INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 40 (2015) 9825–9837

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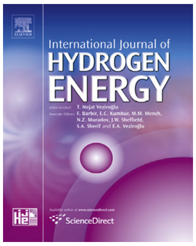

Effects of hydrogen-altered yielding and work hardening on plastic-zone evolution: A finite-element analysis

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ARTICLE INFO

Article history:
Received 28 February 2015
Received in revised form
28 May 2015
Accepted 29 May 2015
Available online 28 June 2015

Keywords:
Hydrogen
Crack-tip plasticity
Diffusion
Bulk
Ductility
Finite elements

ABSTRACT

In the present paper, finite-element analysis of a cracked specimen was conducted using a unified model for the elastic–plastic deformation and hydrogen diffusion. We considered the effects of the hydrogen-reduced yielding strength and work-hardening coefficient and used a comparison parameter in the simulation of the hydrogen-localized plastic zone near a crack tip. We realized two important facts: (1) the normal component of the plastic strain in the direction of remote stress near the crack tip is significantly increased by the reduced work-hardening coefficient at the same stress-intensity factor; (2) the reduced work-hardening coefficient enhances the localization of the plastic zone when compared to the case using the normal component of the crack-tip plastic strain in the direction of remote stress, which probably determines the ductile–brittle transition of the fatigue-crack propagation mode under a hydrogen atmosphere. These results indicate that the reduction in work-hardening coefficient and the utilization of the crack-tip plastic strain as a parameter to organize the data play important roles in the prediction of the transition condition of hydrogen-accelerated fatigue-crack propagation.

Introduction

The establishment of hydrogen-related infrastructures requires a thorough understanding of the effects of hydrogen on mechanical properties. Recently, it has been reported that hydrogen induces softening [1] or hardening [1,2]. More specifically, hydrogen-enhanced local plasticity (HELP) associated with fatigue-crack propagation has drawn attention toward practical applications of hydrogen because fatigue fracture is a major cause of destruction in accidents. For instance, hydrogen uptake is known to accelerate the fatigue-crack propagation rate and drastically deteriorate the fatigue life owing to a change in the crack-propagation mode [3,4]. The brittle- or brittle-like-crack propagation rate in the fatigue-crack mode is around 10 times faster than that in the ductile mode [4]. Therefore, understanding the ductile–brittle transition condition is essential to the prediction of fatigue life in a hydrogen environment.

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http://dx.doi.org/10.1016/j.ijhydene.2015.05.187

Nomenclature

b_0	initial radius of blunting crack tip, (m)
C_L	hydrogen concentration, (m^{-3})
C_{LB}	initial hydrogen concentration at lattice sites on crack flank surface, (m^{-3})
C_T	hydrogen concentration at trap sites, (m^{-3})
D_L	lattice diffusivity, ($m^2\ s^{-1}$)
$D_L{}^*$	effective diffusion coefficient
E	Young's modulus, (GPa)
J	hydrogen flux, ($s^{-1}\ m^{-2}$)
K_T	equilibrium constant
K_I	mode I stress intensity factor, (MPa $m^{1/2}$)
n	work-hardening exponent
N_L	number of lattice sites per unit volume, (m^{-3})
N_T	number of trap sites per unit volume, (m^{-3})
r_0	radius of crack model, (m)
r	distance from the crack tip, (m)
R	gas constant, (J $mol^{-1}\ K^{-1}$)
T	temperature, (K)
$t_{\varepsilon=0.6}$	time when crack-tip plastic strain reaches 0.6
t_f	total loading time
u_x	displacement in x-direction, (m)
u_y	displacement in y-direction, (m)
V_H	partial molar volume, ($m^3\ mol^{-1}$)
W_B	trap-binding energy, (J mol^{-1})
δ_x	plastic-zone width along x-axis
δ_y	plastic-zone width along y-axis
δ_{x0}	plastic-zone width along x-axis without hydrogen effect
δ_{y0}	plastic-zone width along y-axis without hydrogen effect
δ_{x1}	plastic-zone width along x-axis with hydrogen effect
δ_{y1}	plastic-zone width along y-axis with hydrogen effect
δ_θ	plastic-zone width along θ-axis
δ_r	plastic-zone width along r-axis
ε_p	equivalent plastic strain
ε_0	initial yield strain
ζ	coupling-effect parameter
η	coupling-effect parameter
θ	angle of crack model at the crack tip
θ_L	occupancy of lattice sites
θ_T	occupancy of trap sites
ν	Poisson's ratio
ξ	coupling-effect parameter
ρ	material density, (kg m^{-3})
σ_h	hydrostatic stress, (MPa)
σ_Y	yield strength, (MPa)
σ_0	initial yield strength, (MPa)

From the viewpoint of ductile–brittle transition in a hydrogen environment, the formation of brittle striation as a result of transgranular-crack propagation was reported in single crystalline Fe–Si [5] and commercial polycrystalline ferritic steels [4] which have a bcc crystal structure. Although transgranular-crack propagation was observed to show a brittle-like feature on the fracture surface, the propagation path was not along any identical crystallographic planes such as $\{110\}_\alpha$ for cleavage fracture [5]. Instead, Nishikawa et al. [6] proposed a ductile propagation mechanism in terms of the formation and coalescence of microvoids [7] associated with HELP [8–10] to explain the propagation of brittle-like cracks. This model could explain the brittle-like fractographic feature as well as the acceleration of the crack propagation rate. Therefore, we assume that the main factors triggering brittle-like fatigue-crack propagation are the extents of plastic strain and hydrogen localizations, which promote the HELP effect near a crack tip. Based on this assumption, a method for predicting the transition in crack-propagation mode was examined in this study.

Up to the present time, the effect of hydrogen on mechanical properties has been analyzed by the finite-element method (FEM) [11–15] or molecular dynamics (MD) [16]. FEM can be used to calculate the relatively macro- or mesoscopic distributions of plastic strain and hydrogen at a crack tip; however, it cannot describe the dislocation slip [17] and inhomogeneous distribution of hydrogen around dislocations. On the other hand, MD has been used to clarify the microscopic behavior [16] and fracture criterion [18] in a hydrogen environment, although MD has a disadvantage regarding atomic-scale analysis because of the limit on the number of atoms in a model. Hence, the selection of the method of simulation is critical to the development of an accurate model of the real hydrogen effect on an identical scale. When a plastic zone needs to be analyzed with the effect of stress-assisted hydrogen diffusion near a crack tip, mesoscopic to macroscopic scale analysis, namely FEM, is considered an appropriate approach [11–15]. More specifically, the ductile–brittle transition noted in this study requires a FEM-scale analysis that would elucidate the hydrogen-related factors on a scale of 30.0 μm (plastic-zone size on steels at $K_I = 40.0$ MPa $m^{1/2}$) to 150 mm (the distance at which the displacement is not affected by the plastic zone at a crack tip): hydrogen distribution, plastic-zone size, plastic strain distribution, and coordination state of hydrogen such as dislocations. FEM has been successfully applied to analysis of the plastic zone with hydrogen diffusion near a crack tip [11–15]. However, we noticed a remaining issue in terms of this plastic-zone analysis, namely, simulation of the decrease in plastic-zone size in the loading direction, which plays an important role in the HELP effect. We expect a simulation of a localized plastic zone would allow us to precisely estimate the transition condition and fatigue life.

We focused on the effects of hydrogen on plastic deformation and determining a comparison parameter for solving the remaining issue of plastic-zone size. Here, the yield strength and work-hardening coefficient are considered to be mechanical factors that dominate the plastic-zone evolution. In particular, the effect of the work-hardening coefficient has never been introduced to simulations of the HELP phenomenon. Additionally, based on the propagation mechanisms of ductile and brittle-like cracks, we compared the plastic-zone size by using a new parameter, a normal component of the crack-tip plastic strain in the direction of remote stress to determine the transition of the fatigue-crack propagation mode as shown in Fig. 1(b). By coupling FEM with a simulation of stress-induced hydrogen diffusion in this study, we