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

Part I *Hydrided region in an infinite solid or at a free surface*

E. SMITH
Manchester University – UMIST Materials Science Centre, Grosvenor Street, Manchester, M1 7HS, UK

In the context of modelling delayed hydride cracking (DHC), this paper shows that with a lenticular shaped hydrided region, i.e. one whose length is large compared with its thickness, the compressive stress σ_H induced within the region by hydriding is markedly influenced by the unconstrained transverse precipitation strains as well as the unconstrained normal strain. For the case of DHC initiation at a planar surface or the surface of a very blunt flaw, the values of σ_H obtained by assuming (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, are approximately equal. This means that assuming the strain is entirely in the normal direction allows for both precipitation strain scenarios.

1. Introduction

Delayed hydride cracking (DHC) can occur in a zirconium alloy if the hydrogen concentration is sufficient for the terminal solid solubility limit (TSS) of hydrogen in zirconium to be exceeded. It is caused by the diffusion of hydrogen atoms to a stress concentration, preferential precipitation and growth of hydride platelets in favourably oriented grains, followed by fracture of a hydrided region which consists of a distribution of hydride platelets within a zirconium alloy matrix. A hydrided region is usually lenticular in shape (its length is large compared with its thickness), and the tensile stress due to the applied loadings, enhanced in the vicinity of a stress concentration, must over-ride the induced compressive stress within a hydrided region to a sufficient extent for the region to fracture and so lead to DHC initiation. The induced compressive stress arises from the unconstrained expansion strains associated with the precipitation of a hydride platelet. In the context of modelling DHC, it is therefore important to quantify the compressive stress (normal to the hydrided region) distribution 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.

In determining the magnitude of the compressive 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 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 co-workers [7, 8] in their DHC modelling work; they assume a normal strain of 5.4%, but neglect the effect of the in-plane expansion strains in their calculations. The objective of the present paper is to explore, with regard to a lenticular shaped two-dimensional hydrided region, the effect of the various unconstrained expansion strain components on the magnitude of the compressive stress within a hydrided region.

2. A general two-dimensional hydrided region

Fig. 1 shows a general two-dimensional symmetric hydrided region with length $2L$ and maximum thickness $t = 2h$. The compressive stress σ_H at the centre of the region, i.e. the position x, due to the four edge dislocations of Burger's vector b_* situated in the symmetric positions as indicated, is

$$\sigma_H = \frac{E_0 b_*}{\pi} \times \frac{x_1(3x_2^2 + x_1^2)}{(x_2^2 + x_1^2)^2} \quad (1)$$

where $E_0 = E/(1 - \nu^2)$, E being the Young's modulus and ν being the Poisson's ratio. (It is assumed that both the hydrided region and the surrounding material have the same elastic constants). Thus if e_{22}^u is the unconstrained expansion strain (in the direction

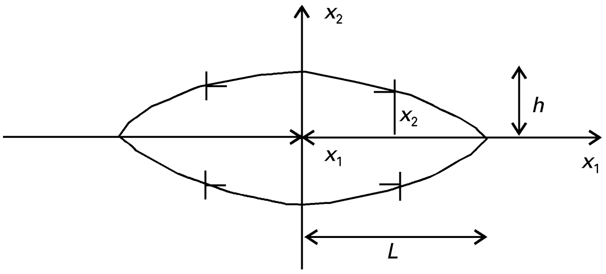

Figure 1 A general two-dimensional symmetric hydrided region of maximum thickness $t = 2h$ and length $2L$.

normal to the region) associated with hydride precipitation, the compressive stress σ_H at x arising from this e^u_{22} strain is that due to a continuous distribution of edge dislocations (with Burger's vectors as shown in Fig. 1) around the boundary of the region, such that $-e^u_{22}\delta x_2/b_*$ dislocations each of Burger's vector b_* are contained within an element of vertical length δx_2. Thus σ_H is given by the expression

$$\sigma_H = -\frac{E_0 e^u_{22}}{\pi}\int_{x_1=0}^{L}\frac{x_1(3x_2^2 + x_1^2)}{(x_2^2 + x_1^2)^2}\,dx_2 \tag{2}$$

Similarly the compressive stress σ_H at the centre of the region x due to four edge dislocations of Burger's vector b_* situated in the same symmetric positions as indicated in Fig. 1, but with their extra half planes in the vertical direction and pointing inwards into the region, is

$$\sigma_H = \frac{E_0 b_*}{\pi}\times\frac{x_2(x_2^2 - x_1^2)}{(x_2^2 + x_1^2)^2} \tag{3}$$

Thus if e^u_{11} is the unconstrained expansion strain, in the direction of the plane of the region, associated with hydride precipitation, the compressive stress σ_H at x is that due to a continuous distribution of edge dislocations, with Burgers vector's, as mentioned earlier in this paragraph, around the boundary of the region, such that $e^u_{11}\delta x_1/b_*$ dislocations, each of Burger's vector b_*, are contained within an element of horizontal length δx_1. Thus, σ_H is given by the expression

$$\sigma_H = \frac{E_0 e^u_{11}}{\pi}\int_{x_1=0}^{L}\frac{x_2(x_2^2 - x_1^2)}{(x_2^2 + x_1^2)^2}\,dx_1 \tag{4}$$

It therefore follows that, if hydride precipitation is associated with an unconstrained expansion strain e^u_{22} in the direction normal to the plane of the region together with an unconstrained expansion strain e^u_{11} in the direction of the plane of the region, the compressive stress σ_H at x due to the hydrided region is given by the sum of the separate contributions of Equations 2 and 4, i.e.

$$\sigma_H = -\frac{E_0 e^u_{22}}{\pi}\int_{x_1=0}^{L}\frac{x_1(3x_2^2 + x_1^2)}{(x_2^2 + x_1^2)^2}\,dx_2 + \frac{E_0 e^u_{11}}{\pi}\int_{x_1=0}^{L}\frac{x_2(x_2^2 - x_1^2)}{(x_2^2 + x_1^2)^2}\,dx_1 \tag{5}$$

This is an expression which, in principle, gives σ_H for any shape of symmetric hydrided region, i.e. for any given relation between x_2 and x_1.

3. The special case of a constant thickness hydrided region

For the special case of a hydrided region with constant thickness $t = 2h$ and length $2L$, Equation 5 simplifies to

$$\sigma_H = \frac{E_0 e^u_{22}}{\pi}\int_{x_2=0}^{h}\frac{L(3x_2^2 + L^2)}{(x_2^2 + L^2)^2}\,dx_2 + \frac{E_0 e^u_{11}}{\pi}\int_{x_1=0}^{L}\frac{h(h^2 - x_1^2)}{(h^2 + x_1^2)^2}\,dx_1 \tag{6}$$

which simplifies with $\beta = h/L = t/2L$, to

$$\sigma_H = \frac{E_0 e^u_{22}\beta}{\pi}\int_{w=0}^{1}\frac{(3\beta^2 w^2 + 1)}{(\beta^2 w^2 + 1)^2}\,dw + \frac{E_0 e^u_{11}}{\pi}\int_{w=0}^{1/\beta}\frac{(1 - w^2)}{(1 + w^2)^2}\,dw \tag{7}$$

We are interested in the characteristics of a lenticular region for which $h/L = \beta$ is small, when evaluation of the integrals in Equation 7 to terms of order β easily gives

$$\sigma_H = \frac{E_0\beta}{\pi}(e^u_{22} + e^u_{11}) = \frac{E_0 t}{2\pi L}(e^u_{22} + e^u_{11}) \tag{8}$$

4. The special case of an elliptically cylindrical hydrided region

For an elliptically cylindrical hydrided region whose boundary is given by the equation

$$\frac{x_1^2}{L^2} + \frac{x_2^2}{h^2} = 1 \tag{9}$$

then again, with $h/L = \beta$, and after substituting $x_1 = L\sin\theta$ and $x_2 = L\cos\theta$, Equation 5 simplifies to

$$\sigma_H = \frac{E_0 e^u_{22}\beta}{\pi}\int_0^{\pi/2}\frac{\cos^2\theta(3\beta^2\sin^2\theta + \cos^2\theta)\,d\theta}{(\beta^2\sin^2\theta + \cos^2\theta)^2} + \frac{E_0 e^u_{11}\beta}{\pi}\int_0^{\pi/2}\frac{\cos^2\theta(\beta^2\cos^2\theta - \sin^2\theta)\,d\theta}{(\beta^2\cos^2\theta + \sin^2\theta)^2} \tag{10}$$

Let the integral I be given by the expression

$$I = \int_0^{\pi/2}\frac{\cos^2\theta(3\beta^2\sin^2\theta + \cos^2\theta)\,d\theta}{(\beta^2\sin^2\theta + \cos^2\theta)^2} \tag{11}$$

which simplifies to

$$I = \int_0^{\pi/2}\frac{(1 + \cos 2\theta)[(1 + 3\beta^2) + (1 - 3\beta^2)\cos 2\theta]\,d\theta}{[(1 + \beta^2) + (1 - \beta^2)\cos 2\theta]^2} \tag{12}$$

whereupon the substitution $\phi = 2\theta$ gives

$$\frac{2(1 + \beta^2)^2 I}{(1 + 3\beta^2)} = \int_0^{\pi}\frac{(1 + \cos\phi)(1 + A\cos\phi)\,d\phi}{(1 + B\cos\phi)^2} \tag{13}$$

with $A = (1 - 3\beta^2)/(1 + 3\beta^2)$ and $B = (1 - \beta^2)/(1 + \beta^2)$. Thus

$$\frac{2(1+\beta^2)^2 I}{(1+3\beta^2)} = \int_0^\pi \left\{ a + \frac{b}{(1 + B\cos\phi)} + \frac{c}{(1 + B\cos\phi)^2} \right\} d\phi \quad (14)$$

with

$$\left.\begin{aligned} a &= \frac{A}{B^2} \\ b &= \frac{(A+1)}{B} - \frac{2A}{B^2} \\ c &= 1 + \frac{A}{B^2} - \frac{(A+1)}{B} \end{aligned}\right\} \quad (15)$$

Evaluation of the integrals in Equation 14 gives

$$\frac{2(1+\beta^2)^2 I}{(1+3\beta^2)} = \pi a + \frac{\pi b}{(1-B^2)^{1/2}} + \frac{\pi c}{(1-B^2)^{3/2}} \quad (16)$$

whereupon Equations 15 and 16 give the integral I as

$$I = \frac{\pi}{2} \times \frac{(1+2\beta)}{(1+\beta)^2} \quad (17)$$

Now let the integral J be given by the expression

$$J = \int_0^{\pi/2} \frac{\cos^2\theta(\beta^2\cos^2\theta - \sin^2\theta)\, d\theta}{(\beta^2\cos^2\theta + \sin^2\theta)^2} \quad (18)$$

which simplifies to

$$J = \int_0^{\pi/2} \frac{(1+\cos 2\theta)[(1+\beta^2)\cos 2\theta - (1-\beta^2)]\, d\theta}{[(1+\beta^2) - (1-\beta^2)\cos 2\theta]^2} \quad (19)$$

whereupon the substitution $\phi = 2\theta$ gives

$$\frac{2(1+\beta^2)^2 J}{(1-\beta^2)} = \int_0^\pi \frac{(1+\cos\phi)(C\cos\phi - 1)}{(1 - D\cos\phi)^2} d\phi \quad (20)$$

with $C = (1 + \beta^2)/(1 - \beta^2)$ and $D = (1 - \beta^2)/(1 + \beta^2)$. Thus

$$\frac{2(1+\beta^2)^2 J}{(1-\beta^2)} = \int_0^\pi \left\{ d + \frac{e}{(1 - D\cos\phi)} + \frac{f}{(1 - D\cos\phi)^2} \right\} d\phi \quad (21)$$

with

$$\left.\begin{aligned} d &= \frac{C}{D^2} \\ e &= -\frac{(C-1)}{D} - \frac{2C}{d^2} \\ f &= -1 + \frac{C}{D^2} + \frac{(C-1)}{D} \end{aligned}\right\} \quad (22)$$

Evaluation of the integrals in Equation 21 gives

$$\frac{2(1+\beta^2)^2 J}{(1-\beta^2)} = d + \frac{e}{(1-D^2)^{1/2}} + \frac{f}{(1-D^2)^{3/2}} \quad (23)$$

whereupon Equations 22 and 23 give the integral J as

$$J = \frac{\pi}{2} \times \frac{1}{(1+\beta)^2} \quad (24)$$

It follows from Equations 10, 11, 17, 18 and 24 that

$$\sigma_H = \frac{E_0 \beta}{2(1+\beta)^2} [(1+2\beta) e^u_{22} + e^u_{11}] \quad (25)$$

simplifying when $\beta = h/L = t/2L$ is small, i.e. for a lenticular shaped hydrided region, to

$$\sigma_H = \frac{E_0 \beta}{2}(e^u_{22} + e^u_{11}) = \frac{E_0 t}{4L}(e^u_{22} + e^u_{11}) \quad (26)$$

5. Application of Eshelby's ellipsoidal inclusion solutions

Eshelby [9] has presented a general analysis which gives, as a special case, the (uniform) stresses and strains within a two-dimensional elliptically cylindrical region which, when unconstrained, is subjected to prescribed transformation strains. We are interested in the p_{22} stress for the case where the elliptically cylindrical hydrided region's boundary is given by Equation 9, with the cylinder axis being the x_3 axis, when the unconstrained transformation strains are e^u_{11}, e^u_{22} and e^u_{33}, the unconstrained transformation shear strains being zero. In this case, the non-zero strains are e^c_{11} and e^c_{22} and the p_{22} stress is then given by the relation

$$p_{22} = \lambda(e^c_{11} - e^u_{11}) + (\lambda + 2\mu)(e^c_{22} - e^u_{22}) \quad (27)$$

where λ and μ are the Lamé constants, it being assumed that the hydrided region and the surrounding matrix have the same elastic constants. The non-zero strains e^c_{11} and e^c_{22} are related to the unconstrained transformation strains e^u_{11}, e^u_{22} and e^u_{33} by the relations [9]

$$e^c_{11} = S_{1111} e^u_{11} + S_{1122} e^u_{22} + S_{1133} e^u_{33} \quad (28)$$

$$e^c_{22} = S_{2211} e^u_{11} + S_{2222} e^u_{22} + S_{2233} e^u_{33} \quad (29)$$

with

$$\left.\begin{aligned} S_{1111} &= QL^2 I_{11} + RI_1 \\ S_{1122} &= Qh^2 I_{12} - RI_1 \\ S_{1133} &= \left(\frac{Q}{3} - R\right) I_1 \\ S_{2211} &= QL^2 I_{21} - RI_2 \\ S_{2222} &= Qh^2 I_{22} + RI_2 \\ S_{2233} &= \left(\frac{Q}{3} - R\right) I_2 \end{aligned}\right\} \quad (30)$$

where

$$\left.\begin{aligned} I_1 &= \frac{4\pi h}{(h+L)}, \quad I_2 = \frac{4\pi L}{(h+L)} \\ I_{12} &= I_{21} = \frac{4\pi}{3(h+L)^2}, \quad I_{11} = \frac{4\pi}{3L^2} - I_{12}, \\ I_{22} &= \frac{4\pi}{3h^2} - I_{12} \end{aligned}\right\} \tag{31}$$

and

$$Q = \frac{3}{8\pi(1-\nu)}, \quad R = \frac{(1-2\nu)}{8\pi(1-\nu)} \tag{32}$$

It follows from Equations 27–32, together with use of the standard relations between the various elastic constants, that the compressive stress $\sigma_H = -p_{22}$ within the hydrided region, for the limiting case where h/L is small, is given by the expression

$$\sigma_H = \frac{E_0 h}{2L}(e^u_{11} + e^u_{22} + 2\nu e^u_{33}) = \frac{E_0 t}{4L}(e^u_{11} + e^u_{22} + 2\nu e^u_{33}) \tag{33}$$

This expression is consistent with Equation 26 for the special case where the strain e^u_{33} is zero.

6. Discussion

The analyses in this paper have shown, both for a constant thickness hydrided region (Section 3) and an elliptically cylindrical region (Sections 4 and 5), that when the region is lenticular shaped as is the case in practice, i.e. when the region length is large compared with its thickness, then the compressive stress σ_H within the hydrided region is influenced by the unconstrained transverse strains as well as the unconstrained normal strain. This conclusion follows automatically from Equation 8, for the case of a constant thickness hydrided region, and from Equations 26 and 33 for the case of an elliptically cylindrical region. The compressive stress σ_H refers to the region centre, but the stress is the same at the positions indicated (see Fig. 2) for hydrided regions at a free surface, since the models of isolated regions can be cut at their mid-points without affecting the results. Thus Equation 8 gives the compressive stress σ_H at the position x for a hydrided region of constant thickness $t = 2h$ and length L (Fig. 2a), while Equations 26 and 33 give σ_H at position x for an elliptically cylindrical region of maximum thickness $t = 2h$ and length L (Fig. 2b). These relations should also be approximately applicable for hydrided regions emanating from a very blunt flaw provided that the ratio of hydrided region length to flaw root radius is not too large.

Another important feature of this paper's results is that with regard to the modelling of DHC initiation at a planar surface or at the surface of a very blunt notch, the values of σ_H are approximately the same (see for example Equation 33) irrespective of whether (a) the overall unconstrained expansion strain ($\sim$17%) is confined entirely to the normal direction [1], or (b) the overall unconstrained expression strain is partitioned

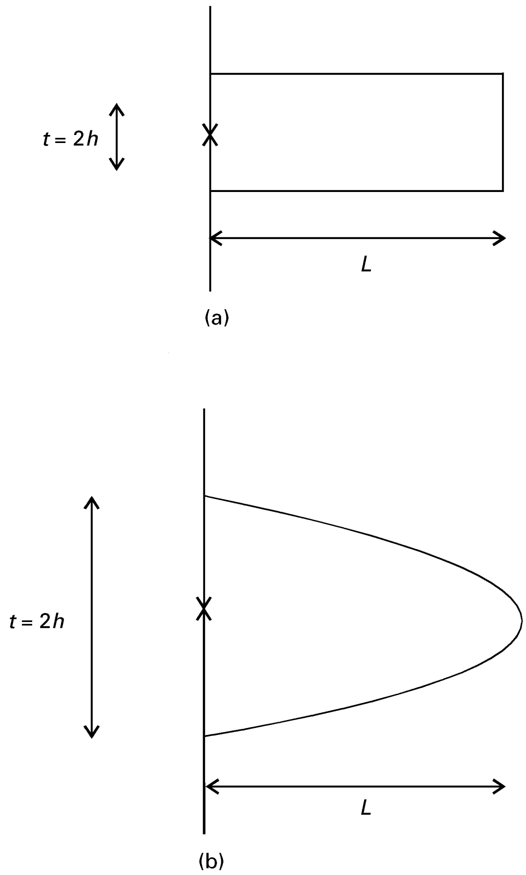

Figure 2 Hydrided regions at a planar surface: (a) constant thickness region, (b) elliptically cylindrical region.

approximately equally between the three orthogonal directions [6]. This means that the procedure adopted by the author [2–5], somewhat fortuitously with hindsight, i.e. assuming a 17% strain in the normal direction with the transverse strains being zero, allows for both possible precipitation strain scenarios.

Before closing this discussion, it is worth recording that when the total hydride unconstrained expansion strain is confined to the direction normal to a hydrided region, i.e. $e^u_{11} = e^u_{33} = 0$ and $e^u_{22} \neq 0$, Equation 7 gives, with $\beta = h/L = t/2L$

$$\sigma_H = \frac{E_0 e^u_{22}\beta}{\pi}\int_{w=0}^{1}\frac{(3\beta^2 w^2 + 1)}{(\beta^2 w^2 + 1)^2}\,dw \tag{34}$$

for a hydrided region with constant thickness t and length $2L$, simplifying to [4]

$$\sigma_H = \frac{E_0 e^u_{22}}{\pi}\left\{2\tan^{-1}\left(\frac{t}{2L}\right) - \frac{\left(\frac{t}{2L}\right)}{\left[1 + \left(\frac{t}{2L}\right)^2\right]}\right\} \tag{35}$$

while Equation 10, again with $\beta = h/L = t/2L$, gives

$$\sigma_H = \frac{E_0 e^u_{22} t}{4L} \times \frac{\left(1 + \frac{t}{L}\right)}{\left(1 + \frac{t}{2L}\right)^2} \tag{36}$$

for an elliptically cylindrical region with thickness t and length $2L$. Equations 35 and 36 apply to all values of the ratio t/L. Now in his modelling work [2–5], the author has simplified the description of a hydrided region associated with an unconstrained expansion strain e^{u}_{22}, by replacing the dislocations that are distributed along the boundary of the hydrided region by super-dislocations that lie along the central plane $x_2 = 0$ of the region. Thus, with regard to a hydrided region of constant thickness $t = 2h$ and length $2L$ in an infinite solid, there are two super-dislocations each of total Burger's vector $e^{u}_{22}t$ situated at the ends of the region and the compressive stress σ_H at the region centre is then given by the very simple expression

$$\sigma_H = \frac{E_0 e^{u}_{22}}{2\pi L} \qquad (37)$$

Comparison of Equations 35 and 37 shows that the super-dislocation description gives σ_H to an accuracy of better than 1% when $L/t > 5$, i.e. for a 2 μm thick hydrided region when $L > 10$ μm. With a general symmetrical hydrided region, if instead of the four edge dislocations in Fig. 1, we have two edge dislocations of Burger's vector $2b_*$ situated at a distance x_1 from the centre of the region, either side of the centre, and along the major axis $x_2 = 0$, the compressive stress σ_H at x due to this super-dislocation description is

$$\sigma_H = -\frac{E_0 e^{u}_{22}}{\pi} \int_{x_1=0}^{L} \frac{dx_2}{x_1} \qquad (38)$$

a relation which arises from the first term on the right-hand side of Equation 5 by allowing $x_2 \to 0$ in the integral. This expression is clearly simpler than the first term on the right-hand side of Equation 5, and gives σ_H for any arbitrarily (albeit symmetric) shaped hydrided region, i.e. for any given relation between x_2 and x_1. Thus with the elliptically cylindrical region described by Equation 9, use of the super-dislocation description gives the stress σ_H at the centre of the region as (see Equations 9 and 38)

$$\sigma_H = \frac{E_0 e^{u}_{22} t}{4L} \qquad (39)$$

whereupon comparison of Equations 36 and 39 shows that the super-dislocation description again gives the stress σ_H to an accuracy of better than 1% when $L/t > 5$. In view of this agreement between the σ_H values obtained using the super-dislocation approach and the exact values for, respectively, a constant thickness hydrided region and an elliptically cylindrical region, the super-dislocation procedure can be used with confidence to give the stress σ_H induced by the unconstrained expansion strain e^{u}_{22}, and thereby used to assess the effect of the shape of a lenticular hydrided region on the criterion for the initiation of delayed hydride cracking. Coupled with the conclusion reached earlier in this paper, the implication is that the super-dislocation approach can be used to provide a reasonable estimate for σ_H with a generally shaped lenticular region that emanates from a planar surface or very blunt flaw, if it transpires that hydride precipitation is associated with essentially a pure dilatation, rather than a normal strain, by regarding the dilatation as a normal strain. The great advantage of the super-dislocation approach is that it is simple and therefore allows for a relatively simple assessment of DHC initiation when a hydrided region has a general shape.

7. Conclusions

1. Theoretical analyses have shown that with a lenticular shaped hydrided region, the compressive stress σ_H induced within the region, as a consequence of the unconstrained precipitation strains, is markedly influenced by the unconstrained transverse strains as well as the unconstrained normal strain.

2. With regard to DHC initiation at a planar surface or the surface of a very blunt flaw, the values of σ_H are approximately the same irrespective of whether (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. This means that assuming the overall strain is confined to the normal direction allows for both precipitation strain scenarios.

3. This second conclusion highlights the usefulness of the super-dislocation description of a lenticular hydrided region for determining σ_H for a generally shaped region.

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