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A coupled elastoplastic-transient hydrogen diffusion analysis to simulate the onset of necking in tension by using the finite element method

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ARTICLE INFO

Article history:

Received 17 August 2009

Received in revised form

4 November 2009

Accepted 5 November 2009

Available online 4 December 2009

Keywords:

Necking

Shear localization

Hydrogen embrittlement

Local flow stress

Coupled analysis

Transient hydrogen diffusion

Finite element

ABSTRACT

Hydrogen-enhanced localized plasticity (HELP) is an acceptable mechanism for hydrogen embrittlement which is based on the experimental observations and the theoretical computations. The underlying principle in the HELP theory is that the presence of hydrogen causes the localization of the slip bands which results in the decrease of the fracture strength. In a sample under plane-strain tensile stress, plastic instability can lead to either the concentration of plastic flow in a narrow neck or bifurcation from homogeneous deformation into a mode of an exclusively localized narrow band of intense shear. Recently, it has been demonstrated that the presence of hydrogen can indeed induce shear banding bifurcation at macroscopic strains. By using a steady-state equilibrium equation for hydrogen diffusion analysis, the effect of hydrogen on the bifurcation of a homogeneous deformation in a plane-strain tension specimen into a necking or a shear localization mode of deformation has already been studied. In the present research, using a transient hydrogen diffusion analysis and introducing a new constitutive equation accompanied by considering the reduction in the local flow stress upon hydrogen dissolution into the lattice, the effect of hydrogen on shear localization is investigated. In addition, progress has been made in that, the changes in the distribution of the total and trapping hydrogen concentrations through the loading time and particularly during the development of the necking event have been determined.

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1. Introduction

Presence of dissolved atomic hydrogen in metals and alloys can severely degrade mechanical properties and fracture toughness, reduce the fracture strength and accelerate the crack growth [1,2]. The role of hydrogen in hydrogen embrittlement, stress corrosion cracking and hydrogen induced cracking has been largely determined. Recently, several

mechanisms have been proposed by different researchers. Among these suggestions, three mechanisms appear to be viable; stress induced hydride formation and cleavage [3], hydrogen induced decohesion [4,5] and hydrogen enhanced localized plasticity (HELP) [6–10].

Hydrogen-enhanced localized plasticity (HELP) is an acceptable mechanism for hydrogen embrittlement which is based on the experimental observations and theoretical

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doi:10.1016/j.ijhydene.2009.11.024

computations. The underlying principle in the HELP theory is that the presence of hydrogen causes the localization of the slip bands which results in the decrease of the fracture strength. According to the HELP theory, the presence of hydrogen in a solid solution increases the dislocation motion, thereby increasing the amount of plastic deformation that occurs in a localized region adjacent to the fracture zone.

Sofronis and McMeeking [11] proposed a finite element model to show the effect of hydrostatic stress and trapping phenomenon on hydrogen distribution in plastically deformed steels. Based on their model, Krom et al., [12] suggested a formulation to provide the hydrogen balance by considering a strain rate factor in the hydrogen transport equation. Kanayama et al., [13] used a different finite element scheme from Krom et al., [12] and applied the Galerkin method in a 3D simulation in order to reconstruct the Sofronis and McMeeking's model [11]. Taha and Sofronis [14] analyzed the material mechanical behavior at a crack tip or a rounded notch with that of hydrogen diffusion.

The underlying principle in the HELP mechanism is the shielding of the elastic interactions between dislocations and obstacles by the hydrogen solutes [6,9,15]. This interaction enhances the dislocation mobility [16,17] and thereby inducing material softening at the micro scale [6]. The detailed mechanism of shear localization and fracture in bulk due to enhanced dislocation mobility is still unclear. Sofronis et al., [18] proposed a model to provide a theoretical explanation for the onset of the shear localization in the presence of hydrogen from a solid mechanics point of view. They modeled the hydrogen effect on material deformation through the hydrogen induced volume dilatation and the reduction in the local flow stress upon hydrogen dissolution into the lattice. Following this work and by using a steady-state equilibrium equation for the hydrogen diffusion analysis, Liang et al., [19] studied the effect of hydrogen on the bifurcation of a homogeneous deformation in a plane-strain tension specimen into a necking or a shear localization mode of deformation.

In the present research, by using a transient hydrogen diffusion analysis and considering the reduction in the local flow stress upon hydrogen dissolution into the lattice, the effect of hydrogen on the shear localization is investigated. In addition, progress has been made in that, by applying the transient analysis, the changes in the distribution of the total and trapping hydrogen concentrations through the loading time and particularly during the necking event have clearly been determined. The plan of the paper is as follows: Section 2 describes the transient hydrogen transport equation. Section 3 introduces a new constitutive law for the elasto-plastic material response in the presence of hydrogen. Section 4 describes the fully coupled analysis procedure, Section 5 explains the model, boundary conditions and the material properties. Finally, Section 6 summarizes the numerical results.

2. Transient hydrogen transport equation

The diffusion formulation is based on Sofronis and McMeeking's paper [11] which uses an equilibrium theory established by Oriani [20,21]. Hydrogen moves through the material by the

normal interstitial lattice site (NILS) diffusion. Transported hydrogen is located either in NILS or in trap sites. The hydrogen concentrations in NILS and trap sites are described, respectively, as follows:

$$C_L = \theta_L N_L \quad (1)$$

$$C_T = \theta_T N_T \quad (2)$$

where θ_L and θ_T are, respectively, the occupancy of lattice sites and the occupancy of trap sites. N_L and N_T are the lattice site and the trap site densities, respectively. Based on Kumnick and Johnson's paper [22] in which the trap site density only depends upon the plastic strain ϵ_p , Sofronis and McMeeking [11], and Krom et al., [12] used the following monotonic increasing function:

$$\log_{10}(N_T) = 23.26 - 2.33 e^{-5.5\epsilon_p}. \quad (3)$$

An expression of the hydrogen concentration in trap sites as a function of concentration in lattice sites under the assumption $\theta_L \ll 1$ was given by Oriani [20]:

$$C_T = \frac{C_L N_T K_T}{K_T C_L + N_L} \quad (4)$$

where K_T is the equilibrium constant such that $K_T = e^{-\Delta E_T/RT}$ with ΔE_T as the trap binding energy. The partial derivative of the hydrogen concentration in trap sites with respect to time is

$$\frac{\partial C_T}{\partial t} = \frac{\partial C_T}{\partial C_L} \frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial N_T} \frac{dN_T}{d\epsilon_p} \frac{\partial \epsilon_p}{\partial t}. \quad (5)$$

The final hydrogen transport equation was presented by Krom et al., [12] as

$$\frac{C_L + C_T(1 - \theta_T)}{C_L} \frac{\partial C_L}{\partial t} - \nabla \cdot (D_L \nabla C_L) + \nabla \cdot \left(\frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h \right) + \theta_T \frac{dN_T}{d\epsilon_p} \frac{\partial \epsilon_p}{\partial t} = 0 \quad (6)$$

where D_L is the constant hydrogen diffusion coefficient, \bar{V}_H the partial molar volume of hydrogen, R the gas constant, T the absolute temperature and $\sigma_h = 1/3\sigma_{ii}$ is the hydrostatic stress which induces a drift for diffusion through the NILS (in the latest term, the summation convention is considered).

A weak form of the diffusion formulation is

$$\left(\left[1 + \frac{N_L K_T N_T}{(K_T C_L + N_L)^2} \right] \frac{\partial C_L}{\partial t}, C_L^* \right)_\Omega + (D_L \nabla C_L, \nabla C_L^*)_\Omega - \left(\frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h, \nabla C_L^* \right)_\Omega + \left(C_L \frac{K_T}{K_T C_L + N_L} \frac{dN_T}{d\epsilon_p} \frac{\partial \epsilon_p}{\partial t}, C_L^* \right)_\Omega = 0 \quad (7)$$

where $(A, B)_\Omega = \int_\Omega A \cdot B d\Omega$ with Ω as a domain and C_L^* as a test function for C_L .

The time-implicit scheme for the advection diffusion equation which has been concluded in Kanayama et al., [13] is as follows:

$$\left(\left[1 + \frac{N_L K_T N_T (\epsilon_p^n)}{(K_T C_L^n + N_L)^2} \right] \left(\frac{C_L^{n+1} - C_L^n}{\Delta t} \right), C_L^* \right)_\Omega + (D_L \nabla C_L^{n+1}, \nabla C_L^*)_\Omega - \left(\frac{C_L^{n+1} D_L \bar{V}_H}{RT} \nabla \sigma_h^n, \nabla C_L^* \right)_\Omega + \left(C_L^{n+1} \frac{K_T}{K_T C_L^n + N_L} 29.508 N_T \times (\epsilon_p^n) e^{-5.5\epsilon_p^n} \frac{\epsilon_p^{n+1} - \epsilon_p^n}{\Delta t}, C_L^* \right)_\Omega = 0 \quad (8)$$

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