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



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#### 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 strain in the direction of remote stress hear 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.

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#### 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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Nomenclature

$b_0$ initial radius of blunting crack tip, (m) $C_L$ hydrogen concentration at lattice sites on crack flank surface, (m <sup>-3</sup> ) $C_{LB}$ initial hydrogen concentration at trap sites, (m <sup>-3</sup> ) $D_L$ lattice diffusivity, (m <sup>2</sup> s <sup>-1</sup> ) $D_L$ *effective diffusion coefficient $E$ Young's modulus, (GPa) $J$ hydrogen flux, (s <sup>-1</sup> m <sup>-2</sup> ) $K_T$ equilibrium constant $K_1$ mode I stress intensity factor, (MPa m <sup>1/2</sup> ) $n$ work-hardening exponent $N_L$ number of lattice sites per unit volume, (m <sup>-3</sup> ) $r_0$ radius of crack model, (m) $r$ distance from the crack tip, (m) $R$ gas constant, ( $J$ mol <sup>-1</sup> K <sup>-1</sup> ) $T$ temperature, (K) $t_{e=0.6}$ 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) $u_y$ glastic-zone width along x-axis $\delta_y$ plastic-zone width along y-axis $\delta_y$ plastic-zone width along y-axis withouthydrogen effect $\delta_{y1}$ plastic-zone width along y-axis with hydrogen $effect$ $\delta_y$ $\delta_y$ plastic-zone width along y-axis $\delta_y$ plastic-zone width along y-axis $\delta_{y1}$ plastic-zone width along y-axis $\delta_y$ plastic-zone width along		
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$u_y$ displacement in y-direction, (m) $V_H$ partial molar volume, (m <sup>3</sup> mol <sup>-1</sup> ) $W_B$ trap-binding energy, (J mol <sup>-1</sup> ) $\delta_x$ plastic-zone width along x-axis $\delta_y$ plastic-zone width along y-axis $\delta_{x0}$ plastic-zone width along x-axis withouthydrogen effect $\delta_{y0}$ plastic-zone width along y-axis withouthydrogen effect $\delta_{y1}$ plastic-zone width along x-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along p-axis $\delta_r$ plastic-zone width along p-axis $\phi_r$ plastic-zone width along r-axis $\epsilon_p$ equivalent plastic strain $\epsilon_0$ initial yield strain $\zeta$ coupling-effect parameter $\eta$ coupling-effect parameter $\eta$ coupling-effect parameter $\theta$ angle of crack model at the crack tip $\theta_L$ occupancy of trap sites $v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_h$ hydrostatic stress, (MPa) $\sigma_0$ initial yield strength, (MPa)	u <sub>x</sub>	displacement in x-direction, (m)
$V_{\rm H}$ partial molar volume, $(m^3 \text{ mol}^{-1})$ $W_{\rm B}$ trap-binding energy, $(J \text{ mol}^{-1})$ $\delta_{\rm x}$ plastic-zone width along x-axis $\delta_{y}$ plastic-zone width along y-axis $\delta_{x0}$ plastic-zone width along x-axis withouthydrogen effect $\delta_{y0}$ plastic-zone width along y-axis withouthydrogen effect $\delta_{x1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{\theta}$ plastic-zone width along $\theta$ -axis $\delta_r$ plastic-zone width along $\theta$ -axis $\delta_r$ plastic-zone width along $\pi$ -axis $\epsilon_{\rm p}$ equivalent plastic strain $\epsilon_0$ initial yield strain $\zeta$ coupling-effect parameter $\eta$ coupling-effect parameter $\theta$ angle of crack model at the crack tip $\theta_{\rm L}$ occupancy of trap sites $v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_{\rm h}$ hydrostatic stress, (MPa) $\sigma_0$ initial yield strength, (MPa)	u <sub>v</sub>	displacement in y-direction, (m)
$W_B$ trap-binding energy, $(f mol^{-1})$ $\delta_x$ plastic-zone width along x-axis $\delta_y$ plastic-zone width along y-axis $\delta_{x0}$ plastic-zone width along x-axis withouthydrogen effect $\delta_{y0}$ plastic-zone width along y-axis withouthydrogen effect $\delta_{y1}$ plastic-zone width along x-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along x-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{\theta}$ plastic-zone width along $\theta$ -axis $\delta_r$ plastic-zone width along $\theta$ -axis $\delta_r$ plastic-zone width along $r$ -axis $\epsilon_p$ equivalent plastic strain $\epsilon_0$ initial yield strain $\zeta$ coupling-effect parameter $\eta$ coupling-effect parameter $\theta$ angle of crack model at the crack tip $\theta_L$ occupancy of trap sites $v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_h$ hydrostatic stress, (MPa) $\sigma_0$ initial yield strength, (MPa)	V <sub>H</sub>	partial molar volume, (m³ mol <sup>-1</sup> )
	WB	trap-binding energy, (J mol $^{-1}$ )
	$\delta_{\mathbf{x}}$	plastic-zone width along x-axis
$\begin{array}{lll} \delta_{x0} & \mbox{plastic-zone width along x-axis without} \\ & \mbox{hydrogen effect} \\ \delta_{y0} & \mbox{plastic-zone width along y-axis without} \\ & \mbox{hydrogen effect} \\ \delta_{x1} & \mbox{plastic-zone width along x-axis with hydrogen} \\ & \mbox{effect} \\ \delta_{y1} & \mbox{plastic-zone width along y-axis with hydrogen} \\ & \mbox{effect} \\ \delta_{\theta} & \mbox{plastic-zone width along $\eta$-axis} \\ \phi_{\mu} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{r} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{r} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{r} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{\rho} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{r} & \mbox{plastic-zone width along $\eta$-axis} \\ \delta_{\rho} & \mbox{coupling-effect parameter} \\ \theta_{\mu} & \mbox{occupancy of trap sites} \\ v & \mbox{Poisson's ratio} \\ \xi & \mbox{coupling-effect parameter} \\ \rho_{\mu} & \mbox{material density, (kg m^{-3})} \\ \sigma_{h} & \mbox{hydrostatic stress, (MPa)} \\ \sigma_{0} & \mbox{initial yield strength, (MPa)} \\ \end{array}$	$\delta_y$	plastic-zone width along y-axis
hydrogen effect $\delta_{y0}$ plastic-zone width along y-axis withouthydrogen effect $\delta_{x1}$ plastic-zone width along x-axis with hydrogeneffect $\delta_{y1}$ plastic-zone width along y-axis with hydrogeneffect $\delta_{\theta}$ plastic-zone width along $\theta$ -axis $\delta_r$ plastic-zone width along $\tau$ -axis $\epsilon_p$ equivalent plastic strain $\epsilon_0$ initial yield strain $\zeta$ coupling-effect parameter $\eta$ coupling-effect parameter $\theta$ angle of crack model at the crack tip $\theta_L$ occupancy of trap sites $v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_h$ hydrostatic stress, (MPa) $\sigma_0$ initial yield strength, (MPa)	$\delta_{\rm x0}$	plastic-zone width along x-axis without
$\begin{array}{lll} \delta_{y0} & \mbox{plastic-zone width along y-axis without} \\ & \mbox{hydrogen effect} \\ \delta_{x1} & \mbox{plastic-zone width along x-axis with hydrogen} \\ & \mbox{effect} \\ \delta_{y1} & \mbox{plastic-zone width along y-axis with hydrogen} \\ & \mbox{effect} \\ \delta_{\theta} & \mbox{plastic-zone width along $\theta$-axis} \\ \delta_{\theta} & \mbox{coupling-effect parameter} \\ \theta & \mbox{angle of crack model at the crack tip} \\ \theta_{L} & \mbox{occupancy of trap sites} \\ v & \mbox{Poisson's ratio} \\ \xi & \mbox{coupling-effect parameter} \\ \rho & \mbox{material density, (kg m^{-3})} \\ \sigma_{h} & \mbox{hydrostatic stress, (MPa)} \\ \sigma_{0} & \mbox{initial yield strength, (MPa)} \\ \sigma_{0} & \mbox{initial yield strength, (MPa)} \\ \end{array}$		hydrogen effect
hydrogen effect $\delta_{x1}$ plastic-zone width along x-axis with hydrogen effect $\delta_{y1}$ plastic-zone width along y-axis with hydrogen effect $\delta_{\theta}$ plastic-zone width along $\theta$ -axis $\delta_{r}$ plastic-zone width along $r$ -axis $\epsilon_{p}$ equivalent plastic strain $\epsilon_{0}$ initial yield strain $\zeta$ coupling-effect parameter $\eta$ coupling-effect parameter $\theta$ angle of crack model at the crack tip $\theta_{L}$ occupancy of lattice sites $\theta_{T}$ occupancy of trap sites $v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_{h}$ hydrostatic stress, (MPa) $\sigma_{0}$ initial yield strength, (MPa)	$\delta_{y0}$	plastic-zone width along y-axis without
$\begin{array}{lll} \delta_{x1} & \mbox{plastic-zone width along x-axis with hydroger} \\ & \mbox{effect} \\ \delta_{y1} & \mbox{plastic-zone width along y-axis with hydroger} \\ & \mbox{effect} \\ \delta_{\theta} & \mbox{plastic-zone width along $\theta$-axis} \\ \delta_{r} & \mbox{plastic-zone width along $r$-axis} \\ \epsilon_{p} & \mbox{equivalent plastic strain} \\ \epsilon_{0} & \mbox{initial yield strain} \\ \xi_{0} & \mbox{coupling-effect parameter} \\ \eta & \mbox{coupling-effect parameter} \\ \theta & \mbox{angle of crack model at the crack tip} \\ \theta_{L} & \mbox{occupancy of lattice sites} \\ \theta_{T} & \mbox{occupancy of trap sites} \\ v & \mbox{Poisson's ratio} \\ \xi & \mbox{coupling-effect parameter} \\ \rho & \mbox{material density, (kg m^{-3})} \\ \sigma_{h} & \mbox{hydrostatic stress, (MPa)} \\ \sigma_{0} & \mbox{initial yield strength, (MPa)} \end{array}$		hydrogen effect
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$\begin{array}{lll} \delta_{y_1} & \text{plastic-zone width along y-axis with hydroger} \\ & \text{effect} \\ \delta_{\theta} & \text{plastic-zone width along $\theta$-axis} \\ \delta_r & \text{plastic-zone width along $r$-axis} \\ \epsilon_p & \text{equivalent plastic strain} \\ \epsilon_0 & \text{initial yield strain} \\ \zeta & \text{coupling-effect parameter} \\ \eta & \text{coupling-effect parameter} \\ \theta & \text{angle of crack model at the crack tip} \\ \theta_L & \text{occupancy of lattice sites} \\ \theta_T & \text{occupancy of trap sites} \\ v & \text{Poisson's ratio} \\ \xi & \text{coupling-effect parameter} \\ \rho & \text{material density, (kg m^{-3})} \\ \sigma_h & \text{hydrostatic stress, (MPa)} \\ \sigma_0 & \text{initial yield strength, (MPa)} \\ \end{array}$		effect
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		effect
$\begin{array}{ll} \delta_r & \mbox{plastic-zone width along r-axis} \\ \epsilon_p & \mbox{equivalent plastic strain} \\ \epsilon_0 & \mbox{initial yield strain} \\ \zeta & \mbox{coupling-effect parameter} \\ \eta & \mbox{coupling-effect parameter} \\ \theta & \mbox{angle of crack model at the crack tip} \\ \theta_L & \mbox{occupancy of lattice sites} \\ \theta_T & \mbox{occupancy of trap sites} \\ \nu & \mbox{Poisson's ratio} \\ \xi & \mbox{coupling-effect parameter} \\ \rho & \mbox{material density, (kg m^{-3})} \\ \sigma_h & \mbox{hydrostatic stress, (MPa)} \\ \sigma_0 & \mbox{initial yield strength, (MPa)} \end{array}$	$\delta_ heta$	plastic-zone width along $\theta$ -axis
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	$\varepsilon_{\mathrm{p}}$	equivalent plastic strain
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$ θ_T $ occupancy of trap sitesvPoisson's ratioξcoupling-effect parameterρmaterial density, (kg m <sup>-3</sup> ) $ σ_h $ hydrostatic stress, (MPa) $ σ_Y $ yield strength, (MPa) $ σ_0 $ initial yield strength, (MPa)	$\theta_{\rm L}$	occupancy of lattice sites
$v$ Poisson's ratio $\xi$ coupling-effect parameter $\rho$ material density, (kg m <sup>-3</sup> ) $\sigma_{\rm h}$ hydrostatic stress, (MPa) $\sigma_{\rm Y}$ yield strength, (MPa) $\sigma_0$ initial yield strength, (MPa)	$\theta_{\mathrm{T}}$	occupancy of trap sites
	ν	Poisson's ratio
$ \begin{array}{ll} \rho & \text{material density, (kg m ^{-})} \\ \sigma_{\rm h} & \text{hydrostatic stress, (MPa)} \\ \sigma_{\rm Y} & \text{yield strength, (MPa)} \\ \sigma_{\rm 0} & \text{initial yield strength, (MPa)} \end{array} $	ξ	coupling-effect parameter
$\sigma_{\rm h}$ hydrostatic stress, (MPa) $\sigma_{\rm Y}$ yield strength, (MPa) $\sigma_0$ initial yield strength, (MPa)	ρ	material density, (kg m <sup>-2</sup> )
$\sigma_{\rm Y}$ yield strength, (MPa) $\sigma_0$ initial yield strength, (MPa)	$\sigma_{ m h}$	nyarostatic stress, (MPa)
$\sigma_0$ initial yield strength, (MPa)	$\sigma_{ m Y}$	yield strength, (MPa)
	$\sigma_0$	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 stressassisted 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  $\mu$ m (plastic-zone size on steels at  $K_{\rm I}$  = 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 Download English Version:

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