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A comparison of the smeared-dislocation and super-dislocation description of a hydrided region in the context of modelling delayed hydride cracking initiation

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In quantifying the stress distribution within a hydrided region in the context of modelling delayed hydride cracking (DHC) initiation in zirconium alloys, this paper highlights the desirability to account for image effects, i.e. the interaction between the hydrided region and any free surface, for example a sharp crack, blunt notch or planar surface. The super-dislocation representation of a finite thickness hydrided region is ideal for accounting for image effects, and adequately accounts for the finite thickness, t, of a hydrided region provided, as is the case in practice, we are concerned with the stress value within the hydride at distances $\gtrsim 0.25t$ from an end of the region.

1. Introduction

There is the potential for a delayed hydride cracking (DHC) fracture mechanism to become operative if the equivalent hydrogen concentration in a zirconium alloy is sufficient for the terminal solubility limit (TSS) of hydrogen in zirconium to be exceeded. This mechanism is caused by diffusion of hydrogen (deuterium) atoms, precipitation and growth of hydride platelets, followed by fracture of the platelets. This process can occur at stress concentrations, and three different types of initiation site in pressure tubes may be identified: (a) a sharp crack or notch, (b) a shallow and very smooth notch such as a fret mark (this is a notch where the stress state at its tip cannot be characterized by a stress intensity factor), and (c) a nominally smooth surface (this could contain flaws $\lesssim 0.1$ mm deep which could be service-induced flaws such as fuel bundle scratches and crevice corrosion pits).

In modelling DHC initiation, it is important to recognize that, for a hydrided region to fracture, the stress due to the applied loadings (enhanced in the vicinity of a stress concentration) must be sufficient for it to over-ride the effect of the compressive stress within a hydrided region that is associated with hydride precipitation. In quantifying the compressive stress distribution within a hydrided region and in order to simplify the considerations, it can be assumed that (a) the hydrided region is two-dimensional, i.e. it is in the form of a strip, (b) the hydrided region is completely hydride and (c) the hydrided region has a constant thickness, t. Against this background two approaches may be used to model the hydride so as to quantify the compressive stress distribution within the hydride. Firstly, the considerations may be based on the known general solution [1–4] for the stress within an inclusion having a rectangular parallelopiped shape, a special case being that of a two-dimensional strip with constant thickness. This description implicitly assumes that the situation at each end of the strip is represented by a smeared distribution (constant density) of dislocations. On the other hand, the smeared distribution of dislocations may be collapsed into a super-dislocation whose Burgers vector is equal to the total Burgers vector of the smeared distribution.

This paper compares the smeared distribution representation and the super-dislocation representation, with the objective of assessing their appropriateness, or otherwise, of accounting for the interaction of a two-dimensional hydrided region with a free surface, i.e. a planar surface, blunt notch or sharp crack.

2. The smeared-distribution and super-dislocation descriptions of a two-dimensional hydrided region

Fig. 1 shows the smeared distribution representation of a two-dimensional hydrided region of thickness, t, and length, L. Assuming that (a) the region is completely hydride, (b) hydride precipitation is associated with a compressive strain, ε, perpendicular to the hydrided region, i.e. a compressive strain in the vertical direction, and (c) the hydride has the same elastic constants as the surrounding matrix, then with the smeared distribution approach the stress distribution is obtained by recognizing that there are two smeared edge dislocation distributions (constant density) at each end of the hydrided region, with the Burgers vectors being as indicated. There is a smeared distribution at the left-hand end such that $f(y)\,\delta y$ dislocations each of Burgers vector, $\boldsymbol{b}$, are contained within an element of length δy and an equivalent distribution of opposite sign dislocations at the right-hand end.

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$f(y)$ is constant and

$$b \int_{y=-t/2}^{+t/2} f(y)\,dy = \varepsilon t \qquad (1)$$

whereupon $f(y) = \varepsilon/b$. The total Burgers vector of each distribution is $\boldsymbol{B}$, which is given by

$$\boldsymbol{B} = \boldsymbol{b} \int_{y=-t/2}^{+t/2} f(y)\,dy = \varepsilon t \qquad (2)$$

using Equation 1. With this approach, the stress distribution within the system and particularly the compressive stress distribution within the hydride are calculated by determining the stresses resulting from these smeared distributions of dislocations. It is the smeared-distribution representation that is implicit in the analyses leading to the known general solution [1–4] for the stresses associated with a finite thickness region. With the smeared-distribution description of the hydrided region (Fig. 1), the shear stress is infinite at the tips of the distributions but, as will be shown in the next section, the compressive stress within the hydrided region is finite immediately adjacent to a distribution.

With the super-dislocation description of the hydrided region, each smeared distribution of dislocations is collapsed into a super-dislocation of Burgers vector, $\boldsymbol{B}$, where $\boldsymbol{B}$ is the total Burgers vector associated with each distribution; $\boldsymbol{B}$ is equal to εt (see Equation 2). Fig. 2 shows the super-dislocation representation of a two-dimensional hydrided region of thickness, t, and length, L. In the next section, we compare the compressive stresses within the hydrided region using these alternative representations.

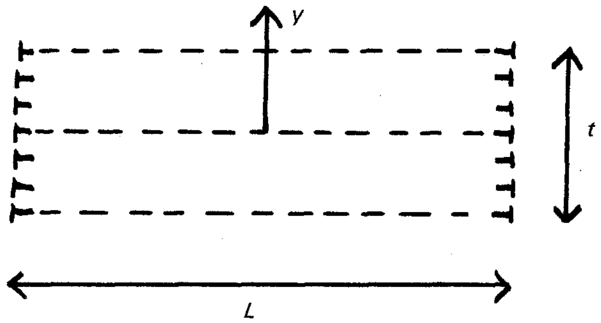

Figure 1 The smeared distribution representation of a two-dimensional hydrided region of thickness, t, and length, L.

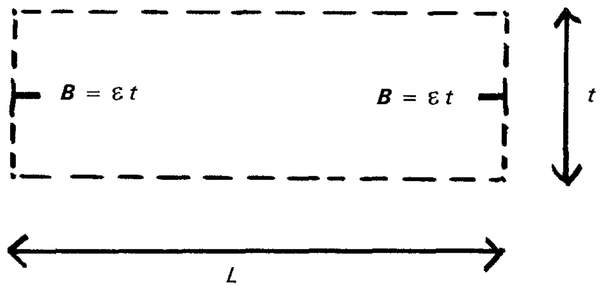

Figure 2 The super-dislocation representation of a two-dimensional hydrided region of a thickness, t, and length, L.

3. Comparison of stresses determined using the two representations

In the light of the comments in Section 1, our concern is with the compressive stress within the hydrided region. For the purposes of this exercise, we need only be concerned with the stresses associated with a single smeared distribution and we will compare these stresses with those obtained by collapsing the distribution into a single superdislocation. Thus (see Fig. 3) we want to know the magnitude of the stress p_{yy} at a distance x from (a) a smeared distribution of edge dislocations, and (b) a super-dislocation.

In the former situation, by using the well-known solution for a single-edge dislocation in an infinite medium [5], the stress, p_{yy}, due to the smeared distribution ($f(y)\,\delta y$ dislocations each of Burgers vector, $\boldsymbol{b}$, are contained within an element of length δy) is given by the expression

$$p_{yy} = -\frac{E_0 x}{4\pi} \int_{-h}^{+h} \frac{(3y^2 + x^2)}{(y^2 + x^2)^2} b f(y)\,dy \qquad (3)$$

where $E_0 = E/(1 - \nu^2)$, E being the Young's modulus and ν being Poisson's ratio. As indicated in the preceding section, $f(y) = \varepsilon/b$, and it thus follows from Equation 3 that

$$p_{yy} = -\frac{E_0 \varepsilon x}{2\pi} \int_0^h \frac{(3y^2 + x^2)\,dy}{(y^2 + x^2)^2} \qquad (4)$$

whereupon substitution of $\lambda = y/x$ gives

$$p_{yy} = -\frac{E_0 \varepsilon}{2\pi} \int_{\lambda=0}^{\lambda=h/x} \frac{(3\lambda^2 + 1)}{(\lambda^2 + 1)^2}\,d\lambda \qquad (5)$$

With $\tan\phi = h/x$ or $\cot\phi = x/h$, evaluation of the integral in Equation 5 gives this relation

$$p_{yy} = -\frac{E_0 \varepsilon}{2\pi}\left(2\phi - \frac{1}{2}\sin 2\phi\right) \qquad (6)$$

This is an analytical expression (valid for all x) that gives the stress within the hydrided region as a function of the distance x from the smeared distribution. The stress is clearly compressive within the hydride, and it is easily seen that the stress, p_{yy}, within the matrix, i.e. to the left-hand side of the distribution in Fig. 3a, is tensile, with p_{yy} being an odd function of x. As $x \to 0$ for positive x, i.e. as we approach the smeared distribution from within the hydride, $\phi \to \pi/2$ and p_{yy} then approaches the finite value $-E_0\varepsilon/2$.

With regard to the super-dislocation representation, the stress p_{yy} is given by the very simple expression.

$$p_{yy} = -\frac{E_0 B}{4\pi x} = -\frac{E_0\,\varepsilon h}{2\pi x}$$

$$= -\frac{E_0 \varepsilon}{2\pi}\tan\phi \qquad (7)$$

because $\boldsymbol{B} = \varepsilon t = 2\varepsilon h$. Equations 6 and 7 allow us to compare the stress values arising from the two approaches at various distances x from the boundary of the two-dimensional hydrided region; the results are shown in Table I. It is immediately seen that the results for the two different representations are in very

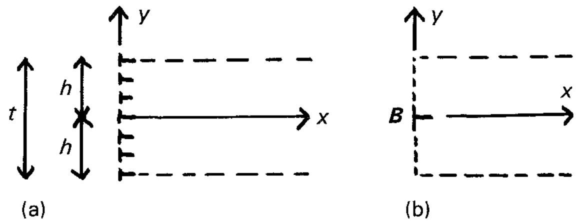

Figure 3 The representations analysed in Section 3.

TABLE I The stress, p_{yy}, at various distances, x, from the boundary of the two-dimensional hydrided region using the two representations (see Fig. 3)

$\frac{x}{t}$	Smeared-distribution $\frac{2\pi\lvert p_{yy}\rvert}{E_0\varepsilon}$	Super-dislocation $\frac{2\pi\lvert p_{yy}\rvert}{E_0\varepsilon}$
0	3.1419	∞
0.25	1.8145	2.0000
0.50	1.0709	1.0000
0.75	0.7146	0.6667
1.00	0.5274	0.5000

close accord for $x/t \gtrsim 0.25$, i.e. they differ by less than 10%, and the results become progressively closer as x increases. We therefore conclude that the super-dislocation description of a hydrided region adequately accounts for the finite thickness of the hydrided region provided that the concern is with the stress value at distances $\gtrsim 0.25t$ from the end of the hydrided region. In practice, this will be the case, for at the limit of $x = 0.25t$ when the compressive stress within the hydride is $\sim E_0\varepsilon/\pi$ using either representation, then with $E_0 = 80 \times 10^3$ MPa and with Weatherly's value [6] of 0.17 for ε, we see that the compressive stress is ~ 4000 MPa; this is much greater than the tensile stress that is likely to be generated as a consequence of the applied loadings, even allowing for constraint effects in the vicinity of a sharp crack tip. Consequently, we will always be interested in the situation where $x > 0.25t$ and then the super-dislocation and smeared distribution approaches give essentially the same results.

It should be pointed out that the conclusion that the super-dislocation description of a hydrided region adequately accounts for the region's finite thickness provided that we are concerned with the stress within the hydride at distances $\gtrsim 0.25$t from an end of the region, has been reached by considering models of the end region in an infinite solid. It is quite clear, however, that the same conclusion carries over to the situation where a hydrided region spreads from a free planar surface or the surface of a blunt flaw, provided the hydrided region length is greater than $0.25t$ and we are interested in the determination of the stress at a distance greater than $0.25t$ from the end of the hydrided region within the solid's interior. It is also valid for the case where there is a hydrided region in the vicinity of a sharp crack tip, with the region extending from the maximum hydrostatic stress position, which is at a finite distance from the crack tip, into the body of the material; in this case the super-dislocation representation will be appropriate provided that the distance between the hydrostatic stress peak and the crack tip is $\gtrsim 0.25t$. (The sharp crack tip situation will receive further consideration in the next section).

4. The necessity to account for the interaction between a hydrided region and free surfaces – image effects

An important attribute of the super-dislocation description of a hydrided region is that one can easily account for image effects, i.e. the interaction between a hydrided region and free surfaces; the author believes that it is very important to give due recognition to these interaction effects.

To highlight the importance of these interaction effects, let us consider the situation (Fig. 4) in the vicinity of the tip of a long crack where there is a two-dimensional hydrided region of thickness, t, which extends from a distance, l, ahead of the crack tip to infinity. Against the background of the preceding section's comments it is good enough to use the super-dislocation representation for the hydrided region when $l \gtrsim 0.25t$. Now if dislocation–crack surface interaction is not taken into account, the stress, p_{yy}, at a distance x within the hydrided (see Fig. 4) is

$$p_{yy}(\text{no int}) = -\frac{E_0\varepsilon t}{4\pi}\frac{1}{x} \tag{8}$$

On the other hand, when interaction between the super-dislocation and the crack surface is taken into account, the stress is

$$p_{yy}(\text{int}) = -\frac{E_0\varepsilon t}{4\pi} \times\left\{\frac{1}{x} - \frac{1}{(x+l)^{1/2}[l^{1/2} + (x+l)^{1/2}]}\right\} \tag{9}$$

whereupon it follows from Equations 8 and 9 that

$$\frac{p_{yy}(\text{no int})}{p_{yy}(\text{int})} = \left(1 + \frac{x}{l}\right)^{1/2} \tag{10}$$

Inspection of Equation 10 shows that neglect of the dislocation–crack surface interaction, i.e. neglect of

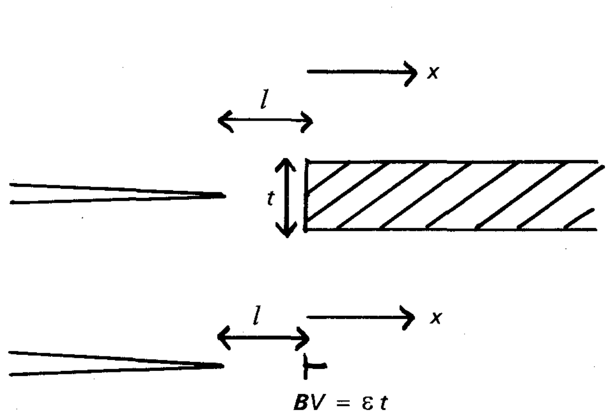

Figure 4 The model of a hydrided region ahead of the tip of a sharp crack.

image effects, can seriously overestimate the compressive stress within the hydrided region. For example, when $x/l = 1$, this stress is overestimated by $\sim 40\%$, and of course to an even greater extent with larger x/l.

To set this conclusion in context, with l being the distance to the hydrostatic stress peak ahead of a plastic-elastic crack, we have $l \sim 2K^2/E_0\sigma_0$ [7], and if $(x + l)$ is the distance to the boundary of the plastic zone as measured along the crack plane, then $(x + l) \simeq 0.032K^2/\sigma_0^2$ [7] (K is the applied crack tip stress intensity and σ_0 is the tensile yield stress of the material). For a crude consideration of DHC initiation in the vicinity of a sharp crack, it may be assumed that the tensile stress normal to the hydride arising from the applied loadings has a constant value, $2.5\sigma_0$, between the hydrostatic stress peak and the plastic zone boundary. That being the case, the region where hydride fracture is most likely to occur, i.e. where the overall stress (applied plus hydride) is a maximum, is at the plastic zone boundary, i.e. where $(x + l)/l \simeq 0.016\, E_0/\sigma_0$; thus with $E_0 \simeq 80 \times 10^3$ MPa and with σ_0 at 250 °C in the range 500–800 MPa on going from unirradiated material to irradiated material, it follows that $x/l \simeq 1$, which is the value used in the preceding paragraph's comparison calculations. Furthermore, with $l \sim 2K^2/E_0\sigma_0$ and with $E_0 = 80 \times 10^3$ MPa, $\sigma_0 = 800$ MPa, it follows that $l \simeq 0.6\ \mu m$ with K as low as $5\ MPa\, m^{1/2}$ (a lower bound experimentally measured threshold K value for DHC crack growth); thus $l/t \simeq 0.3$ for a hydrided region of thickness $t = 2\ \mu m$, whereupon the condition $l/t \gtrsim 0.25$ is satisfied, and consequently, use of the super-dislocation description is justified.

To emphasize further the importance of accounting for interaction with the crack, let us proceed to the extreme situation where there is a two-dimensional hydrided region of thickness, t, immediately adjacent to the crack tip (see Fig. 5), with the hydrided region being infinitely long. With this situation, against the background of the conclusions from the preceding section's arguments, we cannot use the super-dislocation approach to calculate the p_{yy} stress within the hydrided region. Although the super-dislocation approach can be used to calculate p_{yy} at a distance $x \gtrsim 0.25t$ with regard to the contribution stemming from the infinite body situation, problems arise with regard to the image contribution. Regarding the situation as shown in Fig. 5, and using the smeared distribution description, the stress, p_{yy}, for all positive x stemming from the infinite body situation is, of course, given by Equation 6, which is valid for all positive x. With $\cot\phi = x/h$, this relation can be written in the form

$$p_{yy} = -\frac{E_0\varepsilon}{2\pi}\left\{2\cot^{-1}\left(\frac{x}{h}\right) - \frac{(x/h)}{[1 + (x^2/h^2)]}\right\} \tag{11}$$

Again for the infinite body situation, the stress, p_{yy}, on the left-hand side of the smeared distribution is tensile and is equal in magnitude (but not in sign) to the compressive stress on the right-hand side. Thus with reference to Fig. 5, for the case where there is no crack,

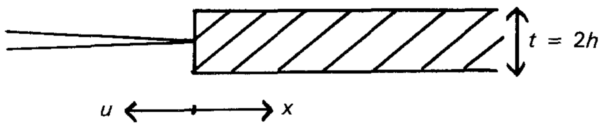

Figure 5 The model of a hydrided region of thickness $t = 2h$ immediately adjacent to the tip of a sharp crack.

the stress on the left-hand side is given by the expression

$$p_{yy} = +\frac{E_0\varepsilon}{2\pi}\left\{2\cot^{-1}\left(\frac{u}{h}\right) - \frac{(u/h)}{[1 + (u^2/h^2)]}\right\} \tag{12}$$

The "image" stress (tensile) within the hydride due to the smeared distribution is then readily obtained by using the solution [8] for point forces applied to the crack surface, with these forces being given by the stress due to the smeared distribution along the crack plane in the absence of the crack. The image contribution is therefore given by the expression

$$p_{yy} = \frac{1}{\pi x^{1/2}}\int_0^\infty \frac{p_{yy}(u)\,u^{1/2}\,du}{(u + x)} \tag{13}$$

with $p_{yy}(u)$ being given by Equation 12, and therefore

$$p_{yy} = \frac{E_0\varepsilon}{2\pi^2}\frac{1}{x^{1/2}}\int_0^\infty \frac{u^{1/2}}{(u + x)} \times \left\{2\cot^{-1}\left(\frac{u}{h}\right) - \frac{(u/h)}{[1 + (u^2/h^2)]}\right\} du \tag{14}$$

Consequently, the total stress within the hydride is given by the sum of the contributions from the infinite body solution (Equation 11) and the image solution (Equation 14), i.e. within the hydride

$$p_{yy} = -\frac{E_0\varepsilon}{2\pi}\left\{2\cot^{-1}\left(\frac{x}{h}\right) - \frac{(x/h)}{[1 + (x^2/h^2)]}\right\} + \frac{E_0\varepsilon}{2\pi^2}\frac{1}{x^{1/2}}\int_0^\infty \frac{u^{1/2}}{(u + x)}\left\{2\cot^{-1}\left(\frac{u}{h}\right) - \frac{(u/h)}{[1 + (u^2/h^2)]}\right\} du \tag{15}$$

It is immediately seen, without proceeding further, that for small x, i.e. within the hydrided region close to the crack tip, the stress is tensile, indeed it increases to plus infinity as $x \to 0$. However, if image effects are not taken into account, then the stress is compressive (see Equation 12) and tends to a finite value as $x \to 0$.

The considerations in this section so far have been with regard to the importance of image effects, i.e. interaction of a hydrided region with a free surface, for the case where there is a hydrided region in the vicinity of a sharp crack tip. Image effects are also important with regard to the situation where there is a hydrided region in the vicinity of a blunt notch and for the extreme limiting case of a hydrided region in the vicinity of a free planar surface. This importance is readily seen with regard to the latter situation. For the case where there is a hydrided region of length, L, and

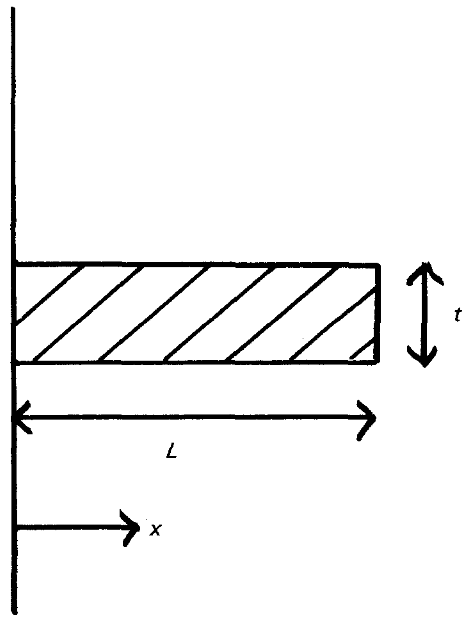

Figure 6 The model of a two-dimensional hydrided region of length, L, and thickness, t, emanating from a free planar surface.

thickness, t, emanating from a free planar surface (Fig. 6), irrespective of whether the smeared-distribution or super-dislocation approach is used, it is quite clear that a physically unrealistic solution for the stress within the hydrided region is obtained if the stress is determined on the basis of there being a smeared distribution or super-dislocation at $x = 0$ and another smeared distribution or super-dislocation at $x = L$, and proceeding on the basis that the smeared distributions or super-dislocations are in an infinite solid. In this case, the stress distribution is obtained by assuming that there is a hydrided region of length $2L$ within an infinite solid, and cutting the solid into two halves; in other words the image stress for the situation in Fig. 6 is provided by an image smeared distribution or super-dislocation at $x = -L$. For sake of consistency, if image effects are taken into account with the planar surface case, they should also be taken into account when considering a sharp crack.

5. Discussion

The present paper, in the context of the problem of DHC initiation, has focused on the modelling of a two-dimensional hydrided region of constant thickness, with regard to the determination of the compressive stress within the hydrided region that is associated with hydride precipitation. The first important conclusion from the report's considerations (see Section 4) is that it is very important to account for image effects, i.e. the interaction between the hydrided region and any surface, whether this be a free planar surface, blunt notch or sharp crack; otherwise one can reach misleading conclusions, regarding the stress distribution within the hydride.

The second important conclusion is that the super-dislocation description of a hydrided region adequately accounts for the finite thickness, t, of the region, provided that we are concerned, as is the case in practice, with the stress within the hydride at distances $\gtrsim 0.25t$ from an end of the region. As demonstrated in Section 3, the super-dislocation description then gives results that accord with those obtained using the smeared-dislocation distribution description of a hydrided region. However, a great virtue of the super-dislocation description is that it is easy to account for image effects, as has been illustrated by the example in the preceding section, i.e. the interaction of a hydrided region with a sharp crack.

Two other added attractions of the super-dislocation procedure are also worth mentioning. Firstly, the considerations in this paper have been concerned with a hydrided region of constant thickness. There is no reason why the characteristics of a variable thickness region cannot be considered; this would merely involve the use of a distribution of super-dislocations along a plane, and again image effects can be taken into account. Secondly, the considerations have been based on the presumption that the hydrided region differs from the surrounding region by a normal compressive strain, but that the elastic properties of the hydrided region and matrix are the same. However, there is no reason why the super-dislocation approach cannot be used to account for different properties of the hydrided region; it is only necessary to introduce non-linearity across the plane joining the super-dislocations via an appropriate stress–displacement law. This is tantamount to introducing a continuous distribution of dislocations along the plane between the super-dislocations at the extremities of the hydrided region.

6. Conclusions

1. In quantifying the stress distribution in a hydrided region, it is very important to account for image effects, i.e. the interaction between the hydrided region and any free surface, for example a sharp crack, blunt notch or planar surface.
2. The super-dislocation representation of a hydrided region is ideal for accounting for image effects.
3. The super-dislocation description adequately accounts for the finite thickness, t, of a hydrided region provided, as is the case in practice, we are concerned with the stress within the hydrided region at distances $\gtrsim 0.25t$ from an end of the region.

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