced crack growth is simulated, under conditions away from hydrogen chemical equilibrium. Then the crack propagates away from the threshold, within stage-I or stage-II regime. The structure of Part II is as follows. In Sect. 2, the boundary value problem and the general structure of the near-tip field are briefly discussed. Details as well as the discussion on the governing and constitutive equations of hydrogen diffusion, hydride precipitation and material deformation are given in Part I [20]. Subsequently a parametric study is presented, in Sect. 3. The combined effect of crack-tip velocity and applied stress intensity factor on the near-tip field is discussed in Sect. 3.1. An important characteristic of the near-tip field is revealed: the field depends on a normalized stress intensity factor, which contains both effects of crack-tip velocity and applied stress intensity factor. In Sect. 3.2, the strong influence of remote hydrogen concentration on the distributions of field quantities, near the crack-tip, is shown. The effects of hydride elastic properties, temperature, solid-solution yield stress as well as of crack face boundary conditions are discussed in Sect. 3.3. The characteristics of the field are used to predict stage-II crack growth velocity in Sect. 4. The predictions are compared with experimental data of single-phase zirconium alloys. A discussion on the development of striations on the fracture surface is also presented. Finally, conclusions are given in section 5.

2 Boundary value problem – general structure of the near-tip field

The boundary value problem is identical to that described in Part I [20]. A crack is moving with a velocity, \( V_c \), in a hydride forming metal, under conditions of plane strain, constant temperature, small-scale yielding and small-scale hydride precipitation. Steady-state crack growth is also assumed. A Cartesian coordinate system, \( (x_1, x_2) \), is considered, with origin at the moving crack tip. \( x_1 \) is the direction of crack propagation. \( (r, \theta) \), is the respective cylindrical coordinate system, where \( r \) is the radial distance from the crack tip and \( \theta \) is the angle, measured from the crack plane.

Far from the crack tip, at a distance which is large compared to the size of the plastic zone, \( r_p \), and the hydride-precipitation zone, \( L_{hz} \), K-field dominates:

\[
\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta), \quad r >> r_p, \quad r >> L_{hz}.
\]

\( L_{hz} \) is measured on the crack plane, ahead of the crack tip (see Fig. 1 of Part I [20]). \( \sigma_{ij} \) is the stress tensor; the italic is the \( \sigma_{ij} \) for an elastic composite material, made of hydrides and a metal. It corresponds to the case of crack growth in an oxide layer in the case of zirconium alloys). A peculiar characteristic of this field is a hydrostatic stress plateau, which dominates in a film on the solid solution with different elastic moduli. In the second case, the composite elastic properties depend on hydride and the solid solution have identical elastic-plastic properties or for an elastic composite material, made of hydrides and solid solution with different elastic moduli. In the second case, the composite elastic properties depend on hydride