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Effect of history on hydrogen assisted cracking

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Abstract

In hydrogen assisted cracking, hydrogenation and crack growth are coupled processes. Consequently, particular histories of stress intensity factor K and crack size evolutions influence crack growth rate v that can occur at the same instantaneous K in a given material. Thus, curve $v = v(K)$ in general does not possess uniqueness as a intrinsic material's property. This paper provides an analytical treatment of the problem by stress-strain assisted diffusion.

1 Introduction

The uniqueness of the crack growth kinetics (CGK) curve $v(K)$ of a given material-environment system is an open question, as shown in many experimental observations [1], which brings doubts on the fracture mechanics approach to environmentally assisted cracking (EAC), even under small scale yielding (SSY). The special case of hydrogen assisted cracking (HAC) is of great interest as far as hydrogen is frequently present in metals from corrosion phenomena or from hydrogenous working agents [2].

The two processes of crack propagation and hydrogen diffusion in metal should not be treated separately but coupled. In terms of the theory of boundary value problems this situation is qualified as diffusion with moving boundary. Thus the crack growth *history* appears as a factor able to affect near-tip hydrogen diffusion, and consequently the kinetics of HAC, apart from the stress-strain field represented by the stress intensity factor (SIF or K).

The objective of the present paper is to elucidate the effect of history of coupled hydrogenation-cracking process on K-dominance during HAC. This would provide more insight on the matter of the uniqueness of CGK curve, i.e., about its character as an intrinsic relationship dependent —by hypothesis— *solely* on the specific material-environment couple.

2 Model assumptions

The analysis is focussed on sustained or quasi-static loading and SSY conditions. It is restricted to a two-dimensional solid with a through-the-thickness opening-mode crack characterised by its length (or depth) l which varies with time t while HAC proceeds, $l = l(t)$.

According to the key concept of the fracture mechanics approach under SSY [3] the K-controlled mechanical autonomy of the near-tip region is supposed to be constantly preserved during crack growth. Despite a nonlinear zone exists close to the crack tip, this region remains so small that it does not sensibly disturb the SIF-dominated elastic solution outside it. This annular K-governed ring shields crack tip from peculiarities of solid's outer geometry and applied loads. Thus, mechanical situation within the nonlinear near-tip region including the fracture process zone (FPZ) is totally K-controlled in the sense that its characteristics (stresses, strains, and mechanical damage if it were involved as an explicit variable) depend on SIF and spatial coordinates x and y with the origin at the crack tip (cf. [3]):

$$\varepsilon_i = \varepsilon_i^*\left(\frac{x}{K^2}, \frac{y}{K^2}\right), \ \sigma_i = \sigma_i^*\left(\frac{x}{K^2}, \frac{y}{K^2}\right) \ \ (i = 1,2,3) \qquad (1)$$

where ε_i and σ_i are principal components of realistic (inelastic) stress-strain field and the asterisks emphasise the pre-determined nature of material's functions in the right-hand parts.

Hydrogen induced fracture depends on hydrogen concentration C at the prospective fracture sites. The local rupture event is associated with some critical combination of mechanical variables (components of stress-strain field) and hydrogen concentration in a relevant material's element (cell, "grain", or point of interest) [4]:

$$C_{cr} = C_{cr}^*\left(\sigma_i, \varepsilon_i\right) \qquad (2)$$

Then the critical concentration (2) is also a K-controlled variable in the same way as the stress-strain field, i.e.

$$C_{cr} = C_{cr}^*\left(\frac{x}{K^2}, \frac{y}{K^2}\right) \qquad (3)$$

Assuming a crack located at y=0 and propagating along x-direction, the criterion of crack growth may be suggested as follows:

$$C(x,t) = C_{cr}\left(\frac{x}{K^2}\right) \qquad (4)$$

where a definite value of $x = x_c$ must be available. It is associated with the concept of a responsible cell, e.g., the worst material unit in the FPZ, or a fixed microstructural length, or other.

The boundary condition for hydrogen diffusion problem is:

$$C(x,t)\Big|_{x=0} = C_\Gamma \tag{5}$$

where surface concentration is related to the stress-strain dependent hydrogen solubility coefficient in the deformed metal. With this boundary condition, hydrogen content throughout the FPZ $C(x,y,t)$ is determined by stress-strain assisted diffusion. In arbitrary fixed coordinate system (x_1,x_2) attached to a solid it proceeds according to:

$$\frac{\partial C}{\partial t} = -\nabla \bullet \left(\frac{D(\varepsilon_p)}{RT} X_\mathrm{D} C \right) \tag{6}$$

with the vector of diffusion driving force:

$$X_\mathrm{D} = -RT\,\nabla ln\left(\frac{C}{K_s(\sigma,\varepsilon_p)} \right) \tag{7}$$

where ∇ is the Hamilton nabla operator, the dot $\bullet$ denotes scalar product of vectors, D is the hydrogen diffusion coefficient (dependent, in general, on plastic strain), R the universal gas constant, T the absolute temperature and K_s the hydrogen solubility coefficient.

With regard to crack growth, two approaches can be considered. According to one of them crack growth proceeds discontinuously by a series of jump-like steps (cf. [4]). The time intervals Δt between discrete crack increments Δl are just the periods of accumulation in FPZ of the amount of hydrogen necessary to satisfy criterion (4). Then, crack growth rate (CGR) is defined as the averaged value:

$$v = \Delta l \,/\, \Delta t \tag{8}$$

Following the other way, crack growth is assumed to go on continuously (cf., e.g., [5]) so that criterion (4) is constantly fulfilled at a distance x_c, i.e., concentration C is there equal to its critical value C_{cr}. The instantaneous CGR is defined as a derivative of crack size:

$$v = dl \,/\, dt \tag{9}$$

In the present study the jump-like treatment is used in qualitative considerations to explain the matter, but the smooth (continuous) crack growth model is used in equations, which allows one to derive conclusions in a more rigourous mathematical manner.

3 *K*-dominance in HAC: the role of coupling of hydrogenation and crack growth processes

In Fig. 1 hydrogen concentration curves near the tip after successive crack increments are schematically shown. The critical point x_c is supposed to coincide with the location of maximum hydrogen concentration and stress. Critical concentration must be attained at this point to produce a rupture event causing jump-like crack increment. All the mentioned variables are assumed to be determined *solely* by material properties and SIF, i.e., they remain constant if $K = const.$ Crack propagation consists of a series of loops (cycles) "hydrogenation – local rupture – crack advance".

During each hydrogenation-fracturing cycle some amounts of hydrogen reach sites of possible subsequent FPZs. Thus, initial conditions for hydrogen diffusion within each particular loop are, in general, different from those of preceding and subsequent cycles (see Fig. 1). Equal SIF values produce not the same CGRs but rather induce a range of feasible velocities.

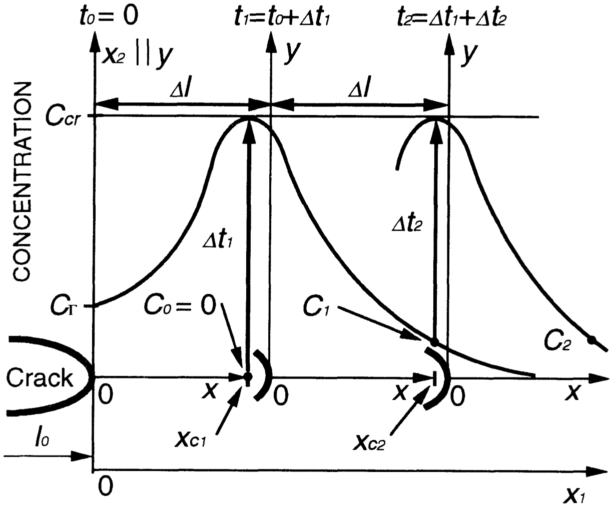

Figure 1: Sketch of metal hydrogenation in the vicinity of the crack tip, with coupling of hydrogenation and crack growth processes.

Presented consideration reveals the coupling of hydrogen diffusion and crack growth processes which mutually influence each other. FPZ hydrogenation appears to be an entire process which runs from the very beginning of metal-environment interaction associated with the HAC process. Near-tip hydrogen diffusion depends on initial

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hydrogen content at the initiation of metal-environment interaction and on the whole HAC history, on elevation of crack size $l = l(t)$ and alterations of SIF $K = K(t)$ in particular. Thus, K-dominance in HAC apparently fails because near-tip diffusion at every instantaneous K proceeds along its specific way which starts at the beginning of a particular run of HAC.

4 Process history and uniqueness of $v(K)$-curve: analytical treatment

Smooth (continuum) modelling of crack growth is convenient for analysis of the role of history of coupled hydrogenation-cracking process in maintenance of SIF control over all crack tip events. Crack size is assumed to be a smooth function $l = l(t)$ and CGR being its ordinary derivative (9). It is suitable to consider the diffusion problem (5)-(7) in a movable coordinate system (x,y) attached to the crack tip. This will cause transformation of the diffusion equation (6) associated with arbitrary stationary coordinates (x_1,x_2) pinned down to a solid. The latter system may be attached so that $x = x_1 - l(t)$, $y = x_2$. Then the total time derivation of concentration is:

$$\dot{C} = \frac{\partial C}{\partial t} - \frac{dl}{dt}\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} - v\frac{\partial C}{\partial x} \qquad (10)$$

After substitution of expression (10) into the left-hand part of equation (6) and performing elementary transformations the modified equation of stress-strain assisted diffusion in moving coordinates can be obtained in a form which slightly differs from the initial one (6):

$$\frac{\partial C}{\partial t} = -\nabla\bullet\left[\left(\frac{D}{RT}X_{\mathrm{D}} - v\right)C\right] \qquad (11)$$

where the vector $\boldsymbol{v} = v\boldsymbol{j}_x$ is independent of spatial coordinates and colinear with x-axis which unit vector is j_x $(\nabla\bullet(\boldsymbol{v}C) = \boldsymbol{v}\bullet\nabla C = v\,\partial C/\partial x)$.

By analogy to the thermodynamic one the fictitious diffusion driving force may be formally introduced into equation (11):

$$X_{\mathrm{D}}^* = X_{\mathrm{D}} - \frac{RT}{D}v \qquad (12)$$

With the use of expression (7) for X_{D} from (12), it yields:

$$X_{\mathrm{D}}^* = -RT\,\nabla\left[ln\left(\frac{C}{K_s}\right) + \frac{v}{D}x\right] = -RT\,\nabla\left[ln\left(\frac{C}{K_s^*}\right)\right] \qquad (13)$$

where formal solubility-like term is:

$$K_s^* = K_s^*(\sigma,\varepsilon_p,v) = K_s(\sigma,\varepsilon_p)\,exp\left(-\frac{v}{D}x\right) \qquad (14)$$

The analogy between diffusion driving forces (7) and (13) is evident. Moreover, the term in brackets in equation (11) may be rewritten in terms of $X_D{}^*$ in accordance with relation (12), and the equation of hydrogen diffusion in moving coordinates takes exactly the same shape as the initial one (6) with the only distinction that it contains correspondent members, i.e., X_D and K_s, with asterisks. After further transformations and assuming a constant hydrogen diffusion coefficient, equation (11) may be reduced to the next linear differential equation with respect to hydrogen concentration:

$$\frac{\partial C}{\partial t} = D\left[\nabla^2 C - \boldsymbol{M}^* \bullet \nabla C - N^* C\right] \tag{15}$$

where vector and scalar coefficients are the following:

$$\boldsymbol{M}^* = \nabla\left[\ln K_s{}^*(\sigma,\varepsilon_p,v)\right] \quad \text{and} \quad N^* = \nabla^2\left[\ln K_s{}^*(\sigma,\varepsilon_p,v)\right] \tag{16}$$

Since near-tip stress-strain field components are controlled by SIF, the equation coefficients (16), apart from spatial coordinates, depend parametrically on SIF and CGR:

$$M^* = M^*(K,v) \quad \text{and} \quad N^* = N^*(K,v) \tag{17}$$

Therefore, the solution of this problem depends not only on SIF, but also on CGR: $C = C(x,t;K,v)$. Thus, hydrogen concentration in the vicinity of the crack tip is determined by diffusion equation (15) with boundary condition (5) and some initial condition with respect to concentration at the beginning of the metal-hydrogen interaction. CGR v becomes one more unknown variable which must be found from the solution of the *coupled* problem of hydrogen diffusion and crack growth. To close the system of equations for this *coupled* diffusion-cracking process, the criterion of crack growth (4) is required. In this case it may be presented in the form:

$$C\,(x_c,t;\,K,v) = C_{cr}\,(K,x_c) \tag{18}$$

It requires that hydrogen concentration reaches its critical value at some known distance x_c from the crack tip.

This formulation of the diffusion-cracking problem is completely closed provided SIF is known, e.g., is maintained constant as in some special types of fracture mechanics test specimen (cf. [6]). For this case, if C is a solution of diffusion equation (15) parametrically dependent on CGR v, the latter can be found from equation (18) as:

$$v = v\,(K,t) \tag{19}$$

i.e., CGR must not be the same for equal values of SIF, but varies with the total HAC process time t.

However, in many practical situations SIF depends on both applied load and crack length and, consequently, equation coefficients (17) too. Hence, crack length l turns to be the additional unknown variable to be determined from the solution of the coupled problem. Differential equation (9) concerning crack size has obvious solution

$$l(t) = l_0 + \int_0^t v\, dt \qquad (20)$$

The problem is finally reduced to the same as for the previous case of $K = const$, but now the left-hand part of equation (18) to determine CGR becomes not a function parametrically dependent on v, but a functional over the whole history of the process involved in relation (20). Correspondingly, CGR as a solution of this coupled diffusion-cracking problem also becomes a functional dependent on the certain process history form its beginning in a particular solid with its individual $K(l)$-variation. It is doubtful that resulting CGR could take the same values at equal instantaneous SIFs if they were approached throughout different process histories. On the contrary, variability of CGR at the same SIF seems to be unavoidable.

5 Concluding remarks

Study of the *effect of history* in HAC reveals that in general the same SIF does not render a single value of CGR. Accordingly, this does not allow a consideration of $v(K)$ plots as intrinsic curves of a particular material-environment system. Instantaneous CGR at each K value is seen to be variable depending on initial conditions and subsequent history of cracking process in terms of time variation of SIF $K(t)$. This follows from the coupled analysis of crack growth and hydrogen accumulation in the near-tip zone and their mutual influences.

However, a lot of test data and engineering experience confirm reasonable uniqueness of CGK curves and applicability of the fracture mechanics approach to HAC for a wide variety of situations. This indicates that intrinsic variability of CGR (not controlled by K) under particular circumstances sometimes can be rather narrow in comparison with a band of inherent random scatter associated with the cracking process itself and errors introduced through crack length measurements in tests and data processing procedures.

As a consequence, a challenge appears for computer simulations to assess the extents of variability of CGR caused by coupling of hydrogenation and crack growth processes in particular cases or structural service conditions.

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