

## On the Validity of the Fracture Mechanics Approach to Hydrogen Assisted Cracking

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### Summary

This paper deals with the meaning and significance of the fracture mechanics approach to hydrogen assisted cracking, analyzing the question of  $K$ -dominance not only over the purely mechanical aspects, but also over the environmental (physico-chemical) events. Two key factors able to violate the uniqueness of the crack growth kinetics curve  $v = v(K)$  are discussed: the role of far field (the stress-strain field which is not  $K$ -dominated) and the effect of the history of hydrogenation and crack growth. The far field is shown to have a minor effect on near-tip hydrogen diffusion, and thus it can only widen the scatter band of crack growth rates in the near-threshold portion of the  $v(K)$ -curve. With regard to the effect of history, the study reveals that hydrogenation and crack growth are coupled processes, one influencing the other, so the crack growth kinetics curve  $v = v(K)$  is not unique, although a special regime of steady-state crack growth is seen to exist in which hydrogen assisted cracking turns out to be a  $K$ -dominated process, and the corresponding plot of the steady-state  $v$  against  $K$  acquires the uniqueness of a material's characteristic curve useful in engineering.

### Introduction

Engineering design frequently involves problems of environmentally assisted cracking (EAC) in materials and structures: stress corrosion cracking, hydrogen assisted cracking (HAC), etc. The linear fracture mechanics approach is effective in material evaluation and structural integrity assessment. Under small scale yielding, the stress intensity factor  $K$  is the only parameter governing the stress-strain state near the crack tip. The key of the approach is the crack growth kinetics curve: a plot of crack growth rate  $v$  vs. stress intensity factor  $K$ , between the threshold  $K_{th}$  and the fracture toughness  $K_c$ .

The idea of *uniqueness* of  $v(K)$ -curves and thresholds  $K_{th}$  as intrinsic characteristics of {material-environment} systems forms the backbone of the approach and ensures the soundness of applications in engineering design. This uniqueness ensures the *similitude* of crack behavior in test specimens and in structural components in service, thereby providing *transferability* of laboratory testing data to real engineering structures.

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The reliability of the fracture mechanics approach to EAC was reviewed in [1], showing that the same  $K$  does not always yield equal crack velocities in a {material-environment} system. A method for engineering safe design is given in [2] based on the *worst* crack tip situation associated with the fastest crack growth rate  $v_m(K)$ . This master curve  $v_m(K)$ , envelope of all  $v(K)$ -curves, is a characteristic of the {material-environment} system: the weakest resistance to EAC.

The present paper elucidates the question of  $K$ -dominance not only over the mechanical aspects of the phenomenon but *also* over the environmental (physico-chemical) events affecting the coupled process of hydrogenation and failure.

### Fracture Mechanics Approach to HAC

To have  $K$ -dominance over the whole HAC process, and thus uniqueness of the  $v(K)$  curve for a given {material-hydrogen} system, two preconditions must be fulfilled (cf. Toribio and Kharin [3] for details and nomenclature):

/1/  $K$ -controlled uniqueness of critical hydrogen concentration  $C_{cr}$  which must be reached at some point of the fracture process zone to cause local fracture and crack advance;

/2/  $K$ -dominance over the process of hydrogenation in the fracture process zone ahead of the crack tip, i.e., uniqueness of the evolution of the distribution of hydrogen concentration  $C(x, t)$ .

While the first precondition is always fulfilled in the framework of linear elastic fracture mechanic analyses under small scale yielding, the achievement of the second one is not guaranteed in all cases. In further sections of this paper, the effects of far field and history are discussed in depth.

However, in spite of the fact that the  $v(K)$ -curve is not always  $K$ -dominated (the second precondition could fail), on assuming sustained loading conditions the threshold  $K_{th}$  is always  $K$ -dominated, because such a threshold is associated with the unique steady-state distribution of hydrogen concentration. This stationary solution of the equation of stress-strain assisted diffusion has the same self-similitude properties as the stress-strain field, and thus only the first precondition is necessary to guarantee the uniqueness of the threshold.

### The Effect of Far Field on $K$ -Dominance in HAC

The matter of  $K$ -dominance with regard to hydrogen diffusion in the near-tip region is addressed in [4]. It is the 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  $\sigma_a$ ) to represent the actual concentration  $C_f$  being driven by the complete mechanical field containing the whole series expansion (i.e., influenced by the non-autonomous *far field*  $\sigma_f$ ). To this end, the discrepancy  $E = C_a - C_f$  between the two concentration distributions

is the subject of interest to estimate the effect of the far field (the remote stress-strain field which is not  $K$ -controlled). As explained in [4], the following equation can be derived for  $E$ :

$$\frac{\partial E}{\partial t} = D[\nabla^2 E - \mathbf{M}_f \bullet \nabla E - N_f E] + \nabla D \bullet [\nabla E - \mathbf{M}_f E] + Q \quad (1)$$

where an additional source-type term arises (cf. [4]):

$$Q = \begin{cases} D\Omega\nabla(\sigma_f - \sigma_a) \bullet C_a \neq 0 & \text{at } r > R_{\text{SIF}} \\ 0 & \text{at } r \leq R_{\text{SIF}} \end{cases} \quad (2)$$

This expression represents the source term for diffusion of discrepancy  $E$  which is the difference between the approximate  $K$ -driven concentration distribution and the exact far-field affected one. With nil initial and boundary conditions for  $E$ , its absolute value increases from zero with time since the source  $Q$  produces this imaginable "diffusible substance" in the solid. This "error" is generated by the source  $Q$  operative at long distances, and it diffuses from there towards the fracture process zone. The effect of the far field on  $K$ -dominance over hydrogen accumulation in the fracture process zone becomes more severe when a greater amount of "error"  $E$  can reach the near-tip region by "virtual" diffusion from the distant source (2) situated at long distance.

After estimation of the sizes of the crack tip zones and analysis of near-tip hydrogen diffusion [4], the time evolution of the asymptotic ( $K$ -driven) concentration  $C_a$  was obtained at the outer border of the fracture process zone where the effect from the source  $Q$  appears first as:

$$C_a(x = R_{\text{FPZ}}, t) = C_a(\tau) = C_\infty(R_{\text{FPZ}}) \operatorname{erfc} \frac{1}{2\sqrt{\tau}} \quad (3)$$

where  $\operatorname{erfc}(\cdot)$  is the complementary error function and  $\tau$  the dimensionless time  $\tau = Dt/R_{\text{FPZ}}^2$ . Fig. 1 shows a plot of  $C_a(\tau)$  (solid line). For  $\tau \geq 130$ , the concentration  $C_a$  in the fracture process zone exceeds 95% of the steady-state level  $C_\infty$ . 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 fracture process zone falls into this 5% strip from the time moment  $t_{\text{SS}}$  (*ss* indicates steady-state) given by:

$$t_{\text{SS}} = 130 \frac{R_{\text{FPZ}}^2}{D} \quad (4)$$

Thus the far field can affect the  $K$ -driven hydrogenation of the fracture process zone well after the transient concentration falls within a 5% scatter band near the

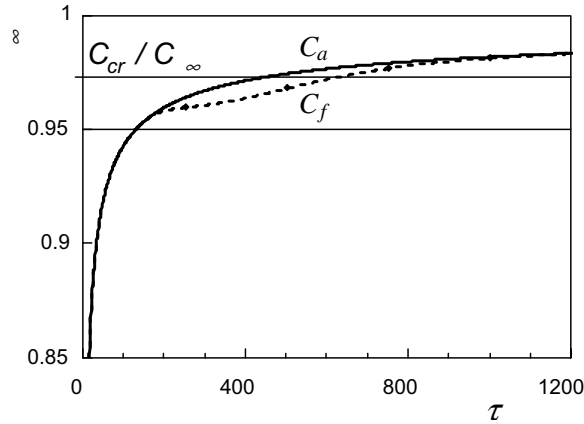


Figure 1: Plot of time evolutions of hydrogen concentration: asymptotically-driven ( $K$ -controlled) concentration  $C_a$  (solid line) and a representative of the family of far-field affected concentration  $C_f$  (dashed line). An example of near-threshold critical concentration level  $C_{cr}$  below the steady-state one  $C_\infty$  at  $K_{th}$  is also shown.

steady-state hydrogen distribution. Within the narrow 5%-width strip in the vicinity of the steady-state limit  $C_\infty$  which defines  $K_{th}$  the supposition about  $K$ -control over hydrogen diffusion may be erroneous, as shown in Fig. 1 where the dashed line represents schematically one of the possible  $C_f$ -curves. This fact can affect the  $v(K)$ -curve only in its near-threshold part, but without affecting the threshold itself which remains  $K$ -controlled, as demonstrated in [4].

### The Effect of History on $K$ -Dominance in HAC

Neither of the two processes of crack propagation and hydrogen diffusion should be considered separated from the other, since the movement of a crack tip is relevant to hydrogen accumulation in the fracture process zone. 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 capable of affecting near tip diffusion and consequently the kinetics of HAC.

The effect of history of the coupled hydrogenation-cracking process on  $K$ -dominance during HAC is addressed in previous research work [5,6]. The first paper [5] develops theoretical bases and a qualitative analysis demonstrating the coupling between hydrogenation and crack growth, so that the crack growth rate in HAC generally is not governed solely by  $K$ . In the second paper [6], the  $K$ -dominance condition is analyzed, as explained in the following paragraphs.

In a moving crack, the diffusion problem may be considered in a coordinate system  $(x, y)$  attached to the crack tip so that  $x = x_1 - a(t)$ ,  $y = x_2$ . This will cause transformation of the diffusion equation associated with the coordinate system  $(x_1,$

$x_2$ ) pinned to the solid. Then the total time derivation of concentration is:

$$\dot{C} = \frac{\partial C}{\partial t} - \frac{da}{dt} \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} - v \frac{\partial C}{\partial x} \quad (5)$$

By analogy with the actual thermodynamic one, the *fictitious driving force* for diffusion may be formally considered:

$$\mathbf{X}_D^* = \mathbf{X}_D - \frac{RT}{D} v \quad (6)$$

This formulation of the diffusion-cracking problem is completely closed if  $K$  is somehow known. For such a case, if  $C$  is a solution of the diffusion equation parametrically dependent on crack growth rate  $v$ , the latter can be found as:

$$v = v(K, t) \quad (7)$$

Therefore, the crack growth rate must not be the same at equal values of  $K$ , but varies with the total HAC process time  $t$ . The  $v$  for a given  $K$  is [6]:

$$v(K, t) = -\frac{D}{x_c} \ln \left[ \frac{C_{cr}(K, x_c)}{C_0 K_S(x_c, K) \operatorname{erfc}\left(\frac{x_c}{2\sqrt{Dt}}\right)} \right] \quad (8)$$

which has physical sense only after some incubation period  $t_{in}$  has elapsed, i.e., at  $t \geq t_{in}$ . This happens for:

$$t_{in} = \frac{1}{4D} \left[ \frac{x_c}{\operatorname{erfc}^{-1}(C_{cr}/C_\infty)} \right]^2 \quad (9)$$

where the function  $\operatorname{erfc}^{-1}(\cdot)$  is the one inverse to  $\operatorname{erfc}(\cdot)$  and  $C_\infty = C_0 K_S(x_c, K)$  is the exact steady-state solution for hydrogen diffusion near a stationary crack.

From relation (8) it follows that the crack growth rate at fixed  $K$  is a rising function of time which starts to increase from  $v = 0$  at  $t = t_{in}$  and asymptotically approaches some *steady-state* value  $v_{SS}$  as  $t \rightarrow \infty$ :

$$v_{SS} = -\frac{D}{x_c} \ln \left[ \frac{C_{cr}(K)}{C_0 K_S(K)} \right] = \frac{D}{x_c} \ln \left[ \frac{C_\infty(K)}{C_{cr}(K)} \right] \quad (10)$$

The steady-state crack growth rate (10) is a single-value function of  $K$ , and thus the crack growth kinetics curve as a plot of  $v_{SS}$  vs.  $K$  possesses the uniqueness of a material's characteristic curve and is really  $K$ -dominated.

### Conclusions

The meaning and significance of the linear elastic fracture mechanics approach to hydrogen assisted cracking was revised for small scale yielding and stationary cracks under sustained or quasi-static loading.

The role of *far field* on near-tip diffusion of hydrogen is of minor importance and can affect the  $v(K)$ -curve only in its near-threshold part, but it has no effect on the threshold itself which is still governed by  $K$ .

The effect of *history* appears in the form of coupling between hydrogen diffusion and crack growth and loss of  $K$ -dominance over the crack growth rate  $v$ , although a  $K$ -controlled steady-state value  $v_{SS}$  does exist.

### Acknowledgement

The authors wish to thank the present financial support of their research by the Spanish Ministry for Education and Science (MEC, Grant BIA2005-08965), and *Junta de Castilla y León* (JCYL; Grants SA078/04 and SA067A05).

### References

1. Toribio, J. and Kharin, V. (1997): "The Reliability of the Fracture Mechanics Approach to Environmentally Assisted Cracking: 1. Uniqueness of the  $v(K)$ -curve", *Materials & Design*, Vol. 18, pp. 87-94.
2. Toribio, J. and Kharin, V. (1997): "The Reliability of the Fracture Mechanics Approach to Environmentally Assisted Cracking: 2. Engineering Safe Design", *Materials & Design*, Vol. 18, pp. 95-101.
3. Toribio, J. and Kharin, V. (1998): "Evaluation of Hydrogen Assisted Cracking: The Meaning and Significance of the Fracture Mechanics Approach", *Nuclear Engineering and Design*, Vol. 182, pp. 149-163.
4. Toribio, J. and Kharin, V. (1997): " $K$ -dominance Condition in Hydrogen Assisted Cracking: The Role of the Far Field", *Fatigue and Fracture of Engineering Materials and Structures*, Vol. 20, pp. 729-745.
5. Toribio, J. and Kharin, V. (1997): "The Effect of History on Hydrogen Assisted Cracking: 1. Coupling of Hydrogenation and Crack Growth", *International Journal of Fracture*, Vol. 88, pp. 233-245.
6. Toribio, J. and Kharin, V. (1997): "The Effect of History on Hydrogen Assisted Cracking: 2. A Revision of  $K$ -dominance", *International Journal of Fracture*, Vol. 88, pp. 247-258.