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# THE SHAPE OF INTERGRANULAR CREEP CRACKS GROWING BY SURFACE DIFFUSION*

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A crack-like creep rupture cavity is considered to extend along the interface between two grains by diffusive transport of material into the boundary ahead of its tip. The shape of the cavity surfaces is determined here on the assumptions that this is governed by surface diffusion, and that steady state conditions prevail, so that the cavity advances as a profile retaining a constant shape near its tip. A second order non-linear differential equation for the profile is derived and a simple approximate solution is given, which is shown to be highly accurate by comparison to a numerical solution. This allows the crack velocity, the radius of curvature adjacent to the tip, and the rate of matter flux into the boundary ahead of the tip to be related to one another and to material constants. The information is useful as boundary conditions to a coupled analysis of diffusion and stress concentration ahead of the cavity, so as to determine the rate of cavity propagation in terms of applied stress.

FORME DES FISSURES INTERGRANULAIRES DE FLUAGE PRODUITES PAR DIFFUSION SUPERFICIELLE

Les auteurs considèrent qu'une cavité de rupture par fluage en forme de fissure se développe suivant l'interface de deux grains par transport de matière par diffusion vers le joint à partir de l'extrémite de la fissure. La forme des surfaces de la cavité est déterminée en supposant qu'elle est régie par la diffusion superficielle et que des conditions d'état stationnaire sont prédominantes, de sorte que la cavité avance en gardant une forme constante au voisinage de son extrémité. Une équation différentielle non linéaire du second ordre est utilisée pour le profil, ce qui permet d'obtenir une solution simple approchée, trés précise d'aprés sa comparaison avec une solution numérique. On peut ainsi relier entre eux la vitesse de la fissure, le rayon de courbure à son extremité, la vitesse du flux de matière vers le joint en avant de la fissure, et les relier également aux constantes du matériau. Les conditions aux limites pour une analyse couplée de la diffusion et de la concentration des contraintes en avant de la cavité peuvent ainsi être obtenues; elles permettent de déterminer la vitesse de propagation de la cavité en fonction de la contrainte appliquée.

DIE GESTALT DER DURCH OBERFLÄCHENDIFFUSION WACHSENDEN INTERGRANULAREN KRIECHRISSE

Ein rißartiger Hohlraum in Kriechproben vergrößert sich entlang der Grenzfläche zwischen zwei Körnern durch Diffusionstransport an seiner Spitze vom Material in die Korngrenze. Die Gestalt der Hohlraumoberflächen wird hier unter der Annahme berechnet, daß Oberflächendiffusion der bestimmende Mechanismus ist und stationäre Bedingungen vorherrschen, so daß sich der rißartige Hohlraum mit konstanter Gestalt an seiner Spitze fortbewegt. Für das Profil wird eine nicht-lineare Differentialgleichung zweiter Ordnung abgeleitet und eine Näherungslösung angegeben, die mit der numerischen Lösung sehr genau übereinstimmt. Somit ist es möglich, eine Beziehung zwischen Rißgeschwindigkeit, Krümmungsradius an der Rißspitze und Materialfluß in die Korngrenze an der Rißspitze einerseits sowie Materialkonstanten andererseits herzustellen. Diese Information ist als Randbedingung für eine gemeinsame Analyse der Diffusion und Spannungskonzentration vor dem Hohlraum sehr nützlich, z.B. zur Bestimmung der Ausbreitungsgeschwindigkeit der Hohlräume als Funktion der angelegten Spannung.

## 1. INTRODUCTION

It is well established that intercrystalline failure normally prevails for ductile materials at high temperatures.[1] This may occur by the formation and growth of sharp cracks or rounded cavities at the grain boundaries.[2] Systematic metallurgical studies suggest that the nucleation of cracks (or voids) is due mainly to grain-boundary sliding while the growth may be due either to plastic flow or to matter transport.[3] The present paper limits the study to the growth of grain-boundary cracks under steady-state conditions, by considering matter flow as the only operating mechanism. An atom lying on the crack surface can migrate by either volume diffusion, surface diffusion, or an evaporation–condensation process. Mullins[4] has set up conditions under which one of the above mechanisms will predominate. Here, it is assumed that the size scale of the crack tip is sufficiently small so that surface diffusion is the dominant mechanism. Furthermore, the two dimensional plane problem is considered in order to simplify the calculations.

## 2. MATHEMATICAL MODEL

Once a crack is nucleated along a grain boundary, it can propagate along it until it meets with an inclusion or a grain-boundary junction. Neglecting the existence of inclusions or junctions, one can adopt the model of a bi-crystal occupying the whole space with its flat grain boundary lying parallel to the $XZ$ plane, as in Fig. 1. Here we choose the $X$-axis to coincide with the lower crack surface at a great distance from the tip, so that the grain boundary plane is $Y = \omega$, where $\omega$ is the crack half-thickness. Also, the crack tip is located at $X = -b$ so that the origin of the

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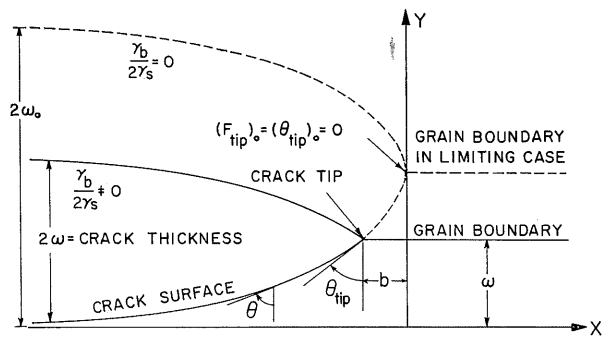


FIG. 1. Coordinate system for crack surface profile.

$X$-axis coincides with where the tip *would* be if our formulae were continued to the point of a vertical tangent at the tip, as illustrated. Of course, $\omega$ and $b$ are unknown *a priori*.

This coordinate system is taken to move through the material with the velocity $V$ of crack advance, and this completely characterizes the problem since we consider only the two dimensional case in steady state. Since the crack surface is assumed to be symmetric with respect to the crack tip, only the lower crack surface need be considered.

### 3. DERIVATION OF EQUATIONS

As previously stated, surface diffusion is assumed to be the only process operating. Denoting the difference in chemical potential per atom between a point of curvature $\kappa$ and a point of zero curvature on the surface by $\Delta\mu$, it may be shown that[5]

$$\Delta\mu = \kappa\gamma_s\Omega \tag{1}$$

where $\gamma_s$ is the surface free energy, which is assumed independent of crystal orientation, and $\Omega$ is atomic volume. Varying curvature along the profile gives rise to gradients of chemical potential which in turn produce a drift of surface atoms with an average velocity given by the Nernst–Einstein relation

$$V_s = -\frac{D_s}{kT}\frac{\mathrm{d}(\Delta\mu)}{\mathrm{d}s}, \tag{2}$$

where $V_s$ is the average surface velocity of atoms, $D_s$ the coefficient of surface diffusion and $\mathrm{d}s$ denotes an element of arc length. Substituting (1) into (2) and setting $J_s = \nu V_s$,

$$J_s = -\frac{D_s\gamma_s\Omega\nu}{kT}\frac{\mathrm{d}\kappa}{\mathrm{d}s}, \tag{3}$$

where $J_s$ is the surface flux of atoms (No. of atoms/unit length per unit time) and $\nu$ the surface concentration of diffusing atoms (No. of atoms/unit area of surface).

The conservation of matter asserts that

$$\frac{\mathrm{d}J_s}{\mathrm{d}s} = \frac{V_n}{\Omega} \tag{4}$$

where $V_n$ is the velocity of the cavity surface in the direction normal to itself. Letting the angle between the surface tangent and $Y$-axis be denoted by $\theta$ (Fig. 1) and assuming that the cavity advances in steady state without change in profile,

$$V_n = V\cos\theta.$$

But $\mathrm{d}s = \mathrm{d}Y/\cos\theta$ and so (4) becomes

$$\frac{\mathrm{d}J_s}{\mathrm{d}Y} = \frac{V}{\Omega}. \tag{5}$$

Hence, since $J_s = 0$ on the flat cavity surface, far behind the tip, where $Y = 0$,

$$J_s = \frac{V}{\Omega}Y \tag{6}$$

which states that atom flux is a linear function of $Y$. Evidently, the flux $J_{tip}$ into the grain boundary at the crack tip can be expressed as

$$J_{tip} = 2(J_s)_{Y=\omega} = \frac{2V\omega}{\Omega}. \tag{7}$$

The combination of the diffusion equation (equation 3) and conservation of mass (equation 6) will yield the governing differential equation required. However, it is found to be useful to introduce a new variable $F$ defined by

$$F \equiv \sin\theta. \tag{8}$$

Then from the definition of curvature,

$$\kappa \equiv \frac{\mathrm{d}\theta}{\mathrm{d}s} = \frac{\mathrm{d}(\sin\theta)}{\cos\theta\,\mathrm{d}s} = \frac{\mathrm{d}F}{\mathrm{d}Y} \tag{9}$$

because $\mathrm{d}Y = \mathrm{d}s\cos\theta$. Introducing the same substitution for $\mathrm{d}s$ and employing (9), the diffusion equation can be written in the form

$$J_s = -\frac{D_s\gamma_s\Omega\nu}{kT}\sqrt{(1-F^2)}\frac{\mathrm{d}^2F}{\mathrm{d}Y^2}. \tag{10}$$

Thus, one has the following governing differential equation after combining equations (6) and (10):

$$\frac{D_s\gamma_s\Omega\nu}{kT}\sqrt{(1-F^2)}\frac{\mathrm{d}^2F}{\mathrm{d}Y^2} + \frac{V}{\Omega}Y = 0. \tag{11}$$

Equation (11) can be non-dimensionalized by introducing a new independent variable $y$ such that

$$y = \left(\frac{VkT}{D_s\gamma_s\Omega^2\nu}\right)^{1/3}Y, \tag{12}$$

and the equation takes the form:

$$\sqrt{(1-F^2)}\,\frac{d^2F}{dy^2}+y=0 \tag{13}$$

together with the initial conditions at $y=0$:

$$F=1, \quad \text{since} \quad \theta=\pi/2 \quad \text{at} \quad y=0;$$
$$\frac{dF}{dy}=0, \quad \text{since} \quad \kappa=0 \quad \text{at} \quad y=0. \tag{14}$$

In addition to (13) and (14), which completely determine the function $F=F(y)$, it is obvious that the condition which fixes the location of the crack tip on the profile is required in order to obtain the complete solution. As in the case of grain-boundary grooving, it is assumed that the local thermodynamic equilibrium conditions always hold at the crack tip so that the equilibrium angle $\theta_{tip}$ remains unchanged at all times. This means that $2\gamma_s \sin\theta_{tip}=\gamma_b$, so that

$$F_{tip}=\frac{\gamma_b}{2\gamma_s} \tag{15}$$

where $\gamma_b$ is grain-boundary energy. This condition shows that $\theta_{tip}$ is only a function of $(\gamma_b/2\gamma_s)$ and is independent of applied stress. Given a material with a known value of $(\gamma_b/2\gamma_s)$, the location of the crack tip on the profile can then be determined by using (15).

## 4. SOLUTION OF EQUATIONS

The nonlinear ordinary differential equation (13) is solved first by expanding $F$ in an infinite power series in $y$, about $y=0$, subject to the initial conditions (14). Details are given in the Appendix; the result is

$$F(y)=1-\tfrac{1}{2}y^2-\frac{1}{8(13)}y^4-\frac{67}{16(31)(13)^2}y^6 - \frac{49463}{8(16)(31)(57)(13)^3}y^8-\cdots \tag{16}$$

Since the coefficients higher than second order term are approximately 0.01, 0.001, 0.0001 and so on, it is sufficient to keep only the first two terms. Thus,

$$F(y)\approx 1-\tfrac{1}{2}y^2. \tag{17}$$

It is convenient to reference results to the limiting case $\theta_{tip}=0$, and we attach the subscript "0" on all quantities referring to this case. Setting $F_{tip}=(F_{tip})_0=0$, the approximation (17) results in $(y_{tip})_0\approx\sqrt{2}$ and, since $Y_{tip}=\omega$, the corresponding crack half-thickness is

$$\omega_0\approx\sqrt{2}\left(\frac{D_s\gamma_s\Omega^2\nu}{VkT}\right)^{1/3} \tag{18}$$

In general, we have from (15) and (17)

$$F_{tip}=\frac{\gamma_b}{2\gamma_s}\approx 1-\tfrac{1}{2}(y_{tip})^2=1-\frac{\omega^2}{\omega_0^2},$$

so that the actual crack half-thickness is

$$\omega\approx\omega_0\sqrt{\left(1-\frac{\gamma_b}{2\gamma_s}\right)}. \tag{19}$$

The corresponding flux rate into the grain boundary ahead of the tip is, from (7)

$$J_{tip}=\frac{2V\omega}{\Omega}\approx 2\sqrt{2}\sqrt{\left(1-\frac{\gamma_b}{2\gamma_s}\right)}\left(\frac{D_s\gamma_s\nu V^2}{\Omega kT}\right)^{1/3}. \tag{20}$$

Also, the crack profile is given by integration of

$$\frac{dx}{dy}=\frac{\sin\theta}{\cos\theta}=\frac{F}{\sqrt{(1-F^2)}}\approx\frac{2-y^2}{y\sqrt{(4-y^2)}} \tag{21}$$

where $x$ is the dimensionless $X$ coordinate, defined as for $Y$ in (12). Requiring that $x=0$ when $y=\sqrt{2}$ (Fig. 2), this gives the profile shape

$$-x\approx\log\left[\frac{2+\sqrt{(4-y^2)}}{(1+\sqrt{2})y}\right]+\sqrt{2}-\sqrt{(4-y^2)}. \tag{22}$$

From (9) the curvature is

$$\kappa=\frac{dF}{dY}\approx -y\frac{dy}{dY}=-\left(\frac{VkT}{D_s\gamma_s\Omega^2\nu}\right)^{2/3}Y. \tag{23}$$

Hence, if $\rho_{tip}$ denotes the radius of curvature adjacent to the crack tip, then

$$\rho_{tip}=-\frac{1}{(\kappa)_{Y=\omega}}\approx\frac{1}{\sqrt{2}\sqrt{\left(1-\frac{\gamma_b}{2\gamma_s}\right)}}\left(\frac{D_s\gamma_s\Omega^2\nu}{VkT}\right)^{1/3},$$

or

$$\rho_{tip}\approx\frac{\omega}{2}\frac{1}{1-\frac{\gamma_b}{2\gamma_s}}. \tag{24}$$

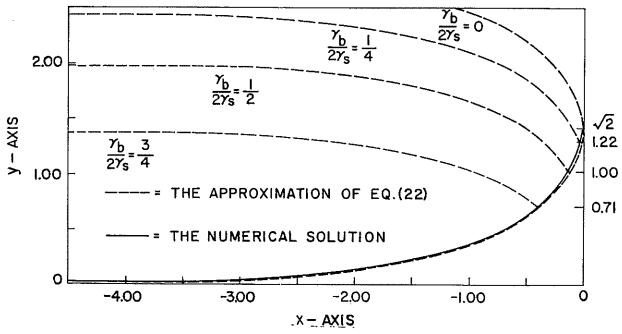


FIG. 2. Crack propagation profile in $x$–$y$ plane.

It is also of interest to note that since $\kappa$ and $J_s$ are both in direct proportion of $Y$, $J_s \approx$ (const.) $\kappa$, and this together with $J_s \propto d\kappa/ds$ means that both $J_s$ and $\kappa$ decay exponentially with arc length as measured from the crack tip, according to our approximation.

All these results are based on replacing the series solution (16) by its dominant terms, (17). A numerical solution to (13) has also been obtained, through the Runge–Kutta method with step size $\Delta y = 0.01$. Figure 2 shows the comparison of this numerical solution (solid line) and the above approximate solution (22) for the crack tip profile. This numerical solution further shows that the precise versions of (18) and of (20) and (24) in the limiting case $\theta_{tip} = 0$ are

$$\omega_0 = \frac{\Omega(J_{tip})_0}{2V} = 1.38\left(\frac{D_s\gamma_s\Omega^2\nu}{VkT}\right)^{1/3}, \qquad (25)$$

$$(\rho_{tip})_0 = \frac{1}{1.52}\left(\frac{D_s\gamma_s\Omega^2\nu}{VkT}\right)^{1/3} = \frac{\omega_0}{2.1}.$$

Hence we see that the exact results are barely distinguishable from the approximate solution based on (17).

## 5. CONCLUSION

We have presented the crack profile shape, and the relation of the crack half-thickness $\omega$, root radius $\rho_{tip}$ adjacent to the crack tip, flux $J_{tip}$ into the grain boundary, and velocity $V$ to one another and to material properties and temperature, assuming steady state conditions. The steady state assumption should be valid when the crack velocity changes little over distance of crack advance equal to several root radii.

Ashby[6] has proposed a creep cracking model which entails transport of matter from the crack surfaces, into and along the grain boundary. The boundary transport is governed by the tensile stress distribution ahead of the crack, and this stress distribution is in turn determined by the applied stress, by the shape of the cavity, and by the dislocational misfit stresses due to matter previously diffused into the boundary. It is possible to solve for the crack shape, as we have here, in terms of crack velocity, without solving the complete problem, so as to relate the velocity to applied stress, temperature, flaw length, etc. Indeed, the relations between $J_{tip}$, $V$ and $\rho_{tip}$ of our solution will enter a more complete analysis as boundary conditions at the moving crack tip. We leave this to future study.

It may also be noted that Ashby[6] derived equations of similar form to (18) and (24) by the approximate procedure of viewing the crack as an ellipse, and writing net diffusion equations based on the extremal differences in curvature, although this procedure does not accurately predict the numerical coefficients which appear from our solution. Further, his colleague H. Frost has obtained analog computer solutions for the tip profile which take a form similar to the exact results.

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## APPENDIX

To seek a solution $F = F(y)$ of the differential equation

$$\sqrt{(1 - F^2)}\frac{d^2F}{dy^2} + y = 0, \qquad (A1)$$

subject to the conditions

$$F(0) = 1, \quad F'(0) = 0, \qquad (A2)$$

assume that $F$ can be expressed in terms of infinite series in $y$, i.e.

$$F(y) = \sum_{n=0}^{\infty} a_n y^n. \qquad (A3)$$

The conditions of equation (A2) require that $a_0 = 1$ and $a_1 = 0$. Thus, equation (A3) leads to

$$1 - F = y^2 G \qquad (A4)$$

where

$$G = -\sum_{n=2}^{\infty} a_n y^{n-2}. \qquad (A5)$$

After substitution of (A4) into (A1), one obtains

$$G^{1/2}(2 - y^2G)^{1/2}(y^2G'' + 4yG' + 2G) = 1$$

or

$$G(2 - y^2G)(y^2G'' + 4yG' + 2G)^2 = 1. \qquad (A6)$$

From (A5), equation (A6) can be expanded into power series in $y$. One can then find the coefficients by requiring that the constant term be 1 and others vanish. The result is

$$a_2 = -\frac{1}{2}, \quad a_3 = 0, \quad a_4 = \frac{-1}{8(13)}, \quad a_5 = 0,$$

$$a_6 = \frac{-67}{16(31)(13)^2}, \quad a_7 = 0, \quad a_8 = \frac{-49463}{8(16)(31)(57)(13)^3}, \text{ etc.}$$

Accordingly, the solution of $F$ written in the form of (A3) is as given in equation (16) of the text.