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Prediction of crack propagation under cyclic loading based on hydrogen diffusion

Q1 X. Xing, W. Chen, H. Zhang*

Q2 Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada T6G 2V4

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ABSTRACT

Previous work on corrosion fatigue of steel has shown that the crack propagation rate is related to ΔK , K_{max} and loading frequency f , in which it can be described in a form of the Paris Law. In current study, fracture mechanics has been employed to explore the hydrogen diffusion effect on crack propagation under cyclic loading. In particular, H potential, diffusivity and hydrostatic stress near crack tip, and the critical loading frequency have been considered in the new model. The predicted crack propagation values have been compared with experimental results of X-65 steel in C-2 and NOVATW solutions, and X-52 steel in C-2 solution and the new model provides physical meanings to rationalize the empirical Paris Law.

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1. Introduction

Hydrogen embrittlement has been well accepted as one of the most severe steel degradation mechanisms [1–4]. There are several theories to illustrate hydrogen embrittlement in steel. Hydrogen Enhanced Local Plasticity (HELP) [5] postulates that hydrogen would not lock dislocations in place and instead it would enhance the movement of dislocations. The increased local plasticity is believed to cause an increase in local stress so that crack can be initiated easily [6,7]. Hydrogen Enhanced Decohesion (HEDE) [8,9] postulates that H atoms in steel would diminish the bonding energy between adjacent iron atoms and this mechanism causes an easier planar failure [10]. Lynch's theory which involves H promoting dislocation nucleation, and facilitating the link up of cracks with voids ahead of cracks is also reasonable in explaining material changing from ductile to brittle as H concentration increases [11].

Near Neutral pH Stress Corrosion Cracking (NNpHSCC) condition Hydrogen effects are more complicated [12,13]. It determines whether cracks can be re-sharpened or blunted in pipeline steel [14]. A recent study has illustrated that there is a minimum loading frequency ($f_{critical}$) under which the crack propagation rate would reach maximum and keep constant [15]. A crack propagation model considering both $f_{critical}$ and hydrogen diffusion can be written as follows:

$$\left(\frac{da}{dN}\right)_{tot} = \left(\frac{da}{dN}\right)_{airfatigue} + \left(\frac{f_{critical}}{f}\right)^{\gamma} \left(\frac{da}{dN}\right)_{HAC}^{max} \quad (1)$$

* Corresponding author.

E-mail address: hao7@ualberta.ca (H. Zhang).

where $(da/dN)_{airfatigue}$ is crack growth due to air fatigue (usually relatively small) and $(da/dN)_{HAC}$ is due to hydrogen assisting cracking. The $(da/dN)_{HAC}$ term takes account for both the HEDE theory and Lynch's theory, where the former expects the accumulation of H at the crack front direction to diminish the free surface energy and cause crack propagation [16,17] and the latter considers the coalescence of the minor defects with cracks due to H effects [18–20]. As hydrogen atoms saturate in the plastic zone, two mechanisms will enhance the crack propagation rate to reach maximum rate, as suggested by the recent experiments [15]. Since both mechanisms are related with hydrogen diffusion, the total hydrogen assisting cracking rate is naturally expected to have a power law relationship with cracking propagation rate based on HEDE. Hence, the main task in this model is to develop the crack propagation rate based on HEDE mechanism.

Considering equilibrium condition, the hydrogen concentration near crack tip is related to the hydrostatic stress distribution [21,22] and can be expressed as

$$c = c_0 \exp\left(\frac{\sigma^{hyd} \Omega}{k_B T}\right) \quad (2)$$

where c_0 is the atomic ratio of H/Fe away from crack tip, Ω is the partial volume of hydrogen, k_B is the Boltzmann constant, and σ^{hyd} is the hydrostatic stress which shown as follows:

$$\sigma^{hyd}(r, \theta) = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = \frac{2(1+\nu)}{3\sqrt{2}\pi r} K_I \cos \frac{\theta}{2} \quad (3)$$

where ν is Poisson's ratio, K_I is the stress intensity, r is the distance from any specific position to crack tip, and θ is the angle between crack front direction and the line from specific position to crack tip. Here we employ the criteria that when the atomic ratio

reaches 1, the free surface forms and the crack propagates [23,24]. Hence, the length of the saturated zone can be estimated as follows:

$$L(K_I) = \left[\frac{4(1+\nu)\Omega}{3\pi k_B T \sqrt{2\pi} \ln(1/c_0)} \right]^2 K_I^2 \quad (4)$$

Therefore, the maximum $(da/dN)_{\text{HEDE}}$ is the difference of $L(K_I)$ as K_I changes from K_{\min} to K_{\max} and the value can be shown as follows:

$$\left(\frac{da}{dN} \right)_{\text{HEDE}}^{\max} = L_{\max} - L_{\min} = \left[\frac{4(1+\nu)\Omega}{3\pi k_B T \sqrt{2\pi} \ln(1/c_0)} \right]^2 \left(\frac{1+R}{1-R} \right) \Delta K^2 \quad (5)$$

where L_{\min} is the saturated length at K_{\min} , L_{\max} is the saturated length at K_{\max} , and R ratio is equal to K_{\min}/K_{\max} . The $(da/dN)_{\text{HEDE}}$ is the crack propagation rate related to hydrogen diffusion. When $f < f_{\text{critical}}$, the $da/dN = (da/dN)_{\max}$, however, when $f > f_{\text{critical}}$, the da/dN value would vary with loading frequency, i.e.,

$$\left(\frac{da}{dN} \right)_{\text{HEDE}} = \left(\frac{da}{dN} \right)_{\text{HEDE}}^{\max} \left(\frac{f_{\text{critical}}}{f} \right)^\gamma \quad (6)$$

The power of loading frequency γ can be fitted from experimental results, which is expected to be related to hydrogen diffusion. The hydrogen concentration in the steel is somehow difficult to quantify and can range from 0 to 5×10^{-4} atomic ratio [25]. To simplify the calculation, the c_0 here is taking a constant at 10 appm which is a reasonable amount around crack tips in steel [16,17].

The plastic zone shape under plain strain condition can be approximated to be a circular region with radius r_p (as shown in Fig.1), which is reasonable because when the H concentration in the circular region reaches equilibrium, its concentration in the plastic zone also reaches saturation. To reach the dynamic equilibrium of hydrogen concentration in the plastic zone during cyclic loading, an annulus region with the inner radius r_p and the outer radius R_{eq} is needed to supply and deplete hydrogen atoms. The hydrogen concentration outside of plastic zone is estimated to be c_0 . Therefore, the minimum time, t_{critical} , for H diffusion in/out of circular region during cyclic load to satisfy the dynamic equilibrium hydrogen concentration in plastic zone is related to critical frequency through $f_{\text{critical}} = 1/(2t_{\text{critical}})$. Hence, the number of hydrogen atoms needed to saturate the plastic zone can be calculated as follows:

$$N(K_I) = \int_{L(K_I)}^{r_p} \left(c_0 \exp\left(\frac{\sigma^{\text{hyd}} \Omega}{k_B T} \right) 2\pi r l_z / (a_0^3 / 2) \right) dr + \frac{4L(K_I)^2 l_z}{a_0^3} \quad (7)$$

where r_p is the plastic zone size based on plain strain condition $(1/6\pi)(K_{\max}/\sigma_{\text{ys}})^2$, a_0 is the lattice parameter, l_z is the thickness of the specimen and $L(K_I)$ is the free surface length where hydrogen

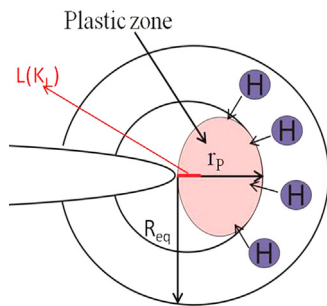


Fig. 1. The schematic of the H enhanced crack propagation model. The pink region is the plastic zone, in which the size is equal to r_p . The annulus region in which the inner radius equaling to r_p and the outer radius equaling R_{eq} is the zone supplying and depleting hydrogen atoms to the plastic zone during cyclic loading. $L(K_I)$ is the length of a free surface (the distance that crack propagates) covered by hydrogen atoms.

concentration is equal to 1. As K_I changes from K_{\min} to K_{\max} , the hydrogen numbers change in the circular region with radius r_p is $N(K_{\max}) - N(K_{\min})$. This difference can be calculated by changing K_I in Eq. (7) from K_{\min} to K_{\max} , and the exchanging of H atoms in plastic zone would be supplied or depleted by an annulus region of which inner radius equals to r_p and the outer radius equals to R_{eq} . Hence, the increase of H atoms in plastic zone during one single cycle of loading should still be equal to the H numbers in this annulus region as follows:

$$N(K_{\max}) - N(K_{\min}) = \frac{2\pi c_0 l_z}{a_0^3} (R_{\text{eq}} - r_p)^2 \quad (8)$$

The average velocity of hydrogen movement \bar{V}_r over position and stress intensity can be estimated from hydrogen chemical potential deduced force and the motivation [16,26]. The hydrogen chemical potential can be shown as follows:

$$\mu = \mu_0 + k_B T \ln \frac{c}{1-c} + \sigma^{\text{hyd}} \Omega \quad (9)$$

and the velocity can be expressed as follows:

$$V_r = \frac{DF_r}{k_B T} = \frac{(1+\nu)\Omega}{k_B T 3\sqrt{2\pi}} \frac{DK_I \cos(\theta/2)}{r^{3/2}} \quad (10)$$

As hydrogen atoms flux into plastic zone during loading, the hydrogen concentration outside the plastic zone is assumed to be a constant c_0 , hence $F_r = -\nabla\mu = -\Omega\nabla\sigma^{\text{hyd}}$. Then the average velocity is

$$\bar{V}_r = \frac{\int_{r_p}^{R_{\text{eq}}} \int_0^\pi \int_{K_{\min}}^{K_{\max}} V_r dK_I d\theta dr}{\pi (R_{\text{eq}} - r_p) (K_{\max} - K_{\min})} \quad (11)$$

The t_{critical} value is equal to the size of the zone which supplies or depletes hydrogen atoms over the average velocity, i.e., $f_{\text{critical}} = (1/2t_{\text{critical}})$, then

$$f_{\text{critical}} = \frac{(1+\nu)\Omega D (K_{\max} + K_{\min}) ((1/\sqrt{r_p}) - (1/\sqrt{R_{\text{eq}}}))}{\pi (R_{\text{eq}} - r_p)^2 k_B T 3\sqrt{2\pi}} \quad (12)$$

In Eq. (12), the f_{critical} is proportional to hydrogen diffusivity, and D is about $2 \times 10^{-11} \text{ m}^2/\text{s}$ [27] when the strain of specimen is equal to zero. However, MD simulation shows that there is an excess volume for hydrogen atoms as the specimen is under tensile strain. Hence, the diffusivity of hydrogen could be almost two orders higher than that value and could reach $1.7 \times 10^{-9} \text{ m}^2/\text{s}$ [28]. Therefore, this D value has been used in current calculation and the HEDE propagation rate could be shown as follows:

$$\left(\frac{da}{dN} \right)_{\text{HEDE}} = \left[\frac{4(1+\nu)\Omega}{3\pi k_B T \sqrt{2\pi} \ln(1/c_0)} \right]^2 \left(\frac{1+R}{1-R} \right) \frac{\Delta K^2}{(f/f_{\text{critical}})^\gamma}, \quad f > f_{\text{critical}} \quad (13)$$

Fig. 2 compares the estimated HEDE crack propagation with experimental results in C-2 and NOVATW solutions [29]. The hollow points (HEDE) and the solid ones (experimental values) have the same trend. The predicted HEDE crack propagation rate and the total crack propagation rate from experiments both show a power law with ΔK . It suggests that the estimated HEDE propagation rate based on hydrogen diffusion and critical loading frequency could be related to the Paris Law and could provide physical meaning for this empirical model in NNpHSCC. The deviation of slope in predicting HEDE propagation rate is proportional to the deviation of experiment crack propagation results.

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