#### On certain aspects of the hydrogen-assisted cracking

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IN THE ARTICLE the geometric and stress distribution characteristics of the fracture process zone are defined. These results are applied to consider the problem of hydrogen assisted cracking under threshold conditions. In particular, the relation of threshold stress intensity factors  $(K_{th})$  vs. hydrogen pressure (p) for elasto-plastic materials is theoretically established in accordance with experiments. As a by-product of the analysis, the mean hydrogen concentration within the process zone is calculated and used to discuss the kinetic conditions of the crack motion.

W pracy określono geometrię i charakterystykę stanu naprężenia w obszarze podlegającym procesowi pękania. Wyniki te zastosowano do rozważenia problemu pękania z udziałem wodoru w warunkach progowych. W szczególności ustalono teoretyczny (zgodny z doświadczeniami) związek między progowymi współczynnikami intensywności naprężenia K<sub>th</sub> a ciśnieniem wodoru p dla materiałów sprężysto-plastycznych. Produktem ubocznym tej analizy jest wartość średniej koncentracji wodoru, którą wykorzystać można w dyskusji warunków ruchu szczeliny.

В работе определены геометрия и характеристика напряженного состояния в области, подлежающей процессу разрушения. Эти результаты применены к рассуждению задачи разрушения с участием водорода в пороговых условиях. В частности установлена теоретическая связь (совпадающая с экспериментами) между пороговыми коэффициентами интенсивности напряжения  $K_{\rm th}$  и давлением водорода *р* для упруго-пластических материалов. Дополнительным продуктом этого анализа является значение средней концентрации водорода, которую можно использовать в обсуждении условий движения трещины.

#### 1. Introduction

THE EMBRITTLING effect of hydrogen on the fracture behaviour of metals has been studied extensively over several decades. Nevertheless it appears that no single unified theory is able to explain and describe this very complex problem. Some of the major aspects of hydrogen embrittlement have been reviewed by several authors, eg, GERBERICH [8], HIRTH and JOHNSON [9], ORIANI and JOSEPHIC [16], BIRNBAUM [5]. Therefore, for the sake of brevity, no attempt will be made here to review the voluminous hydrogen embrittlement literature. The term "Hydrogen Embrittlement" (HE) is used to describe the influence of hydrogen on the nucleation and propagation of cracks in solids. The mechanical process usually associated with HE is subcritical crack growth under an applied stress within a hydrogen environment. Subcritical crack growth denotes slow, stable crack growth occurring at stress intensity factors below the critical stress intensity factor. In the present paper we will limit our considerations to the so-called hydrogen-assisted cracking (HAC), this means to the situation where hydrogen is delivered to the metal system from the external gaseous atmosphere only. The mechanistic interaction between hydrogen and metal is not well understood. The difficulty is mainly due to the fact that the role of hydrogen on the material properties is multifold and cannot be accounted for on the basis of a single fracture mechanism. In particular, the effect of hydrogen on the strength of atomic bonds and the properties of dislocations is not clear. Besides these fundamental problems, the modeling of HE or HAC is further complicated by the fact that it manifests itself in different forms, given different environmental conditions, alloys and testing procedures.

There are two main components defining the process of HAC: 1) the kinetics of hydrogen transfer across the gas-solid interface into the material and hydrogen atoms transfer within the material and 2) the specific mechanism of failure. It is important to distinguish the difference between these factors since the manifestation of embrittlement may vary widely due to different kinetic effects even though the specific mechanism of failure may not change. It is generally accepted, however, that for brittle fracture to occur in a normally ductile material, a critical concentration of hydrogen must accumulate in a process zone (PZ) located ahead of the crack tip. This general idea underlines the computational procedure adopted in the paper in order to verify or predict certain experimentally observed phenomena. Accepting this point of view, we depart, however, from the usually adopted assumption that the critical concentration at a certain point, somewhere ahead of the crack tip, should be utilized in the fracture criterion. This quantity is a very difficult one to be measured experimentally and difficult to be calculated realistically because of the very complex nature of the stress distribution within the degradated region ahead of the crack tip. Instead of the concentration at the particular point ahead of the crack tip, we use in our criterion the notion of the mean critical concentration, calculated over a certain domain which is broadly called the fracture process zone or shortly the process zone.

The plan of the paper is as follows: first the PZ is precisely defined for inert environment, then the results are extended to take into account the influence of the chemically active environment. The so-called scaling procedure is adopted. Scaling coefficients are determined both by macro and microscopic analysis. This leads to the general structure of the K(stress intensity factor) vs.v (crack velocity) curve. Next the p (hydrogen pressure) vs.  $K_{th}$  curve is predicted, the mean hydrogen concentration within PZ is calculated and the threshold stress intensity factor is estimated. Finally the microscopic analysis leads to the formula for the crack tip velocity within the first stage of the crack growth. For the details of certain calculations we refer to the recent papers by NEIMITZ and AIFANTIS [11, 12, 13, 14].

#### 2. Process zone definition

The notion of the PZ is broadly used in fracture mechanics. It consists of a small region surrounding the crack tip. It is a controlling factor for the onset of instability as well as for crack growth. Its size and shape depends on the nature of the material and the level of loading. It has different features for brittle, ductile or environmental fracture. Usually, continuum mechanics arguments are applied outside of this zone, while a distribution of "cohesive" forces is postulated in its interior.

We consider a blunted crack in an elasto-plastic material of length a and tip opening displacement  $\delta_T$ . We replace the "physically" blunted crack by a "mathematically" sharp



FIG. 1. Scheme of the crack tip zone.

one by properly extending the crack faces as shown in Fig. 1. The tip of the physical crack will be called "trailing edge" (TT) as opposed to the mathematical crack tip which will be called "leading edge" (L). The region TTL is referred to as the process zone (PZ). To define it precisely we need to know its length, shape, as well as the distribution of stresses within it. Roughly speaking, its length is motivated by RICE-JOHNSON [20] elastoplastic analysis for blunted crack, its shape by smooth closure condition and SMITH's [21] power representation for the PZ displacements, while the PZ stresses are assumed to vary linearly from a minimum value at the trailing edge to a maximum one at the leading edge. In connection with the Rice and Johnson findings we assume here that in the absence of environmental and chemical factors the leading edge of the crack is identified with the point of maximum stresses. Thus, according to the above mentioned results, only the length of the PZ changes with the external loading but not the maximum of the stress at its ending tip. This behaviour is in qualitative agreement with the plastic zone defined by DUGDALE [7] or cohesive zone defined by PANASYUK [17]. Indeed, in Dugdale's model the length of the plastic zone is a function of the crack tip opening displacement which, in turn, is an increasing function of external loading. In connection with the above discussion, the essential difference, in the basic concept, of the present PZ definition from many earlier theories should be pointed out. We present the point of view here that the PZ in the elasto-plastic material extends over a strongly degradated domain ahead of the crack tip and is not necessarily identified with the distance between microstructural inhomogeneities. The length of the PZ is a result of the synergistic action of stresses and environment, thus, is the function of the external loading, temperature, concentration of chemical species as well as the "macroscopic" properties of the material.

The distribution of stresses within the PZ is assumed to vary linearly from a minimum value at the trailing edge to a maximum one at the leading edge and this latter value does not depend on external loading. In particular, we assume that the stress distribution f(x) in the region TTL is given by the formula

(2.1) 
$$f(x) = \sigma_T + \left(\frac{\sigma_L - \sigma_T}{r_p}\right) x,$$

where  $\sigma_L$  and  $\sigma_T$  denote the maximum (leading edge) and minimum (trailing edge) values, respectively, and  $r_p$  is the PZ length. Taking into account the geometry depicted in Fig. 1, the simple relation for  $r_p$  can be written in the form

(2.2) 
$$r_p = \delta(2\nu + 0.5),$$

and the coefficient v is to be found from the model. Moreover, we assume the following relations for  $\sigma_L$  and  $\sigma_T$ :

(2.3) 
$$\sigma_L = \xi \sigma_y, \quad \sigma_T = \eta \sigma_y,$$

where  $\xi$  is given by the Rice and Johnson analysis and  $\eta$  is to be defined later.

Having the length of the PZ and stress distribution within it available, we must now define its shape. Motivated by SMITH'S [21] analysis and the smooth closure condition, we assume that the displacement distribution u(x) within the PZ varies in a power-law fashion as follows:

(2.4) 
$$u(x) = u_T \left(\frac{r_p - x}{r_p}\right)^m,$$

where  $u_T$  is the value of the displacement u(x) at the trailing edge  $(u_T = u(0) = \delta_T/2)$ and the coefficient m is assumed to be larger than one (m > 1) in order to satisfy the smooth closure condition. The relations (2.1) to (2.4) define completely the characteristics of the PZ provided that the coefficients  $\eta$ , m and v are known. The values of these coefficients will be obtained as a result of certain "consistency" relations. First, the consistency relation has been obtained by eliminating plastic singularity, similarly to BARENBLATT'S [4] approach but replacing the elastic stress field by the HRR plastic field ahead of the modified, mathematically sharp crack and unknown cohesive stress distribution by the one assumed as in the relation (2.1). Both Barenblatt's and Dugdale-Panasyuk's analyses were performed for the elastic material. Elimination of elastic singularity was obtained by superposing the two independent solutions: one for the body loaded at infinity and the second for loading applied on the crack faces. The same procedure was adopted to calculate displacements of the crack faces. In this case the exact solution for the body loaded on the crack faces was superimposed on the approximate, one-term solution for the body loaded at infinity. The physical situation that we consider involves small deformations without unloading. Thus, in analogy to elasticity, we assume that the above procedure is valid independently of whether the loads are applied on the boundaries of the specimen or on the crack faces. Nevertheless, the situation here is more complicated since neither approximate nor exact solutions for a crack loaded on its faces are known. To solve the problem we simply adopt the assumptions (2.1) to (2.3) listed earlier with the unknown coefficients left to be calculated later. Thus, the displacements of the crack faces due to the forces applied to its surfaces can be written in the form

(2.5) 
$$u_{PZ}(x) = u_{\infty}(x) - u(x),$$

where  $u_{\infty}(x)$  is the known elasto-plastic solution due to external loading applied at infinity and u(x) is given by Eq. (2.4). After certain calculations we obtain (NEIMITZ and AIFANTIS [11]) the first "consistency" relation which, evaluated at the onset of crack growth, can be written in the form

(2.6) 
$$m_{c} = \left[\frac{1}{(\xi - \eta_{c})}\left\{(q_{c}^{\omega} - 1)\eta_{c} - \frac{1}{d_{n}}\right\} + \frac{q_{c}^{\omega}}{1 + \omega}\right]^{-1} - 1,$$

where  $\omega = 1/(n+1)$ , *n* is an exponent in the Ramberg-Osgood constitutive relation,  $d_n$  is a numerical coefficient and  $q = 4\nu + 1$ , the subscript *c* denotes that the particular coefficient has been evaluated at the onset of the crack growth. The second "consistency" relation is obtained by considering the energy balance at the crack tip, right at the onset of instability. As was originally shown by RICE [19] one may calculate the *J* integral by evaluating it along a contour  $\Gamma$  surrounding the crack tip and essentially shrinking its size down to the upper and lower surfaces of the PZ. This procedure reduces the original definition of the *J*-integral

(2.7) 
$$J_{\infty} = \int_{\Gamma} \left( W dy - \frac{\partial \mathbf{u}}{\partial x} \cdot \mathbf{t} \, ds \right),$$

where W is the strain energy density, **u** the displacement vector, **t** the traction, and ds the differential element of  $\Gamma$ , to the following formula:

(2.8) 
$$J = -\int_{\Gamma} f(x_1) \frac{\partial u}{\partial x_1} dx_1 = -2 \int_{0}^{T_p} f(x_1) \frac{\partial u}{\partial x_1} dx_1,$$

with  $f(x_1)$  obtained from Eq. (2.7) and u from Eq. (2.4) by changing the coordinate x to  $x_1$   $(x_1 = r_p - x)$ . At the onset of crack motion the above relation expresses the energy balance at the crack tip. Thus we have formally

(2.9) 
$$2\int_{0}^{\beta c} f_{c}(x_{1}) \frac{\partial u_{c}}{\partial x_{1}} dx_{1} = J_{\infty c},$$

where  $f_c$  and  $u_c$  are expressed in the form

(2.10) 
$$f_c(x_1) = \sigma_L - \left(\frac{\sigma_L - \sigma_{Tc}}{r_{pc}}\right) x_1,$$

(2.11) 
$$u_c(x_1) = u_{Tc} \left(\frac{x_1}{r_{pc}}\right)^{m_c}.$$

The quantity  $J_{\infty c}$  is a material parameter usually termed "energy release rate". It can be expressed in terms of the critical crack opening displacement as follows:

(2.12) 
$$J_{\infty c} = \left(\frac{\delta_c}{d_n}\right)\sigma_y.$$

On substituting Eqs. (2.10), (2.11) and (2.12) into Eq. (2.9) one obtains the following "consistency" relation between  $m_c$  and  $\eta_c$ :

(2.13) 
$$m_c = \left[\frac{1}{(\xi - \eta_c)} \left(\frac{1}{d_n} - \eta_c\right)\right]^{-1} - 1.$$

Finally, the third "consistency" relation has been evaluated by introducing the definition of the crack opening angle (COA). As a result of extensive theoretical and experimental works, it has been shown by several investigators that the COA serves as an important parameter to characterize subcritical crack growth. The definition of the COA is a difficult and non-unique problem. It depends to a certain degree on the fancy of the particular investigator. In most of the presented theories the COA is identified directly or indirectly with the ratio  $\delta_c/r_{pc}$ . In contrast to the above procedures, here we present the point of view that the COA should not only be a function of the ratio  $\delta_c/r_{pc}$ , but also depend on the PZ profile. As it was shown previously, this profile is completely determined by  $m_c$ , provided that  $\eta_c$  and  $r_{pc}$  are given. Motivated by this discussion, it would not be unreasonable to define here the COA as the average of the COA's along the whole profile. With these assum ptions the COA =  $\theta$  is equal for small angles  $(\tan \theta \simeq \theta)$ 

$$\theta = \frac{m_c}{q_c}.$$

Equations (2.6), (2.13) and (2.14) can be solved simultaneously to render the values of  $m_c$ ,  $\eta_c$  and  $\nu_a$  in terms of material parameters n,  $\sigma_y/E$  and  $\theta$ . Indeed, the above equations can be cast in the following convenient form:

(2.15) 
$$Am_c^{\omega} + Bm_c^{\omega-1} + C = 0,$$

(2.16) 
$$\eta_c = \frac{m_c + (1 - \xi d_n)}{m_c d_n},$$

(2.17) 
$$v_c = \frac{1}{4} \left( \frac{m_c}{\theta} - 1 \right),$$

where the material coefficients A, B, C are given by the expressions

(2.18) 
$$A = [(\omega+1)^{-1} - (1-\xi d_n)^{-1}]\theta^{-\omega},$$

$$(2.19) B = -\omega \theta^{-\omega},$$

(2.20) 
$$C = 2(1 - \xi d_n)^{-1}.$$

The numerical results for  $m_c$ ,  $\eta_c$  and  $\nu_c$  were given by NEIMITZ and AIFANTIS [11]. Example values are presented in Fig. 2.



FIG. 2. Examples values of  $m_c$ ;  $\eta_c$  and  $\nu_c$ .

In the case when environmental effects in the form of high temperature or corrosion are important, the process zone should be properly modified. Such modification is necessary in order to take into account the fact that the critical zone of material degradation ahead of the crack tip may now be different from that defined by  $r_p$ . Accepting this point of view, it has been postulated that the new process zone in the presence of environment can be determined by proper scaling of the parameters defining it in the absence of environment. The scaling coefficients will then depend on the structure of the stress field and the evolution of the relevant microstructure ahead of the crack tip, and their precise evaluation will rest upon theoretical arguments pertaining to this structure. Basing on these ideas we can now proceed formally and write

$$(2.20a) r_{pc}^{h} = \lambda_{1c} r_{pc}$$

$$(2.20b) \qquad \qquad \delta^h_{Tc} = \lambda_{2c} \, \delta_{Tc},$$

$$(2.20c) m_c^h = \lambda_{3c} m_c$$

(2.20d) 
$$\sigma_{Tc}^{h} = \lambda_{4c} \sigma_{Tc}$$

where  $\lambda_{1c}$ ,  $\lambda_{2c}$ ,  $\lambda_{3c}$ ,  $\lambda_{4c}$  are scaling coefficients, to be calculated. Similar relations are also true for the arbitrary moment but omitting the subscript c. It turns out that the scaling coefficients  $\lambda_{1c}$ ,  $\lambda_{2c}$  and  $\lambda_{3c}$  can be calculated from the "macroscopic" approach. In contrast, the calculation of the  $\lambda_{4c}$  coefficient is based on microscopic arguments. The first relation between  $\lambda_{1c}$  and  $\lambda_{2c}$  can be obtained by adopting the idea of a stepwise crack motion and the geometrical considerations on the shape and size of the PZ before and after jump (NEIMITZ and AIFANTIS [12]). Let us assume that at a reference time  $t_1$  the crack length is  $a_1$  and the initial mean concentration of hydrogen within the PZ is  $C_0$ . As time progresses the microstructure evolves under the synergistic action of the applied stress and environment and eventually reaches a critical value  $C_c$  at a moment  $t_2$ . Within this period  $\Delta t =$  $t_2 - t_1$ , the crack does not advance but its tip opening  $\delta_T^h$  and its PZ length  $r_p^h$  increase up to their critical values  $\delta_{Tc}^{h}$  and  $r_{pc}^{h}$  and its shape changes accordingly from  $m^{h}$  to  $m_{c}^{h}$ . At that critical moment the crack jumps spontaneously by a distance  $\Delta a = a_2 - a_1$ , so that the crack length is  $a_2$  at time  $t_2$ . We assume that after the jump is completed the material ahead of the crack tip is in identical conditions like those at the reference state. Thus the concentration begins to build up again from the initial ground value  $C_0$  until critical conditions are again reached and the whole process is repeated. The average crack velocity is then naturally defined by the ratio  $\Delta a/\Delta t_{\rm cr}$ . The geometrical analysis of the PZ just before and after jump leads to the relation between  $\lambda_{1c}$  and  $\lambda_{2c}$ :

(2.21) 
$$\lambda_{1c} = \lambda_{2c} \left[ 1 - \left( \frac{\delta_T}{\lambda_{2c} \delta_{Tc}} \right)^{1/m} \right],$$

or, introducing the relation

(2.22) 
$$\lambda_{10} = \lambda_{1c} \left(\frac{K_c}{K}\right)^2,$$

one obtains

(2.23) 
$$\lambda_{10} = \lambda_{2c} \frac{\delta_{Tc}}{\delta_T} - \left(\lambda_{2c} \frac{\delta_{Tc}}{\delta_T}\right)^{\frac{m-1}{m}},$$

and the length of the jump  $\Delta a$  is equal

$$(2.24) \Delta a = \lambda_{10} r_p$$

The second relation between  $\lambda_{10}$  and  $\lambda_{2c}$  in conjunction with the one already given, will eventually determine the unknown parameters of the theory. This is accomplished by considering the energy balance within the PZ. Indeed, in the absence of environment, instability occurs when a critical energy which is provided by the external load alone and commonly known as "energy release rate" is accumulated within the PZ. This energy can be computed in terms of the familiar path-independent or J integral by letting its contour to shrink down to the upper and lower surfaces of the PZ. In the presence of environment, the cracking process proceeds at smaller load levels than the corresponding ones in the absence of it. Thus, energy accumulated within the PZ due to the external loading only is now smaller than before. As a result, the "extra" energy required for fracture is delivered to the system by the chemomechanical action generated by the environment. Indeed, this chemomechanical action alters the original size and shape of the PZ, as well as the stress distribution within it. If the appropriate J-integral for the environmental conditions is denoted by  $J_c^h$ , it is reasonable to assume the equality

$$(2.25) J_c = J_c^h.$$

This relation can be evaluated provided that the functions  $u_c(x)$ ,  $u_c^h(x)$ ,  $f_c(x)$ ,  $f_c^h(x)$ ,  $r_{pc}$ and  $r_{pc}^h$  are known, as is the case here. After evaluation we obtain

(2.26) 
$$\lambda_{2c} = \frac{\sigma_{Tc} + (\sigma_L - \sigma_{Tc}) (m_c + 1)^{-1}}{\sigma_{Tc}^h + (\sigma_L - \sigma_{Tc}^h) \gamma^{-1} [\lambda_{10}^{\gamma} - (\lambda_{10} - 1)^{\gamma}] \lambda_{10}^{(1-\gamma)}},$$

where  $\gamma = \lambda_{3c}m_c + 1$ . The numerical solution of Eqs. (2.23) and (2.26) is given by NEIMITZ and AIFANTIS [12] for various values of  $\lambda_{3c}$  and  $\lambda_{4c}$ .

The value of the third scaling coefficient  $\lambda_{3c}$  has been estimated by determining its upper limit. On the basis of the observation that the COA decreases with hydrogen pressure, it can be argued that the range of the scaling coefficient  $\lambda_{3c}$  is

$$\frac{1}{m_c} \leqslant \lambda_{3c} \leqslant 1$$

It follows from the condition that  $\theta^h \leq \theta$  and  $m_c \geq 1$  from the smooth closure condition. Evaluating the right hand side of the inequality (2.27), we obtain

(2.28) 
$$m_c^h < m_c \left\{ 1 - \left[ \lambda_{2c} \left( \frac{K_c}{K} \right)^2 \right]^{-1/m} \right\}$$

which is the upper limit for  $m_c^h$ . Evaluating the left hand side of the inequality (2.27), we adopt the point of view that it characterizes the stage of subcritical growth commonly known as region I in the v vs. K graph. In this region the predominant mechanism of fracture is "brittle" or "intergranular" in contrast to the "ductile" or "transgranular" observed for higher K in region II and the "tearing" mechanism of region III. The transition from region I to region II is achieved when the condition  $m_c^h \ge 1$  becomes an equality. In physical terms, this means that as a result of the synergistic action of load and environment the PZ forces become too small to keep crack faces together in a smooth closure

manner. As a matter of convenience, with no consequence to the essence of the analysis, we will assume that the value of  $m_c^h$  remains constant (= 1) after it reaches its terminal unit value. An explicit relation of the transition from region I to region II in terms of the external loading can be found in the form

(2.29) 
$$\lambda_{2c} \left(\frac{K_c}{K}\right)^2 \ge \left(\frac{m_c}{m_c-1}\right)^m.$$

For particular values of  $m_c$  and m we can determine the value of external load ( $K_{I-II}$ ) where the transition occurs. Some numerical values for the transition points were given by NEIMITZ and AIFANTIS [12] where a remarkable agreement with experimental results is noted.

Finally, to complete the PZ definition for environmental cracking, the  $\lambda_{4c}$  coefficient should be estimated. An estimation of  $\lambda_{4c}$  was accomplished by NEIMITZ and AIFANTIS [13] by considering the detailed evolution of the prevailing degradation process. It turns out that  $\lambda_{4c}$  is in the range between 1 and 2.5. Even though the values of  $\lambda_{4c}$  within this range do not affect significantly the calculation of  $\lambda_{10}$  and  $\lambda_{2c}$  a more detailed calculation was proposed in the above mentioned report. The method was based on the assumptions (i) that the trailing edge stresses in the absence and presence of environment  $\sigma_T$  and  $\sigma_T^h$ relate through the mean concentration of hydrogen within the PZ which, for critical conditions, was assumed to be a material constant and (ii) that the critical values of the trailing edge stresses  $\sigma_{Tc}$  and  $\sigma_{Tc}^h$  are related through the local concentration of hydrogen at the tip of the crack. It turns out with the help of experimental data that the  $\lambda_{4c}$  coefficient is the function of hydrogen pressure and is in the rnage 1.1 to 1.25 for Oriani and JOSEPHIC [16] experimental data, and 1.2 to 1.5 for AKHURST and BAKER [3] experiment.

To complete the general structure of the v vs. K curve, the second transition point  $(K_{II-III})$  should be estimated in addition to the one  $(K_{I-II})$  already given. To accomplish it, one can notice the term  $(\lambda_{10}-1)^{\gamma}$  in the denominator of the relation (2.26). Since  $\gamma$  and  $\lambda_{10}$  are independent parameters, it follows that  $\lambda_{2c}$  may take imaginary values unless  $\lambda_{10}$  remains always larger than 1. In view of Eq. (2.23)

(2.30) 
$$\lambda_{10} = \lambda_{2c} \left(\frac{K_c}{K}\right)^2 - \left[\lambda_{2c} \left(\frac{K_c}{K}\right)^2\right]^{\frac{m-1}{m}} \ge 1.$$

The value of  $K_{II-III}$  (the second transition point from "ductile" to "tearing" type of fracture is obtained in terms of K when the inequality becomes equality. Physically the violation of the condition (2.30) means that the crack jump  $\Delta a$  is smaller than  $r_p$  since we have  $\Delta a = \lambda_{10} r_p$ . Therefore, the finite jump model is not applicable and the mode of fracture changes from a "discontinuous" or tearing one.

#### 3. Application of the PZ concept to the HAC

The concept of the PZ can be directly applied to analysis of the HAC. In particular, the p vs.  $K_{th}$  (threshold stress intensity factor) graph can be obtained utilizing AIFANTIS' [1] equilibrium solution for the hydrogen distribution in a stressed solid in the form (3.1)  $\rho = \rho_0 (1 + \beta \sigma^0)^{\alpha}$ ,

where  $\varrho$  denotes the local equilibrium hydrogen concentration ahead of the crack tip,  $\varrho_0$  its boundary value just below the crack surface,  $\sigma^0$  is the trace of the stress tensor and  $\alpha$ ,  $\beta$  are phenomenological coefficients. First, we note that  $\varrho_0$  can be expressed by Sivert's law

$$(3.2) \varrho_0 = k \sqrt{P},$$

where k is an equilibrium constant and P the external pressure. Secondly, we recall the structure of the stress field within the PZ which was discussed earlier and is depicted in Fig. 3. The point T indicates the trailing edge, L the leading edge of the crack (or the tip



FIG. 3. Scheme of the stress distribution within PZ at the presence of hydrogen environment.

of the PZ) in the absence of environment, and  $L^{h}$  the tip of the PZ in the presence of hydrogen. The maximum of the PZ forces occurs in L and thus we have two regions I and II within which the stress gradient is positive and negative, respectively. Specifically the stress distribution f(x) within the PZ is given by the formula

(3.3) 
$$\sigma_{22} = f(x) = \begin{cases} \sigma_{Tc}^h + \frac{\sigma_L - \sigma_{Tc}^h}{r_p} x, & 0 \le x \le r_p, \\ \sigma_L + \frac{\sigma_L - \sigma_y}{R_p} (x - r_p), & r_p \le x \le \lambda_{10} r_p. \end{cases}$$

For simplicity the stresses within region II was assumed to vary from the maximum value  $\sigma_L$  to a minimum one  $\sigma_{22} = \sigma_y$  at the tip of the plastic zone  $R_p$  ( $\gg r_p$ ). For small scale yielding  $R_p$  is given by the formula

(3.4) 
$$R_p = \frac{1}{3\pi} \left( \frac{K}{\sigma_y} \right)^2.$$

Having  $\sigma_{22}$  thus available, we can compute the trace of the stress tensor  $\sigma^0$  by utilizing Tresca's yield condition as was first done by AKHURST and BAKER [3] to obtain

(3.5) 
$$\sigma^{0} = (1 + \nu^{*}) (2\sigma_{22} - \sigma_{\nu}),$$

where  $\nu^*$  denotes an effective Poisson's ratio varying from 0.3 to 0.5. Upon substitution of Eqs. (3.2), (3.3), (3.4) and (3.5) into Eq. (3.1) we obtain the following relations for the equilibrium concentration of hydrogen

(3.6) 
$$\varrho(x) = \begin{cases} k \sqrt{P} \left( 1 + \beta (1 + \nu^*) \left\{ 2 \left[ \sigma_{Tc}^h + \frac{\sigma_L - \sigma_{Tc}^h}{r_p} x \right] - \sigma_y \right\} \right)^{\alpha}, & 0 \le x \le r_p, \\ k \sqrt{P} \left( 1 + \beta (1 + \nu^*) \left\{ 2 \left[ \sigma_L - \frac{\sigma_L - \sigma_y}{R_p} (x - r_p) \right] - \sigma_y \right\} \right)^{\alpha}, & r_p \le x \le \lambda_{10} r_p. \end{cases}$$

By evaluating Eq. (3.6) at  $x = \lambda_{10}r_p$ , i.e. at the tip of the PZ, we obtain an expression for the ground concentration  $C_0$  which is assumed to be a material constant. In view of Eqs. (1.2), (3.4), and (3.6) this expression reads

(3.7) 
$$\lambda_{10}^{\text{th}} = \left\{ \xi - \frac{1}{2} \left( \frac{1}{\sigma_y \beta (1 + \nu^*)} \left[ \left( \frac{C_0}{k \sqrt{P}} \right)^{1/\alpha} - 1 \right] + 1 \right) \right\} \left\{ \frac{1}{3\pi (2\nu_c + 0.5) d_n} \frac{E}{\sigma_y} \frac{1}{\xi - 1} \right\} + 1,$$

where  $\lambda_{10}$  was replaced by  $\lambda_{10}^{th}$  to indicate evaluation at threshold conditions. On evaluating Eq. (3.7) for two sets of threshold points  $(\lambda_{10}^{th}, P)$  and  $(\lambda_{10}^{th}, P)$  with a superimposed  $\circ$  denoting a reference state, we can eliminate the ground concentration  $C_0$  to obtain

(3.8) 
$$\left(\frac{\mathring{P}}{P}\right)^{1/2\alpha} = \frac{B_0}{1+B_1(B_2-B_3\lambda_{10}^{th})}$$

where

(3.9)  

$$B_{0} = 1 + B_{1}(B_{2} - B_{3} \lambda_{10}^{tn}),$$

$$B_{1} = \sigma_{y}\beta(1 + \nu^{*}),$$

$$B_{2} = 2\xi - 1 + B_{3},$$

$$B_{3} = \frac{6\pi\sigma_{y}}{E}(2\nu_{c} + 0.5)d_{n}(\xi - 1)$$

The quantity  $\lambda_{10}^{th}$  in Eqs. (3.8) and (3.9) is obtained from Eq. (2.23) by evaluating it at threshold conditions, i.e.

(3.10) 
$$\lambda_{10}^{\rm th} = \lambda_{2c}^{\rm th} \left(\frac{K_c}{K_{\rm th}}\right)^2 - \left[\lambda_{2c}^{\rm th} \left(\frac{K_c}{K_{\rm th}}\right)^2\right]^{\frac{m-1}{m}}.$$



FIG. 4. P-Kth curves. a) Akhurst and Baker experiment, b) Oriani and Josephic experiment.

<sup>10</sup> Arch. Mcch. Stos. 1/88

On combining Eqs. (3.8) and (3.10) we can plot the external pressure P vs. the threshold stress intensity factor. It should be pointed out that the results are insensitive to the choice of the reference point  $(\mathring{P}, \mathring{K}_{th})$  as long as this point is obtained from experiment. In Fig. 4 the results are compared with the experimental findings of AKHURST and BAKER [3] and ORIANI and JOSEPHIC [16].

Utilizing the relations (3.6), the mean concentration of hydrogen C can be easily calculated:

(3.11) 
$$C = \frac{1}{r_p^h} \int_0^{r_p^h} \varrho(x) dx.$$

Evaluation of Eq. (3.11) along with the numerical results for Akhurst and Baker, and Oriani and Josephic experimental data was presented by NEIMITZ and AIFANTIS [13]. The ratio of the mean, critical concentration of hydrogen to  $\rho_0$  is a function of K for constant P and varies, e.g. from 43.8 at K = 36 MPa $\sqrt{m}$ ,  $\alpha = 8$ , n = 5 to 48.8 at K == 46.5 MPa $\sqrt{m}$ ,  $\alpha = 8$ , n = 5 for Akhurst and Baker experimental data or from 10.9 at K = 10.0 ksi $\sqrt{in}$ ,  $\alpha = 8$ , n = 5 to 25.2 at K = 17.7 ksi $\sqrt{in}$ ,  $\alpha = 8$ , n = 5 for the Oriani and Josephic experiment.

In the preceding paragraph a jump-like crack kinetics has been postulated with a continuous measure of the crack velocity v given by the relation

$$v = \frac{\Delta a}{\Delta t_{\rm cr}},$$

where  $\Delta a$  is an average length of the crack jump which is here identified with the PZ length  $r_p^h$  and  $\Delta t_{\rm cr}$  is the time interval between two subsequent crack jumps. Indeed,  $\Delta t_{\rm cr}$  is a measure of the time interval which is necessary to build up a critical accumulation of hydrogen atoms within the PZ. Several investigators have utilized the concept of a critical hydrogen concentration at a certain arbitrarily chosen point ahead of the crack tip to formulate a criterium. In contrast to the above models, we adopt the point of view that the mean hydrogen concentration within the PZ should serve as a more suitable parameter to characterize the degradation of the material ahead of the crack tip. In turn, when this quantity reaches a critical value, fracture will occur. Utilizing this concept, NEIMITZ and AIFANTIS [14] have developed a formula for  $\Delta t_{\rm cr}$  and, subsequently, for v for the first domain within v v.s K curve. Neglecting hydrogen transport by dislocations, the formula is as follows

(3.13) 
$$v = \left(\frac{\delta_T}{\lambda_{2c}\delta_{Tc}} + 1\right)\frac{\varrho^*}{C_c}\frac{1}{w}V_h,$$

where  $V_h$  is the mean hydrogen velocity within the PZ, w is the numerical factor describing the shape of the PZ (since  $m^h \ge 1$   $w \le 0.5$ ) and  $\varrho^*$  the local hydrogen concentration at the crack tip. A rigorous calculation of the mean hydrogen velocity  $V_h$  may be a difficult task due to the evolution of the PZ and the mathematical difficulties in obtaining analytical transient solutions to the relevant stress-assisted diffusion equation; this problem was considered by AIFANTIS [2], VAN LEEUWEN [23] and PANASYUK *et al.* [18]. In this connection it should be noted that in such analyses the diffusion coefficients are taken as constants

(VAN LEEUWEN [23], PANASYUK *et al.* [18]) or linearly dependent on stress for elastic deformation (UNGER and AIFANTIS [22]). However, the PZ is a severely plastically deformed zone with numerous inhomogeneities acting as traps for hydrogen atoms. Indeed, this problem has been considered by DARKEN and SMITH [6], ORIANI [15] and JOHNSON and LIN [10] who concluded that diffusivity varies with plastic deformation. In view of the above problems, we have postponed (NEIMITZ and AIFANTIS [14]) a rigorous analysis of the transient diffusion problem to the future and provided a physically motivated approximate scheme for obtaining the velocty  $V_h^*$  and the trapping function  $\Omega$  (in deriving Eq. (3.13) the mean hydrogen velocity  $V_h$  was defined as a product of hydrogen atoms velocity without traps  $V_h^*$  and the so-called trapping function  $\Omega$ ). The formulas that we have proposed are strictly valid for region I where the ratio  $\varrho^*/C_c$  is assumed to be constant. This assumption is motivated by the fact that we view the stage I growth as a sequence of elementary thresholdlike jumps. This assumption becomes less reasonable for stage II and even more so for stage III where the idea of quasi-threshold conditions is certainly violated. The formulas introduced by NEIMITZ and AIFANTIS [14] can be written in the form

(3.14) 
$$V_h = \varkappa K^{2\omega} \left[ M - N \left( \frac{K}{K_{I-II}} \right)^2 \right]^n$$

with

$$m = \left[1 + Q\left(\frac{K}{K_{\rm II-III}}\right)\right],$$

where  $\chi$ ,  $\omega$ , M, N, Q are certain parameters depending on environmental and material properties. A proper selection of coefficients gives a very good agreement of the relation (3.13) with the experimental data.

The present article summarises a series of four articles by Neimitz and Aifantis where the problem of environmental cracking for elastoplastic materials has been studied by means of the PZ concept. Even though several encouraging results have been obtained many more possibilities are left open for further investigation.

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