JOURNAL OF MATERIALS SCIENCE 32 (1997) 1127–1131

The stress in a zirconium alloy due to the hydride precipitation misfit strains

Part II *Hydrided region at a crack tip*

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With regard to the quantitative modelling of delayed hydride cracking (DHC), it has been shown in Part I [9] that when a lenticular shaped hydrided region, i.e. one whose length is large compared with its thickness, forms at a planar surface or at the surface of a very blunt notch, the compressive stress σ_H induced within the region is markedly influenced by the unconstrained transverse precipitation strains as well as the unconstrained normal strain. The σ_H values are approximately the same irrespective of whether we assume that (a) the overall unconstrained expansion strain associated with hydride precipitation is confined entirely to the normal direction or (b) the strain is partitioned approximately equally between the three orthogonal directions. Thus, assuming the strain to be entirely in the normal direction allows for both precipitation strain scenarios.

The paper extends the considerations in Part I to the case where there is a hydrided region immediately ahead of a sharp crack, i.e. the other extreme to that considered in the earlier work, a model situation that simulates the behaviour of a growing DHC crack. In this case the normal stress within the region immediately ahead of the crack tip is not compressive but tensile, and is influenced by the unconstrained transverse precipitation strains, though not to the same extent as is the hydride induced stress associated with a hydrided region that emanates from a planar surface. Assuming the strain to be entirely in the normal direction overestimates the local stresses, and therefore unlike the planar surface situation, the assumption does not allow for both precipitation strain scenarios. It is therefore important to input the correct unconstrained precipitation strain tensor, if we require a reasonably accurate quantitative picture of DHC crack growth.

1. Introduction

If the hydrogen concentration in a zirconium alloy is sufficient for the terminal solid solubility (TSS) to be exceeded, delayed hydride cracking (DHC) can occur in a zirconium alloy. DHC is caused by the diffusion of hydrogen atoms to a stress concentration, preferential precipitation and growth of hydride platelets leading to the formation of a lenticular shaped hydrided region (one whose length is large compared with its thickness), and finally fracture of the region (DHC initiation). The stress due to the applied loadings (enhanced in the vicinity of a stress concentration) when combined with the stress induced by hydriding must be sufficient to fracture the region (the hydriding induced stress arises as a result of the unconstrained expansion strains associated with the precipitation of a hydride platelet). With regard to the modelling of DHC, it is important to quantify the hydride induced compressive stress (normal to the hydrided region) within a lenticular hydrided region, and in order to simplify the considerations, we will assume that the region is fully hydrided and has a two-dimensional profile.

When determining the magnitude of the hydride induced stress, it is important to input the correct unconstrained expansion strains associated with hydride formation. This poses a problem because, though it is generally believed that the overall unconstrained expansion strain, i.e. the sum of the strains in the three mutually orthogonal directions, is about 17%, there is dispute as to whether all this strain is confined to the direction normal to the plane of a lenticular hydrided region as suggested by Weatherly [1], and as assumed by the author [2–5] in his DHC initiation modelling work, or whether it is partitioned approximately equally between the three directions as suggested by Carpenter [6], and as implicitly assumed by Shi and Puls [7, 8] in their DHE modelling work, since they assume a normal strain of 5.4%, but neglect the effect of the in-plane expansion strains.

An earlier paper [9] (Part I) by the author has shown that when a lenticular shaped hydrided region forms at a planar surface or at the surface of a very blunt notch, the compressive stress σ_H induced within the hydrided region is markedly influenced by the unconstrained transverse precipitation strains as well as the unconstrained normal strain. The σ_H values obtained by assuming either Weatherly's or Carpenter's precipitation strain scenarios are approximately equal, whereby assuming [2–5] the overall strain to be confined to the normal direction allows for both precipitation strain scenarios.

The present paper extends the earlier work [9] to the case where there is a (constant thickness) hydrided region immediately ahead of a sharp crack, a model situation that is relevant to the behaviour of a growing DHC crack. In this case the normal stress within the hydrided region immediately ahead of the crack tip is not compressive but tensile, and though being influenced by the unconstrained transverse precipitation strains, the effect is not as great as that for a hydrided region ahead of a planar surface or very blunt notch. In the case of a crack, assuming the strain is confined to the normal direction overestimates the local stress, and therefore unlike the free surface situation, this assumption does not allow for both precipitation strain scenarios. The implication is that it is important to input the correct unconstrained precipitation strain tensor, if we require a reasonably accurate quantitative picture of DHC crack growth in zirconium alloys.

2. A hydrided region associated with an unconstrained normal expansion strain

Fig. 1 shows a two-dimensional hydrided region with length s and constant thickness $t = 2h$, immediately ahead of the tip of a semi-infinite crack in an infinite solid. The material within the region is assumed to be fully hydrided and, when unconstrained, is associated with an expansion strain e^{u}_{22} in the x_2 direction normal to the plane of the region with the other unconstrained strains being assumed to be zero. The strain e^{u}_{22} can be represented by smeared edge dislocation distributions (constant density) at each end of the hydrided region (see Fig. 1). As a measure of the stress within the hydrided region and how this is affected by e^{u}_{22}, we will determine the crack tip stress intensity K; this is positive, implying a tensile p_{22} stress immediately ahead of the crack tip; this p_{22} stress decreasing and eventually becoming compressive upon moving away from the crack tip into the hydrided region. The determination of K for the configuration in Fig. 1 can be broken down into the determination of K for the two separate configurations in Fig. 2a and b, and subtracting the K value for the configuration in Fig. 2b from that for the configuration in Fig. 2a. In fact, we need only determine K for the Fig. 2a configuration, since K for the Fig. 2b configuration is obtained by letting $s \to 0$.

As regards the determination of K for the Fig. 2a configuration, we can represent the unconstrained normal expansion strain e^{u}_{22} by a smeared edge dislocation distribution (constant density) at the end of the hydrided region. Thus $f(x_2)\delta x_2$ dislocations each of Burger's vector b are contained within an element of length δx_2, with the total Burger's vector B in the distribution being

$$B = b \int_{x_2=-t/2}^{+t/2} f(x_2)\,dx_2 = e^{u}_{22} t = 2e^{u}_{22} h \qquad (1)$$

With this approach, the stress distribution in the solid, and in particular the crack tip stress intensity is calculated by determining the stresses resulting from the smeared distribution of dislocations, as modified by the interaction of the distribution with the crack. Using the well-known solution for a single edge dislocation in an infinite solid [10], the stress p_{22} due to the smeared distribution at a distance u behind the crack

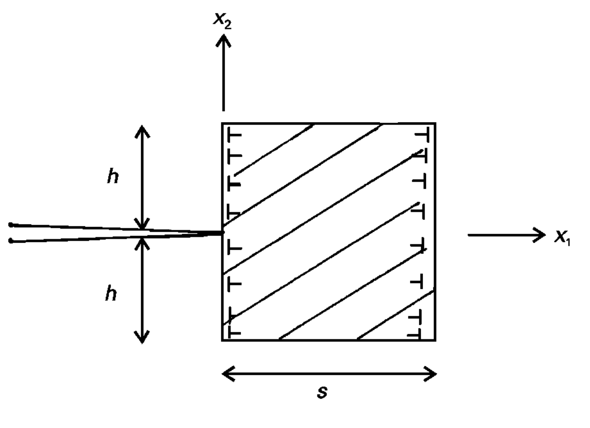

Figure 1 A hydrided region of length s and thickness $t = 2h$ immediately ahead of a crack tip; the region is associated with an unconstrained expansion strain e^{u}_{22} in the x_2 direction.

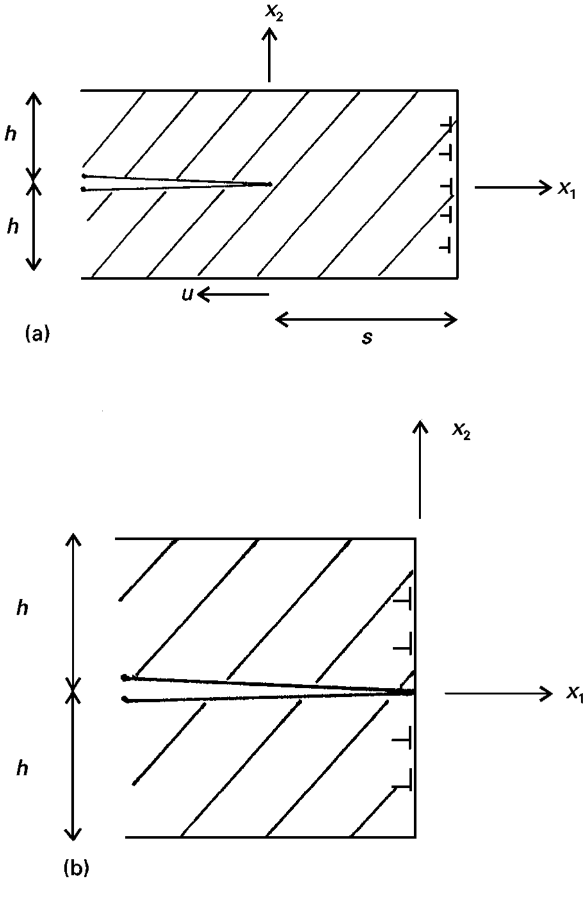

Figure 2 The determination of K for the configuration in Fig. 1 is obtained by subtracting the K value for the configuration in (b) from the K value for the configuration in (a).

tip in the crack's absence is

$$p_{22}(u) = -\frac{E_0(u+s)}{4\pi}\int_{-h}^{+h}\frac{[3x_2^2+(u+s)^2]}{[x_2^2+(u+s)^2]^2}\,b\mathrm{f}(x_2)\,\mathrm{d}x_2 \tag{2}$$

where $E_0 = E/(1-\nu^2)$, E being the Young's modulus and ν being Poisson's ratio (the elastic constants of the hydrided region and the surrounding material are assumed to be the same). Since $b\mathrm{f}(x_2) = e_{22}^{\mathrm{u}}$, it follows from Equation 2 that

$$p_{22}(u) = -\frac{E_0 e_{22}^{\mathrm{u}}(u+s)}{2\pi}\int_0^h \frac{[3x_2^2+(u+s)^2]}{[x_2^2+(u+s)^2]^2}\,\mathrm{d}x_2 \tag{3}$$

whereupon evaluation of the integral gives

$$p_{22}(u) = -\frac{E_0 e_{22}^{\mathrm{u}}}{2\pi}\left[2\cot^{-1}\frac{(u+s)}{h} - \frac{[(u+s)/h]}{1+[(u+s)/h]^2}\right] \tag{4}$$

It follows from standard results [11] that the crack tip stress intensity for the configuration is

$$\mathrm{K} = \left(\frac{2}{\pi}\right)^{1/2}\int_0^\infty \frac{p_{22}(u)\mathrm{d}u}{u^{1/2}} \tag{5}$$

$$= -\left(\frac{2}{\pi}\right)^{1/2}\frac{E_0 e_{22}^{\mathrm{u}}}{2\pi} \times \int_0^\infty \frac{1}{u^{1/2}}\left[2\cot^{-1}\frac{(u+s)}{h} - \frac{[(u+s)/h]}{1+[(u+s)/h]^2}\right]\mathrm{d}u \tag{6}$$

With $\lambda = (u+s)/h$ and $\mu = s/h$, this expression for K can be written as

$$-\frac{2\pi}{E_0 e_{22}^{\mathrm{u}}}\left(\frac{\pi}{2h}\right)^{1/2}K = \int_\mu^\infty \frac{1}{(\lambda-\mu)^{1/2}}\left[2\cot^{-1}\lambda - \frac{\lambda}{(1+\lambda^2)}\right]\mathrm{d}\lambda \tag{7}$$

and since

$$[(\lambda-\mu)^{1/2}\cot^{-1}\lambda]_\mu^\infty = 0 = \int_\mu^\infty \frac{\cot^{-1}\lambda\,\mathrm{d}\lambda}{2(\lambda-\mu)^{1/2}} - \int_\mu^\infty \frac{(\lambda-\mu)^{1/2}}{(1+\lambda^2)}\mathrm{d}\lambda \tag{8}$$

equation 7 for K becomes

$$\frac{-2\pi}{E_0 e_{22}^{\mathrm{u}}}\left(\frac{\pi}{2h}\right)^{1/2}K = \int_\mu^\infty \frac{(3\lambda-4\mu)}{(\lambda-\mu)^{1/2}(1+\lambda^2)}\mathrm{d}\lambda \tag{9}$$

If we now let $(\lambda-\mu)^{1/2} = x$ and $\mu = a^2$, Equation 9 becomes

$$-\frac{\pi}{E_0 e_{22}^{\mathrm{u}}}\left(\frac{\pi}{2h}\right)^{1/2}K = \int_0^\infty \frac{(3x^2-a^2)\mathrm{d}x}{[x^4+2a^2x^2+(a^4+1)]} \tag{10}$$

with $b^4 = (a^4+1)$, the integral in Equation 10 is readily evaluated using standard procedures to give

$$-\frac{\pi}{E_0 e_{22}^{\mathrm{u}}}\left(\frac{\pi}{2h}\right)^{1/2}K = \frac{\pi}{2}\left[\frac{3}{2} - \frac{a^2}{2(a^4+1)^{1/2}}\right]\left[\frac{(a^4+1)^{1/2}+a^2}{2}\right]^{-1/2} \tag{11}$$

or, with $\mu = s/h = a^2$,

$$K = -\left\{\left[\frac{3E_0 e_{22}^{\mathrm{u}} h^{1/2}}{2\pi^{1/2}}\right]\left[1 - \frac{\mu}{3(\mu^2+1)^{1/2}}\right]\right\} \times [(\mu^2+1)^{1/2}+\mu]^{-1/2} \tag{12}$$

As a check, for the limiting case where s is large, i.e. $\mu = s/h$ is large, Equation 12 reduces to the value

$$K = -\frac{E_0 e_{22}^{\mathrm{u}}(2h)}{(8\pi s)^{1/2}} \tag{13}$$

which is the expression appropriate [3] to the situation where the smeared distribution of dislocations at the end of the region is replaced by a superdislocation of Burger's vector $B = 2he_{22}^{\mathrm{u}}$; when the end of the region is sufficiently removed from the crack tip, this replacement is appropriate.

The value of K as given by Equation 12 refers to the configuration in Fig. 2a, whereupon the K value relevant to the configuration in Fig. 2b is (see Equation 12 with $\mu = s/h \to 0$)

$$K = -\frac{3E_0 e_{22}^{\mathrm{u}} h^{1/2}}{2\pi^{1/2}} \tag{14}$$

It therefore follows that the K value appropriate to the configuration in Fig. 1 is given from Equations 13 and 14 by the relation

$$K = \frac{3E_0 e_{22}^{\mathrm{u}} h^{1/2}}{2\pi^{1/2}}\,1 - \left[\frac{\left\{1 - \frac{\mu}{3(\mu^2+1)^{1/2}}\right\}}{[(\mu^2+1)^{1/2}+\mu]^{1/2}}\right] \tag{15}$$

with $\mu = s/h$. For the special case where the hydrided region length is infinite, i.e. $s \to \infty$ or $\mu = s/h \to \infty$, this expression simplifies to

$$K_\infty = \frac{3E_0 e_{22}^{\mathrm{u}} h^{1/2}}{2\pi^{1/2}} \tag{16}$$

3. A hydrided region associated with an unconstrained pure dilatation

Rose [12] has presented an expression which gives the K value appropriate to the situation where there is a pure dilatation $e_{\mathrm{T}}^{\mathrm{u}}$ within the hydrided region, i.e. $e_{\mathrm{T}}^{\mathrm{u}} = e_{11}^{\mathrm{u}} + e_{22}^{\mathrm{u}} + e_{33}^{\mathrm{u}}$, with $e_{11}^{\mathrm{u}} = e_{22}^{\mathrm{u}} = e_{33}^{\mathrm{u}}$. This expression applies to any contour B that defines the front of the region (see Fig. 3) and is

$$K = -\frac{E_0(1+\nu)e_{\mathrm{T}}^{\mathrm{u}}}{3}s^{1/2}A \tag{17}$$

with

$$A \equiv Re\left[\int_B \frac{\mathrm{d}Y}{(2\pi Z)^{1/2}}\right] \tag{18}$$

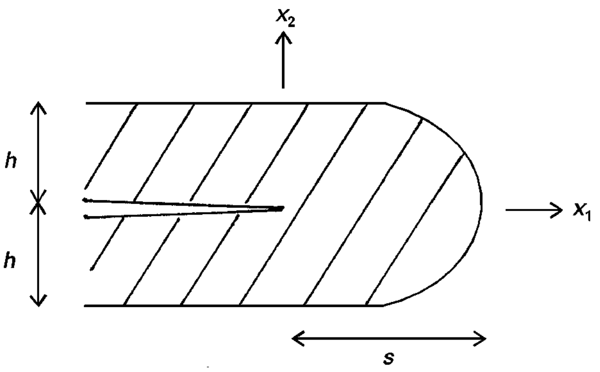

Figure 3 A general hydrided region, with the front edge being defined by the contour *B*.

where distances are normalized with respect to the length s, i.e. $Z = z/s = (x_1 + ix_2)/s$ and $Y = x_2/s$. It thus follows from Equation 18 for a region with a planar front, i.e. that shown in Fig. 2a, with the front being at a distance s from the crack tip, that with $\mu = s/h$

$$A = \frac{2}{(2\pi)^{1/2}} Re\left[\int_0^{1/\mu} \frac{\mathrm{d}Y}{(1+iY)^{1/2}}\right] \tag{19}$$

$$= \frac{2}{\pi^{1/2}}\left[\left(1+\frac{1}{\mu^2}\right)^{1/2} - 1\right]^{1/2} \tag{20}$$

whereupon Equations 17, 18 and 20 give

$$K = -\frac{2E_0(1+\nu)e_{\mathrm{T}}^{\mathrm{u}}h^{1/2}}{3\pi^{1/2}}[(1+\mu^2)^{1/2} - \mu]^{1/2} \tag{21}$$

It then follows, by adopting similar arguments to those used in the preceding section, that the K value appropriate to the hydrided region shown in Fig. 1, but for a situation where the hydriding is associated with an unconstrained pure dilatation, is given by the expression

$$K = \frac{2E_0(1+\nu)e_{\mathrm{T}}^{\mathrm{u}}h^{1/2}}{3\pi^{1/2}}\{1 - [(1+\mu^2)^{1/2} - \mu]^{1/2}\} \tag{22}$$

with $\mu = s/h$. For the special case where the hydrided region length is infinite, i.e. $s \to \infty$ or $\mu = s/h \to \infty$, the expression simplifies to

$$K_\infty = \frac{2E_0(1+\nu)e_{\mathrm{T}}^{\mathrm{u}}h^{1/2}}{3\pi^{1/2}} \tag{23}$$

4. Discussion

Sections 2 and 3 have been concerned with the determination of the stress intensity at the tip of a crack, immediately in front of which is a constant thickness ($2h = t$) hydrided region of length s for the cases where the region is associated with (a) an unconstrained normal expansion strain and (b) an unconstrained pure dilatation. The relevant stress intensities are given by respectively Equations 15 and 22 and they provide a measure of the local tensile stresses within the hydrided region immediately ahead of the crack tip. To effect a comparison of the stress intensities for the two unconstrained precipitation strain scenarios, and thereby assess the likely effect of the transverse strains, it is convenient to compare the stress intensities for the limiting case where the hydrided region length is infinite in extent, when the stress intensities are given by, respectively, Equations 16 and 23. Thus with the pure dilatation scenario for which $e_{11}^{\mathrm{u}} = e_{22}^{\mathrm{u}} = e_{33}^{\mathrm{u}} = e_{\mathrm{T}}/3$, Equation 23 gives, with Poisson's ratio $\nu = 1/3$, $K_\infty = 0.50E_0\varepsilon_{\mathrm{T}}\,h^{1/2}$, while Equation 16 with $e_{22}^{\mathrm{u}} = e_{\mathrm{T}}/3$ gives K_∞, for the normal expansion strain scenario, as $K_\infty = 0.28E_0\varepsilon_{\mathrm{T}}h^{1/2}$. Comparison of the two K_∞ values leads to the conclusion that the transverse expansion strains do affect the local stress within the hydrided region, though not to the same extent as with a hydrided region emanating from a free surface where the three expansion strains have roughly equivalent effects on the local stress [9].

If, instead of the pure dilatation scenario where $e_{11}^{\mathrm{u}} = e_{22}^{\mathrm{u}} = e_{33}^{\mathrm{u}} = e_{\mathrm{T}}/3$ and for which $K_\infty = 0.50\,E_0\varepsilon_{\mathrm{T}}h^{1/2}$, we assume that the overall strain is confined to the normal direction, i.e. $e_{22}^{\mathrm{u}} = e_{\mathrm{T}}$ in Equation 16, then $K_\infty = 0.84E_0e_{\mathrm{T}}h^{1/2}$ and we therefore see that there is a marked overestimation of K_∞, in contrast to the situation where a hydrided region emanates from a free surface when the hydride induced stress values are approximately the same. We therefore conclude that it is important to know and input the correct unconstrained precipitation strain tensor if a reasonably accurate quantitative picture of DHC crack growth is required.

5. Conclusions

1. Theoretical analyses have shown that with regard to a constant thickness hydrided region ahead of a crack tip, the local stress within the hydrided region immediately ahead of the tip is significantly influenced by the unconstrained transverse precipitation strains.
2. Assuming that the unconstrained precipitation strain is entirely in the normal direction overestimates the local stress, and therefore unlike the free surface situation, the assumption does not allow for both Weatherly and Carpenter's precipitation strain scenarios.
3. It is therefore important to know and input the correct unconstrained precipitation strain tensor, so as to provide a reasonably accurate quantitative picture of DHC crack growth.

Acknowledgements

This work was performed for Ontario Hydro Technologies through funding from the CANDU Owners Group. The author thanks numerous colleagues within Ontario Hydro Technologies, Atomic Energy of Canada Limited and Professor R.L. Eadie, University of Alberta, for valuable discussions over the last few years, in the general area of delayed hydride cracking.

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Received 24 June
and accepted 31 July 1996