

K-DOMINANCE CONDITION IN HYDROGEN ASSISTED CRACKING: THE EFFECT OF FAR FIELD ON HYDROGEN TRANSPORTATION TO FRACTURE SITES**J. Toribio* and V. Kharin***

Hydrogen assisted cracking in metals is analyzed on the basis of K -dominance over *both* stress-strain state and hydrogen diffusion in the fracture process zone. The discrepancy in the crack tip zone between the far-field affected diffusion and the asymptotically driven (K -controlled) one is elucidated. The *far field* (i.e., the stress-strain field which is not K -dominated) is shown to have a minor effect on near-tip hydrogen diffusion. It can only widen the scatter band of crack growth rates in the near-threshold portion of the crack growth kinetics curve.

INTRODUCTION

Hydrogen assisted cracking (HAC) in metals has been widely analyzed on the basis of fracture mechanics concepts. The key of the approach is the hypothesis of *mechanical autonomy* of the crack tip zone, which implies that the stress-strain state within this zone depends *only* on the material itself and on some single variable providing cumulative characterisation of loading intensity (Kanninen and Popelar (1)). Assuming the maintenance of the small scale yielding (SSY) condition, the stress intensity factor (SIF) K is usually considered to be the adequate variable which *solely* governs the mechanical situation near the crack tip.

The idea of crack tip autonomy must be completed with the presumption of *physico-chemical autonomy* of the crack tip region with respect to both hydrogen accumulation and hydrogen induced damage in the fracture process zone (FPZ), according to Panasyuk and Kharin (2). These two processes are supposed to depend *only* on material, K -dominated mechanical state and crack tip environment. However, the K -dominance over hydrogen effects has never been verified.

This paper tries to overcome this deficiency by analyzing the effect of the remote stress-strain field which is not K -dominated (the *far field*) on hydrogen accumulation in the FPZ by stress-strain assisted diffusion which is supposed to be the rate-determining step of hydrogen supply to fracture sites in HAC under sustained or quasi-static loading conditions.

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STATEMENT OF THE PROBLEM

The concept of K -dominance may be interpreted as follows: there is a region of characteristic size R_{SIF} (Fig. 1) around the crack tip where the elastic stress-strain state is K -dominated, i.e., adequately represented *solely* by the universal $r^{-1/2}$ singular term of the complete series solution. In addition, a nonlinear region (the FPZ of size R_{FPZ}) does exist in the vicinity of the crack tip where microscopic damage proceeds. This region is usually surrounded by the plastic zone of size R_Y . The whole inelastic zone (FPZ plus plastic region) may be so small that it does not sensibly disturb the linear elastic solution outside this special area (SSY condition). When this happens, the K -dominated annular elastic region still exists at distances from crack tip $R_Y < r \leq R_{SIF}$. Outside this region (at $r > R_{SIF}$) the remote stress-strain field (*far field*) is not governed by K .

When using a fracture criterion based on a critical concentration of hydrogen, if stress-strain fields possess K -dominated autonomy near the crack tip, then K -control is acquired afterwards as a legacy by the critical hydrogen concentration distribution. Therefore, to elucidate the matter of SIF control over HAC requires a revision of K -drive over hydrogen accumulation in the FPZ by stress- and strain-assisted diffusion.

The equation of stress *and* strain assisted diffusion in terms of hydrogen concentration C takes the form (Toribio and Kharin (3)):

$$\frac{\partial C}{\partial t} = D [\nabla^2 C - M \cdot \nabla C - NC] + \nabla D \cdot [\nabla C - MC] \quad (1)$$

where D is the diffusion coefficient, t the time and:

$$M = \nabla \ln K_s(\sigma, \epsilon_p) \text{ and } N = \nabla^2 \ln K_s(\sigma, \epsilon_p) \quad (2)$$

in which K_s is the solubility, σ the hydrostatic stress and ϵ_p the plastic strain.

THE EFFECT OF FAR FIELD ON HYDROGEN DIFFUSION

The matter of K -dominance with respect to hydrogen diffusion in the near-tip zone is a question of the accuracy of the approximate hydrogen concentration distribution C_a governed by the K -dominated component of the near-tip stress-strain field (i.e., by the *asymptotic* term) to represent the actual one C_f being driven by the complete mechanical field containing the whole series (i.e., influenced by the non-autonomous *far field*). To this end, the discrepancy $T = C_a - C_f$ between the two concentration distributions is the subject of interest to estimate the effect of the far field (which is not K -controlled) on hydrogenation of FPZ.

In accordance with the general form of the equation of stress-strain assisted diffusion (1), the equations to obtain the far-field affected concentration C_f (exact) and the near-tip asymptotically driven one C_a (approximate) are:

$$\frac{\partial C_f}{\partial t} = D [\nabla^2 C_f - M_f \cdot \nabla C_f - N_f C_f] + \nabla D \cdot [\nabla C_f - M_f C_f] \quad (3)$$

$$\frac{\partial C_a}{\partial t} = D [\nabla^2 C_a - M_a \bullet \nabla C_a - N_a C_a] + \nabla D \bullet [\nabla C_a - M_a C_a] \quad (4)$$

where coefficients M and N with subindices f and a are determined by their corresponding mechanical fields (the complete and the asymptotic ones).

The following equation can be derived with regard to discrepancy:

$$\frac{\partial T}{\partial t} = D [\nabla^2 T - M_f \bullet \nabla T - N_f T] + \nabla D \bullet [\nabla T - M_f T] + Q \quad (5)$$

where an additional source-type term arises:

$$Q = -D (\Delta M \bullet \nabla C_a + \Delta N C_a) - \nabla D \bullet \Delta M C_a \quad (6)$$

With regard to the source term (6) some simplifications can be made, after which one arrives to (Kharin and Toribio (4)):

$$Q = \begin{cases} \frac{DV_H}{RT} \nabla(\sigma_f - \sigma_a) \bullet \nabla C_a \neq 0 & \text{at } r > R_{SIF} \\ 0 & \text{at } r \leq R_{SIF} \end{cases} \quad (7)$$

The last expression represents the source term for diffusion of discrepancy T , whose absolute value is the difference between the approximate K -driven concentration distribution and the exact far-field affected one. With zero initial and boundary conditions for T , its absolute value increases with time. This "error" is generated by the source Q operative at $r > R_{SIF}$, and it diffuses from there towards the FPZ. The effect of the far field on K -dominance over hydrogen accumulation in the FPZ becomes more severe when a greater amount of "error" T can reach the region $r < R_{FPZ}$ by diffusion from the distant source situated at $r > R_{SIF}$.

ASSESSMENT OF K-DOMINANCE CONDITIONS IN HAC

The question of K -dominance in HAC means assuring the exclusive SIF control *simultaneously* with respect to both the mechanical situation and hydrogen diffusion in the FPZ. Equation (5) for the discrepancy T between the asymptotically driven concentration and the far- field affected one allows an analysis of this item in general terms.

Requirements of K -based linear fracture mechanics involve ensuring that the size of the crack tip plastic zone R_Y at a given SIF value K is small compared with dimensions of the solid and with the crack size (cf. (1)). Using this condition, as well as large-strain elastoplastic solutions for cracks by Mc Meeking (5) and simulations of crack tip damage process by Tvergaard and Hutchinson (6) and Narasimhan (7), the following estimation seems to be reasonable (4):

$$\frac{R_{SIF}}{R_{FPZ}} \geq 0.1 \frac{E}{\sigma_Y} > 10 \quad (8)$$

which is quite adequate for steels since they usually have $\sigma_Y < E/100$.

The ratio (8) allows an assessment of the role of the far field in hydrogen accumulation in the FPZ. The disturbance T of the K -driven concentration C_a must arrive into FPZ situated at $r < R_{FPZ}$ emanating from the distant source Q located at $r > R_{SIF}$. Thus, the effect must be strongly dependent on the diffusion distance from this source to the FPZ.

A transient analytical solution of near-tip hydrogen diffusion problem is available only for the stress-assisted case in one-dimensional cases (Kharin (8)). An upper estimate may be:

$$C_a(x,t) = C_0 \exp\left(\frac{V_H \sigma_a(x)}{RT}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (9)$$

where erfc is the complementary error function, C_0 is the concentration for the material free of stress and V_H the partial molar volume of hydrogen. This may be rewritten as a function of the steady-state solution C_∞ as follows:

$$C_a(x,t) = C_\infty(x) \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (10)$$

A conservative estimation of the earliest time limit t_Q^* (*lower bound*) from which a noticeable disturbance of near-tip K -controlled hydrogenation may be anticipated, thus producing lack of SIF-dominance over diffusion in the FPZ, has been calculated by Toribio and Kharin (9):

$$t_Q^* > \frac{R_{SIF}^2}{2D} \quad (11)$$

It is important to know the time evolution of the K -driven concentration (10) at the outer border of the FPZ where the effect from the source Q appears first, i.e., at $x = R_{FPZ}$. Introducing the dimensionless time $\tau = Dt/R_{FPZ}^2$ we have:

$$C_a(x=R_{FPZ}, t) = C_a(\tau) = C_\infty(R_{FPZ}) \operatorname{erfc}\left(\frac{1}{2\sqrt{\tau}}\right) \quad (12)$$

Fig. 2 shows a plot of this function $C_a(\tau)$ (solid line). It can be concluded that approximately for $\tau \geq 130$, the concentration C_a in the FPZ (i.e., for $x \leq R_{FPZ}$) exceeds 95% of the steady state level C_∞ . From then on, its further variation lies within a 5%-scatter band near this hydrogenation limit, i.e., the increase of K -driven concentration in the FPZ falls into this 5% strip from the time moment t_{ss} (where the subindex *ss* indicates steady state) given by:

$$t_{ss} = 130 \frac{R_{FPZ}^2}{D} = 260 \left(\frac{R_{FPZ}}{R_{SIF}}\right)^2 \frac{R_{SIF}^2}{2D} \quad (13)$$

Comparing relations (11) and (13) and using the estimation (8), the time at which the source of discrepancy arises is:

$$t_Q^* \geq t_{ss} \left(\frac{1}{16.1} \frac{R_{SIF}}{R_{FPZ}}\right)^2 \geq t_{ss} \left(\frac{1}{161} \frac{E}{\sigma_Y}\right)^2 \quad (14)$$

and therefore:

$$t_Q^* > t_{ss} \quad \text{if} \quad E / \sigma_Y > 161 \quad (15)$$

which is valid for most engineering alloys. It means that the far field can affect the K -driven hydrogenation of FPZ well after the transient concentration falls within a 5% scatter band near the steady state hydrogen distribution. Before this there is no reason to anticipate a discrepancy between concentrations C_a and C_f in the FPZ.

CONCLUSIONS

The K -dominance condition in HAC was elucidated by means of an analysis of stress-strain assisted diffusion of hydrogen in the vicinity of a crack tip, to determine the effect of the far-field on hydrogen accumulation in the FPZ under sustained or quasi-static loading and SSY conditions. The influence of the *far field* on near-tip hydrogen diffusion is of minor importance and thus standard linear fracture mechanics preconditions for describing the mechanical state in the crack-tip FPZ using K seem to remain valid to ensure a negligible effect of diverse far-field stress distributions on the kinetics of near-tip hydrogenation

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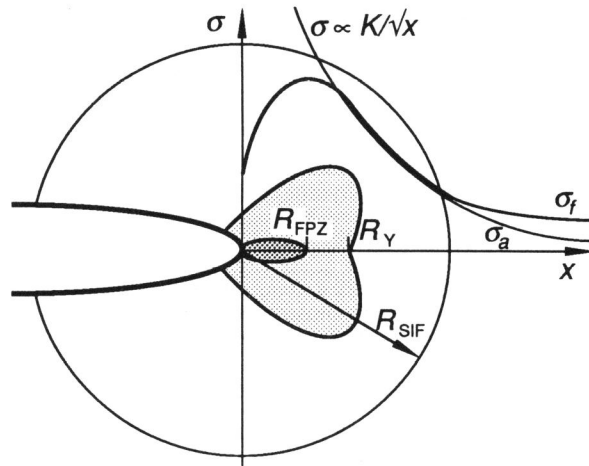


Figure 1 Sketch of specific zones and stress state in the vicinity of the crack tip.

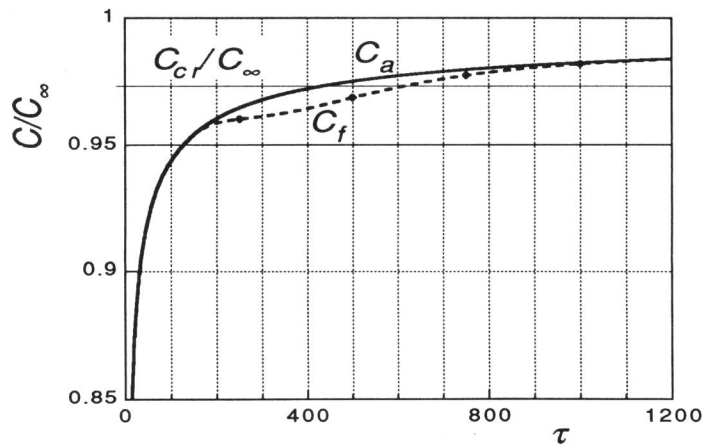


Figure 2 Plot of hydrogen concentration evolutions: K -driven concentration C_a (solid line) and a representative of the family of far-field affected concentration C_f (dashed line). For the purposes of discussion, an example of critical concentration level C_{cr} below the steady-state one C_∞ is also shown.