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Theory of bending of polycrystalline beams by creep at low stress

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Attempts to extend diffusion creep theory from simple grain geometries to more complex polycrystalline structures generally make the assumptions that the vacancy creation (or annihilation) rate is constant over each grain face and that the volume of each grain is conserved. These assumptions do not permit grain rotation, a common feature of polycrystalline creep, nor is diffusion allowed to occur between individual grains. These two aspects are investigated theoretically in this paper, for the specific case of the grain boundary diffusion controlled bending of a polycrystalline beam consisting of a set of orthorhombic grains of dimensions X , Y and Z , with the Z dimension, parallel to the axis of bending, assumed large such that two-dimensional diffusion predominates. The grains are aligned with continuous boundaries across the beam height.

For grains highly elongated along the beam length ($X \gg Y$), the derived rotation rate is identical to that for a bicrystal having the same height as the beam. For smaller X , diffusion in boundaries along the beam length make increasing contributions and the rotation rate increases. The novel prediction is made that the non-conservation of grain volume is an inevitable consequence of the grain boundary diffusion controlled deformation of this particular polycrystalline configuration.

1. Introduction

The theory of diffusion creep was originally developed for simple grain geometries such as the 'bamboo' structures used in early experimental studies [1]. These structures are circular wires having a single grain per cross section and tested in simple tension. Subsequent attempts to extend the theory to polycrystalline materials have proved more complex. The analysis by Greenwood [2] of the lattice diffusion creep of a three-dimensional array of orthorhombic grains, satisfied all the necessary physical requirements and predicted creep rates under multi-axial stresses as a function of the grain dimensions X , Y and Z . A similar

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3 analysis for the grain boundary diffusion case was achieved by using numerical methods [3].
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5 Both these analyses assumed that the boundaries on each grain face acted either as a source or
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7 sink for vacancies and that the vacancy creation or annihilation rate was constant over each
8
9 face. However, such an assumption does not allow for the possibility of grain rotation, a
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11 feature that is commonly observed during the creep of polycrystalline materials with grain
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13 structures more complex than the uniform geometry used in the above models. A second
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15 assumption in the analyses was that creep occurred at constant grain volume, so that no
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17 diffusion was allowed between individual grains.

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19 By relaxing the first of the above conditions and allowing the vacancy creation rate to vary
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21 linearly with distance along a boundary, leads naturally to the possibility of relative rotation
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23 of grains about their common boundary. Analyses have been presented for the diffusion
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25 controlled rotation about the common boundary of a bicrystal, for the cases where both grain
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27 boundary and lattice diffusion predominate [4-7].

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29 In the present paper, the analysis of diffusion controlled rotation is extended from the
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31 bicrystal case, to that of an array of orthorhombic grains under an applied bending moment.
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33 The validity of the second of the above assumptions, namely that deformation occurs at
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35 constant grain volume, is evaluated. The work was stimulated by recent experimental
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37 measurements of the deflection rates of polycrystalline beams at low stresses [8].
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40 41 **2. Analysis**

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44 Consider a cantilever beam of height h , consisting of an array of orthorhombic grains of
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46 dimensions X , Y and Z arranged as shown schematically in Fig.1, under an applied bending
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48 moment M . At elevated temperatures, the bending moment leads to stress-directed vacancy
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50 flow, which causes a local redistribution of the boundary stresses, grain rotation and creep
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52 bending of the beam. It is assumed that the stresses are too low for dislocation creep
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54 mechanisms to operate and the temperature to be sufficiently low for boundary diffusion to
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56 predominate.
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58 59 **2.1 Diffusion in the y -direction**

60

The analysis is simplified by considering the case where $Z \gg X$ and Y , so that diffusion occurs predominantly in one dimension along each boundary. For rotation to occur about the vertical boundary AB , vacancies must be created at a rate that varies linearly along AB , so that:

$$\beta(y) = \beta_{\max} \left(\frac{2y}{h} - 1 \right) \quad (1)$$

where β_{\max} is the vacancy creation rate at $y = h$, with an annihilation rate $-\beta_{\max}$ at $y = 0$. Note that the relative normal velocity between grains $v(y) = \omega\Omega\beta(y)$ where ω is the grain boundary width and Ω the atomic volume. This may be expressed as a local creep rate in the x -direction at a position y , such that: $\dot{\epsilon}_x(y) = v(y) / X = \omega\Omega\beta(y) / X$.

The equation governing steady state diffusion along the boundary is given by:

$$D_V \frac{d^2 C}{dy^2} + \beta_{\max} \left(\frac{2y}{h} - 1 \right) = 0 \quad (2)$$

where C is the vacancy concentration and D_V the grain boundary vacancy diffusion coefficient. For the n^{th} grain, this equation may be solved by integrating twice with the boundary conditions $C = C_{n-1}$ at $y = y_{n-1}$ and $C = C_n$ at $y = y_n$ to give the result:

$$\begin{aligned} C(y) = & \left(\frac{y - y_{n-1}}{Y} \right) C_n - \left(\frac{y - y_n}{Y} \right) C_{n-1} \\ & - \frac{\beta_{\max} h^2}{6D_V} \left\{ 2 \left(\frac{y}{h} \right)^3 - 3 \left(\frac{y}{h} \right)^2 - \left(\frac{y}{Y} \right) \left(2 \left(\frac{y_n^3 - y_{n-1}^3}{h^3} \right) - 3 \left(\frac{y_n^2 - y_{n-1}^2}{h^2} \right) \right) \right\} \\ & + \frac{\beta_{\max} h^2}{6D_V} \left\{ \left(\frac{y_n}{Y} \right) \left(2 \left(\frac{y_{n-1}}{h} \right)^3 - 3 \left(\frac{y_{n-1}}{h} \right)^2 \right) - \left(\frac{y_{n-1}}{Y} \right) \left(2 \left(\frac{y_n}{h} \right)^3 - 3 \left(\frac{y_n}{h} \right)^2 \right) \right\} \end{aligned} \quad (3)$$

The local stress at the grain boundary is related to the vacancy concentration according to:

$$\sigma(y) = \frac{kT}{\Omega} \ln \left(\frac{C(y)}{C_{EQ}} \right) \approx \frac{kT}{\Omega} \left(\frac{C(y)}{C_{EQ}} - 1 \right) \quad (4)$$

where k is Boltzmann's constant, T the absolute temperature and C_{EQ} the equilibrium vacancy concentration. The approximation $\ln(\alpha) \sim (\alpha - 1)$ is used since in cases of practical importance $\sigma\Omega \ll kT$. The moment about the position $y = 0$ can be calculated using equations (3 & 4). Thus, for the n^{th} grain, the moment M_n is given by:

$$\frac{M_n}{Z} = \int_{y_{n-1}}^{y_n} y \sigma(y) dy = \frac{kT}{\Omega} \int_{y_{n-1}}^{y_n} y \left(\frac{C(y)}{C_{EQ}} - 1 \right) dy \quad (5)$$

This evaluates to:

$$\frac{M_n}{ZY^2} = \frac{\sigma_{n-1}(3n-2) + \sigma_n(3n-1)}{6} + \frac{\beta_{\max} Y^2 kT}{360D_g} \left(15 - 30n - 60\left(\frac{n}{N}\right) + \frac{16}{N} + 60\left(\frac{n^2}{N}\right) \right) \quad (6)$$

where $\sigma_n = (C_n/C_{EQ} - 1)kT/\Omega$, $\sigma_{n-1} = (C_{n-1}/C_{EQ} - 1)kT/\Omega$ and $D_g (= D_V C_{EQ} \Omega)$ is the grain boundary diffusion coefficient of atoms. The moment exerted over the entire boundary is:

$$\frac{M_N}{ZY^2} = \frac{1}{ZY^2} \sum_{n=1}^{n=N} M_n = \sum_{n=1}^{n=N} n\sigma_n + \frac{\beta_{\max} Y^2 kT}{360D_g} \sum_{n=1}^{n=N} \left(15 - 30n - 60\left(\frac{n}{N}\right) + \frac{16}{N} + 60\left(\frac{n^2}{N}\right) \right) \quad (7)$$

which reduces to:

$$\frac{M_N}{ZY^2} = \sum_{n=1}^{n=N} n\sigma_n + \frac{\beta_{\max} Y^2 kT}{D_g} \left(\frac{5N^2 - 4}{360} \right) \quad (8)$$

For a bicrystal, $N = 1$, $h = Y$ and $\sigma_n = \sigma_{n-1} = 0$ (since $C = C_{EQ}$ at $y = 0$ and $y = Y$). The rotation rate is then given by:

$$\dot{\theta} = \tan^{-1} \left(\frac{2\beta_{\max} \omega \Omega}{Y} \right) \approx \frac{2\beta_{\max} \omega \Omega}{Y} = \frac{720M\omega\Omega D_g}{Zh^5 kT} \quad (9)$$

This rate is identical to that predicted previously for a bicrystal [3].

2.2 Diffusion in the x-direction

The equation governing diffusion along boundaries in the x -direction is given by:

$$D_V \frac{d^2 C}{dx^2} + \xi_n = 0 \quad (10)$$

where ξ_n is the vacancy creation rate along the n^{th} boundary. In this case the creation rate is independent of distance since, with the grain configuration considered, no rotation occurs about the longitudinal boundaries. The equation may be solved with the boundary conditions $dC/dx = 0$ at $x = X/2$ and $C = C_n$ at $x = 0$ (or $x = X$), to give the result:

$$[C(x)]_n = C_n + \frac{\xi_n X^2}{2D_V} \left\{ \left(\frac{x}{X}\right) - \left(\frac{x}{X}\right)^2 \right\} \quad (11)$$

The stresses over the boundary must sum to zero, so that:

$$\frac{kT}{\Omega} \int_0^X \left(\frac{C_n}{C_{EQ}} - 1 + \frac{\xi_n X^2}{2D_V C_{EQ}} \left\{ \left(\frac{x}{X}\right) - \left(\frac{x}{X}\right)^2 \right\} \right) dx = 0 \quad (12)$$

which evaluates to:

$$\sigma_n = - \frac{\xi_n X^2 kT}{12D_g} \quad (13)$$

Similar analysis for the $(n-1)^{\text{th}}$ boundary reveals:

$$[C(x)]_{n-1} = C_{n-1} + \frac{\xi_{n-1} X^2}{2D_V} \left\{ \left(\frac{x}{X} \right) - \left(\frac{x}{X} \right)^2 \right\} \quad (14)$$

and:

$$\sigma_{n-1} = -\frac{\xi_{n-1} X^2 kT}{12D_g} \quad (15)$$

2.3 Diffusion fluxes at the nodes

For the n^{th} node (at $y = y_n$), the vacancy flow in the y -direction in the boundary of the n^{th} grain is given by:

$$\frac{\Phi_n}{Z} = -\omega D_V \left(\frac{dC}{dy} \right)_{y=y_n} \quad (16)$$

Using equations (3) and (4), this gives:

$$\frac{\Phi_n}{Z} = -\left(\frac{\sigma_{n+1} - \sigma_n}{Y} \right) \frac{\omega D_g}{kT} + \omega \beta_{\max} h^2 \left\{ \left(\frac{y_n^2}{h^3} - \frac{y_n}{h^2} \right) - \frac{1}{Y} \left(\frac{y_{n+1}^3 - y_n^3}{3h^3} - \left(\frac{y_{n+1}^2 - y_n^2}{2h^2} \right) \right) \right\} \quad (17)$$

Since $h = NY$, $y_n = nY$ and $y_{n+1} = (n+1)y$, this reduces to:

$$\frac{\Phi_n}{Z} = -\left(\frac{\sigma_{n+1} - \sigma_n}{Y} \right) \frac{\omega D_g}{kT} + \omega \beta_{\max} Y \left(-\frac{n}{N} + \frac{1}{2} - \frac{1}{3N} \right) \quad (18)$$

Similarly, for the $(n-1)^{\text{th}}$ grain, the flow at the node position $y = y_n$ is:

$$\frac{\Phi_{n-1}}{Z} = -\left(\frac{\sigma_n - \sigma_{n-1}}{Y} \right) \frac{\omega D_g}{kT} + \omega \beta_{\max} Y \left(\frac{n}{N} - \frac{1}{2} - \frac{1}{3N} \right) \quad (19)$$

For diffusion in the x -direction at node n , the diffusion flows are derived from equations (11), (14) and (4) to give:

$$\frac{\Psi_{x=0}}{Z} = -\omega D_V \left(\frac{dC}{dx} \right)_{x=0} = -\frac{\xi_n \omega X}{2} = \frac{6\sigma_n \omega D_g}{XkT} \quad (20)$$

and

$$\frac{\Psi_{x=X}}{Z} = -\omega D_V \left(\frac{dC}{dx} \right)_{x=X} = \frac{\xi_n \omega X}{2} = -\frac{6\sigma_n \omega D_g}{XkT} \quad (21)$$

For conservation of matter at the node n , it is required that:

$$\Phi_n - (\Psi_{x=X} - \Psi_{x=0}) = \Phi_{n-1} \quad (22)$$

which gives:

$$\left(\frac{\sigma_{n-1} + \sigma_{n+1}}{2}\right) = \sigma_n \left(1 + 6\frac{Y}{X}\right) + \frac{\beta_{\max} Y^2 kT}{2D_g} \left(1 - \frac{2n}{N}\right) \quad (23)$$

2.4 Rotation at boundary AB in a beam with $N = 2$

Equations (8, 13 & 23) provide the basis for solving the diffusion problem for beams with different numbers of grains in the cross section AB. For $N = 2$, there is just one horizontal boundary, located at $y_n/h = 1/2$. Since $C = C_{EQ}$ at both $y = 0$ and $y = h$ then $\sigma_0 = \sigma_2 = 0$.

Equations (8) and (23) then reveal that $\sigma_1 = 0$ and

$$\beta_{\max} = \frac{45MD_g}{2ZY^4kT} \quad (24)$$

This gives rise to a rotation rate:

$$\dot{\theta} = \frac{2\omega\Omega\beta_{\max}}{h} = \frac{45M\Omega\omega D_g}{ZY^4hkT} \quad (25)$$

Since $h (= NY) = 2Y$, the rate is identical to that of a bicrystal given by equation (9).

The variation of local stress along the boundary AB may be deduced from equations (3, 4 & 24) to give:

$$\sigma(y) = -\frac{60M}{Zh^2} \left(\frac{y}{h}\right) \left(1 - \frac{y}{h}\right) \left(1 - \frac{2y}{h}\right) \quad (26)$$

This is again identical to the result for the stress variation along the boundary of a bicrystal undergoing grain rotation [3]. The stress $\sigma(y)$ takes maximum and minimum values of $\pm 10M/3^{1/2}Zh^2$, at the positions $(y/h) = (1 \pm 1/3^{1/2})/2$.

There is no diffusion flow in the x -direction since $C_{h/2} = C_{EQ}$ and therefore $\sigma_1 = 0$. The flow in the y -direction at the node located at $y = h/2$ may be calculated from either equation (18) or (19) and is given by:

$$\Phi_{h/2} = -\frac{\omega Y Z \beta_{\max}}{6} = -\frac{15M\omega D_g}{4Y^3kT} \quad (27)$$

This diffusion flow represents the transfer of material from grains in the lower ($y < h/2$) to those in the upper ($y > h/2$) half of the beam. This material transfer requires that grain volume is not conserved during the diffusion controlled bending of this particular polycrystalline configuration.

2.5 Rotation at boundary AB in a beam with $N = 4$

Equations (8, 13 & 23) again provide the necessary equations to effect a solution, namely:

$$\sigma_2 - 2\left(1 + 6\frac{Y}{X}\right)\sigma_1 + \sigma_0 = \frac{\beta_{\max} Y^2 kT}{2D_g} \quad (28)$$

$$\sigma_3 - 2\left(1 + 6\frac{Y}{X}\right)\sigma_2 + \sigma_1 = 0 \quad (29)$$

$$\sigma_4 - 2\left(1 + 6\frac{Y}{X}\right)\sigma_3 + \sigma_2 = -\frac{\beta_{\max} Y^2 kT}{2D_g} \quad (30)$$

$$\frac{M}{ZY^2} = \sigma_1 + 2\sigma_2 + 3\sigma_3 + \left(\frac{5N^2 - 4}{360}\right) \frac{\beta_{\max} Y^2 kT}{D_g} \quad (31)$$

Simultaneous solution of equations (28-31) and also noting that $\sigma_0 = \sigma_4 = 0$, give the results:

$$\sigma_1 = -\sigma_3 = -\frac{45}{128} \frac{M}{ZY^2} \left(\frac{1}{1 + 57Y/32X} \right) \quad (32)$$

$$\sigma_2 = 0 \quad (33)$$

$$\beta_{\max} = \frac{45MD_g}{32ZY^4 kT} \left(\frac{1 + 6Y/X}{1 + 57Y/32X} \right) \quad (34)$$

The rotation rate becomes:

$$\dot{\theta} = \frac{720M\Omega\omega D_g}{Zh^5 kT} \left(\frac{1 + 6Y/X}{1 + 57Y/32X} \right) \quad (35)$$

For large X , when $Y/X \rightarrow 0$, like the previous case for $N = 2$, the rotation rate reduces to that for a bicrystal of height h . For smaller X , the stresses at the nodes vary according to equation (32) and the rotation rate increases, eventually reaching the limit $45M\Omega\omega D_g/19ZY^5 kT$ when $\sigma_1 \rightarrow -15MX/76ZY^3$ and $\sigma_3 \rightarrow +15MX/76ZY^3$ respectively.

2.6 Rotation at boundary AB in a beam with $N = 6$

Using a similar method of solution gives the results:

$$\sigma_1 = -\sigma_5 = -\frac{25}{162} \frac{M}{ZY^2} \left(\frac{1 + 24Y/5X}{1 + 476Y/81X + (176/27)(Y/X)^2} \right) \quad (36)$$

$$\sigma_2 = -\sigma_4 = -\frac{10}{81} \frac{M}{ZY^2} \left(\frac{1 + 3Y/X}{1 + 476Y/81X + (176/27)(Y/X)^2} \right) \quad (37)$$

$$\sigma_3 = 0 \quad (38)$$

$$\beta_{\max} = \frac{5MD_g}{18ZY^4kT} \left(\frac{1+16Y/X+48(Y/X)^2}{1+476Y/81X+(176/27)(Y/X)^2} \right) \quad (39)$$

The rotation rate is:

$$\dot{\theta} = \frac{720M\Omega\omega D_g}{Zh^5kT} \left(\frac{1+16Y/X+48(Y/X)^2}{1+476Y/81X+(176/27)(Y/X)^2} \right) \quad (40)$$

The limiting value when $X \ll Y$ is $15M\Omega\omega D_g / 22ZY^5kT$.

The variation of stress along the boundary AB , calculated from equations (3), (4) and (36-40), is plotted in Fig.2 for three values of the ratio Y/X . The stress is represented in the normalised form $\sigma(y)/\sigma_{ref}$, where $\sigma_{ref} = 10M/3^{1/2}Zh^2$ is the maximum value of stress for the bicrystal case derived from equation (26)

When $X \gg Y$, negligible diffusion occurs along boundaries in the x -direction and the stress variation along AB is identical to that for an equivalent bicrystal of height h , given by equation (26). The stresses σ_1 , σ_2 and σ_3 given by equations (36–38) all reduce to values identical to those for a bicrystal, calculated from equation (26), at corresponding positions $y/h = 1/6, 1/3$ and $1/2$.

For the equi-axed case ($X = Y$), the influence of diffusion in the x -direction now reduces the values of σ_1 , σ_2 and σ_3 and in the extreme case where $X \ll Y$, σ_1 , σ_2 and σ_3 tend to zero.

2.7 Non-conservation of grain volume during creep

It is clear by observation from Fig.2, that the stress gradient (and therefore the vacancy concentration gradient) along the boundary AB at the centre position ($y = h/2$) is non-zero. This means that vacancy flow must occur between the top and bottom half of the beam. This can occur only if individual grain volume is not conserved during creep bending of the beam. These changes in grain volume can be assessed quantitatively, using the example of a beam with an even number of grains over its height, by calculating the vacancy flux at the position $y = h/2$ from equation (19). Thus:

$$\frac{\Phi_{y=h/2}}{Z} = \frac{\sigma_{(N-2)/2}\omega D_g}{YkT} - \frac{\omega\beta_{\max}Y}{3N} \quad (41)$$

For $N = 2$, the vacancy flow at the centre $\Phi_{N=2} = -\omega\beta_{\max} ZY / 6 = -\omega\beta_{\max} Zh / 12$. This is identical to the flow that occurs at $h/2$ for a bicrystal of equivalent height $h = Y$. Thus the grain defined by $n = 1$ changes volume at a rate $-\Phi\Omega$ per second and grain $n = 2$ at a rate $+\Phi\Omega$.

For $N = 4$, the flow at $y = h/2$ is:

$$\Phi_{y=h/2} = -\frac{\omega\beta_{\max} ZY}{12} \left(\frac{1 + 3Y / 2X}{1 + 6Y / X} \right) \quad (42)$$

and for $N = 6$:

$$\Phi_{y=h/2} = -\frac{\omega\beta_{\max} ZY}{12} \left(\frac{1 + 40Y / 9X + (16/3)(Y / X)^2}{1 + 16Y / X + 48(Y / X)^2} \right) \quad (43)$$

The rate of change in volume of an individual grain during deformation can be calculated from the creep rates in the orthogonal directions $\dot{\epsilon}_x$ and $\dot{\epsilon}_y$ as follows:

$$\dot{V} = XYZ(\dot{\epsilon}_x + \dot{\epsilon}_y) \quad (44)$$

Taking the example where $N = 6$, the creep rates for grains $n = 3$ and 2 respectively are given by:

$$(\dot{\epsilon}_x)_3 = -\frac{1}{6} \frac{\beta_{\max} \Omega \omega}{X} = -\frac{5}{108} \left(\frac{M}{ZY^2} \right) \frac{\Omega \omega D_g}{XY^2 kT} \left(\frac{1 + 16Y / X + 48(Y / X)^2}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (45)$$

$$(\dot{\epsilon}_x)_2 = -\frac{1}{2} \frac{\beta_{\max} \Omega \omega}{X} = -\frac{15}{108} \left(\frac{M}{ZY^2} \right) \frac{\Omega \omega D_g}{XY^2 kT} \left(\frac{1 + 16Y / X + 48(Y / X)^2}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (46)$$

$$(\dot{\epsilon}_y)_3 = \frac{(\xi_3 + \xi_2) \omega \Omega}{2Y} = \frac{20}{27} \left(\frac{M}{ZY^2} \right) \frac{\Omega \omega D_g}{X^2 Y kT} \left(\frac{1 + 3Y / X}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (47)$$

$$(\dot{\epsilon}_y)_2 = \frac{(\xi_2 + \xi_1) \omega \Omega}{2Y} = \frac{45}{27} \left(\frac{M}{ZY^2} \right) \frac{\Omega \omega D_g}{X^2 Y kT} \left(\frac{1 + 4Y / X}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (48)$$

Using equations (44-48) gives the results:

$$\dot{V}_3 = -\frac{5}{108} \frac{M \Omega \omega D_g}{Y^3 kT} \left(\frac{1}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (49)$$

and

$$\dot{V}_2 = -\frac{5}{36} \frac{M \Omega \omega D_g}{Y^3 kT} \left(\frac{1 + 4(Y / X)}{1 + 476Y / 81X + (176/27)(Y / X)^2} \right) \quad (50)$$

Note also, by symmetry, that $\dot{V}_4 = -\dot{V}_3$ and $\dot{V}_5 = -\dot{V}_2$. The rate of volume change, represented in the dimensionless form $\dot{V}Y^3kT / M\Omega\omega D_g$ is plotted as a function of the aspect ratio Y/X for grains 2 to 5 in Fig.3. The grain volume changes are negative on the compressive side of the beam ($y < h/2$) and positive on the tensile side ($y > h/2$) and the magnitudes are greater in grains located further away from the centre of the beam. The volume changes are greatest as $Y/X \rightarrow 0$, when they take the (dimensionless) values $\pm 5/36$ and $\pm 5/108$ for the outer and inner grains respectively, and they tend to zero as $Y/X \rightarrow \infty$.

3. Discussion

During the creep of polycrystalline materials at low stresses, individual grains undergo shape changes, grain boundary sliding and rotation. These processes interact in a complex way and result in the externally applied stress being shared between the internal grain boundaries such that the shape changes, sliding and rotation occur at matching rates. The theories of shape changes and sliding are well developed, but rotation has received relatively little attention. The present work extends the theory of the diffusion controlled rotation of a bicrystal³⁻⁷ to a simple polycrystalline case. The two dimensional model of a bending beam is chosen for mathematical simplicity and grain boundary diffusion is assumed to dominate so that exact solutions to the diffusion equations can be derived. The structure is chosen such that all the vertical boundaries are aligned, and this introduces an additional simplification in that rotation is required to occur only about these boundaries, with none occurring about those in the horizontal direction. This enables the predictions to relate directly to those for a bicrystal under the limiting conditions $X \gg Y$, when negligible diffusion occurs along boundaries in the x -direction. This is demonstrated by equations (9, 25, 35 & 40), when the rotation rates are shown to converge with those predicted for a bicrystal. Similarly, the stress distribution over the boundary AB also converges to that for a bicrystal given by equation (26) when $X \gg Y$. This is also demonstrated graphically in Fig.2 for the beam with $N = 6$.

The vertical diffusion flux predicted to occur along the boundary AB at the central position ($y = h/2$) is of special interest. Under the limiting conditions $X \gg Y$, this flux is again identical to that for a bicrystal, but the flux also remains finite for all values of Y/X . The existence of this flux is one of the most important results to emerge from the present work. It shows that grain volume is not conserved during the diffusion controlled bending of the polycrystalline

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3 structure considered. This demonstrates theoretically for the first time that the non-
4 conservation of grain volume can be an inevitable consequence of the diffusion controlled
5 deformation of polycrystalline matter.
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10 The present work was stimulated by a recent experimental study on the bending of
11 polycrystalline beams at low stress levels⁸. These experiments showed behaviour resembling
12 the grain rotation in a bicrystal, for structures where a single grain occupied the entire beam
13 cross section in both the y and z -directions and 'continuum' creep behaviour when the grain
14 size was much smaller than the specimen thickness. Behaviour was more complex in the case
15 where grains occupied the entire beam height, but several grains were present in the z -
16 direction. The experiments were performed at high temperatures where lattice diffusion was
17 rate controlling, compared to the present analyses where boundary diffusion is considered.
18 However, the analysis shown in the Appendix for the grain boundary diffusion case also
19 demonstrates convergence towards continuum behaviour when the grain size is much smaller
20 than the beam thickness.
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32 In the earliest analyses of the diffusion creep of polycrystals^{2,3}, neither grain rotation nor the
33 non-conservation of grain volume were predicted because of the simple grain structures and
34 the applied stress systems considered. The analyses assumed an infinite array of identical
35 grains under uniaxial stresses. Under these conditions the vacancy concentrations at each
36 equivalent grain corner were identical throughout the structure and symmetrical around an
37 individual grain, in such a way that there was no driving force for either rotation or inter-grain
38 diffusion leading to non-conservation of grain volume. In real materials, the presence of
39 external surfaces (where the vacancy concentration must always take the equilibrium value),
40 variations in grain size, or indeed in phase differences between grains, will lead to non-
41 symmetrical vacancy concentrations around grains that may result in both grain rotation and
42 volume non-conservation. It is likely that both rotation and non-conservation effects will
43 occur under uniaxial stresses and do not necessarily require bending moments as in the
44 present analysis.
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56 **4. Conclusions**

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59 The theory of grain boundary diffusion controlled bending of a beam consisting of an array of
60 orthorhombic grains of dimensions X , Y and Z has been developed for the case where the

grains are aligned with a continuous boundary across the beam height. The dimension Z , parallel to the axis of bending, is assumed large such that diffusion occurs only in the x and y -directions. For grains highly elongated along the beam length ($X \gg Y$), the rotation rate is predicted to be identical to that of a bicrystal having the same height as the beam. For smaller X , diffusion along boundaries in the x -direction, make additional contributions and the rotation rate then increases. It is shown that diffusion between grains is an inevitable consequence of the deformation for the configuration considered. This demonstrates theoretically for the first time, the non-conservation of individual grain volume during diffusion creep. It is inferred that that non-conservation of individual grain volume may be a more general feature of the diffusional flow of polycrystalline materials.

Acknowledgement

The author is grateful to the Wingate Foundation for the award of a scholarship.

Appendix

Continuum creep bending of a beam.

The analyses presented in the main body of the paper are concerned with the bending of a beam resulting from diffusion controlled rotation localised at boundaries. To provide a comparison, the hypothetical case is now considered where the creep of material is everywhere uniform. For a beam of height h and depth Z , undergoing such *continuum* creep, the rate must vary linearly with y according to the relationship:

$$\dot{\epsilon}(y) = A_c \sigma_y^m = \left(\frac{2y}{h} - 1\right) \dot{\epsilon}_{\max} \quad (\text{A1})$$

where $\pm \dot{\epsilon}_{\max}$ are the creep rates of the outer fibres of the beam, A_c is the creep constant and m is the stress exponent for creep. For $m = 1$, the stress thus varies across the beam according to the relationship:

$$\sigma_y = \frac{\dot{\epsilon}_{\max}}{A_c} \left(\frac{2y}{h} - 1\right) \quad (\text{A2})$$

The bending moment in the beam is given by:

$$M = Z \int_0^h y \sigma_y dy = \frac{Z \dot{\epsilon}_{\max}}{A_c} \int_0^h y \left(\frac{2y}{h} - 1\right) dy = \frac{Zh^2 \dot{\epsilon}_{\max}}{6A_c} \quad (\text{A3})$$

This may be rearranged to give:

$$\dot{\epsilon}_{\max} = A_c \left(\frac{6M}{Zh^2} \right) \quad (\text{A4})$$

Then from equations (A2) and (A4):

$$\sigma_y = \frac{6M}{Zh^2} \left(\frac{2y}{h} - 1 \right) \quad (\text{A5})$$

The stress thus varies linearly over the beam height between the limits $\pm 6M/Zh^2$.

When the grain size of a material is much smaller than its exterior dimensions, diffusion creep may be expected to approximate to continuum flow. For the grain geometry considered in the present paper, the creep rate may be derived by considering diffusion in the two orthogonal boundaries. The diffusion equation can be solved for boundaries in the x -direction as shown in equation (10). Forces may be resolved over the boundary to give:

$$\frac{kT}{\Omega} \int_0^X \left(\frac{C^*}{C_{EQ}} - 1 + \frac{\xi X^2}{2D_v C_{EQ}} \left\{ \left(\frac{x}{X} \right) - \left(\frac{x}{X} \right)^2 \right\} \right) dx = X \sigma_y \quad (\text{A6})$$

where σ_y is the stress in the y -direction. This yields the result:

$$\sigma_y = \sigma^* + \frac{\xi X^2 kT}{12D_g} \quad (\text{A7})$$

where $\sigma^* = (C^*/C_{EQ} - 1)kT/\Omega$ is the stress at the grain corner. Similar analysis for the orthogonal boundaries gives the result:

$$\sigma_x = \sigma^* + \frac{\beta Y^2 kT}{12D_g} \quad (\text{A8})$$

Grain volume conservation requires: $\xi X + \beta Y = 0$ and then solution of equations (A6-A8) gives the results:

$$\beta = -\frac{X}{Y} \xi = \frac{12(\sigma_x - \sigma_y)D_g}{Y^2 kT(1 + X/Y)} \quad (\text{A9})$$

$$\sigma^* = \left(\frac{X/Y}{1 + X/Y} \right) \sigma_x + \left(\frac{1}{1 + X/Y} \right) \sigma_y \quad (\text{A10})$$

The creep rate is given by:

$$\dot{\epsilon}_x = -\frac{X}{Y} \dot{\epsilon}_y = \frac{\beta \omega \Omega}{X} = \frac{12(\sigma_x - \sigma_y) \Omega \omega D_g}{XY^2 kT(1 + X/Y)} \quad (\text{A11})$$

In the present case $\sigma_y = 0$, so that:

$$\dot{\epsilon}_x = \frac{12\sigma_x \Omega \omega D_g}{XY^2 kT(1+X/Y)} = A_c \sigma_x \quad (\text{A12})$$

Using equation (A4) this gives:

$$\dot{\epsilon}_{\max} = \frac{72M\Omega\omega D_g}{Zh^2 XY^2 kT(1+X/Y)} \quad (\text{A13})$$

The rotation rate assuming continuum creep is given by: $\dot{\theta}_c = 2\dot{\epsilon}_{\max} X/h$ and noting that $h = NY$, this gives for equi-axed grains ($X = Y$):

$$\dot{\theta}_c = \frac{72M\Omega\omega D_g}{ZY^2 h^3 kT} = \left(\frac{N^2}{10}\right) \dot{\theta}_{bicrystal} \quad (\text{A14})$$

where $\dot{\theta}_{bicrystal} = 720M\Omega\omega D_g / Zh^5 kT$ is the rotation rate of a bicrystal.

The rotation rate derived in the main body of the paper is of similar form to equation (A14).

Thus equations (25, 35 & 40) may be written in the form: $\dot{\theta} = \zeta \dot{\theta}_{bicrystal}$, where for the equi-axed case ($X = Y$), $\zeta = 1, 2.52$ and 4.85 for $N = 2, 4$ and 6 respectively. Other evaluations not shown here for reasons of space, give $\zeta = 7.99, 11.94$ and 167.1 for $N = 8, 10$ and 40 . The ratio $\dot{\theta} / \dot{\theta}_c = 10\zeta / N^2$ thus evaluates to $2.5, 1.57, 1.35, 1.25, 1.19$ and 1.04 with $N = 2, 4, 6, 8, 10$ and 40 respectively. Thus for equi-axed grains, the behaviour tends towards continuum creep with increasing N values. The ratio $\dot{\theta} / \dot{\theta}_c$ approaches unity for $N > 40$. The stress variation along AB , for the equi-axed case ($X = Y$) where $N = 40$ is shown in Fig.A1 alongside equivalent plots for a bicrystal and for continuum creep.

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Figures

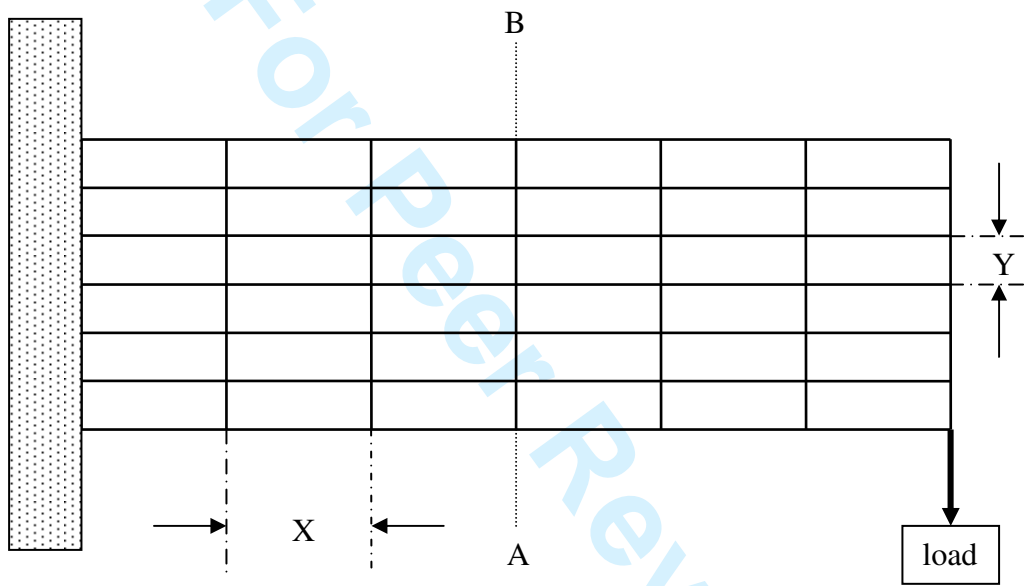


Fig.1 Representation of a simple polycrystalline beam undergoing creep bending.

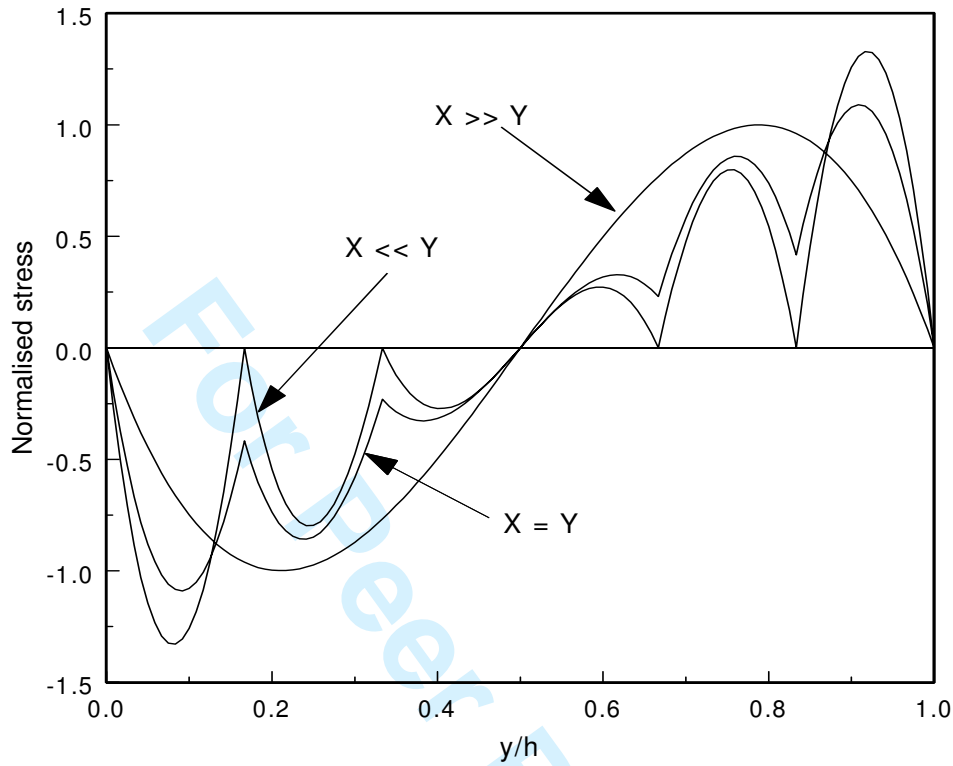


Fig.2 Variation of the local stress $\sigma(y)$ along the boundary AB as a function of the fractional distance y/h , for three different grain aspect ratios Y/X as labelled. The stress is represented in the normalised form $\sigma(y)/\sigma_{ref}$, where $\sigma_{ref} = 10M/3^{1/2}Zh^2$.

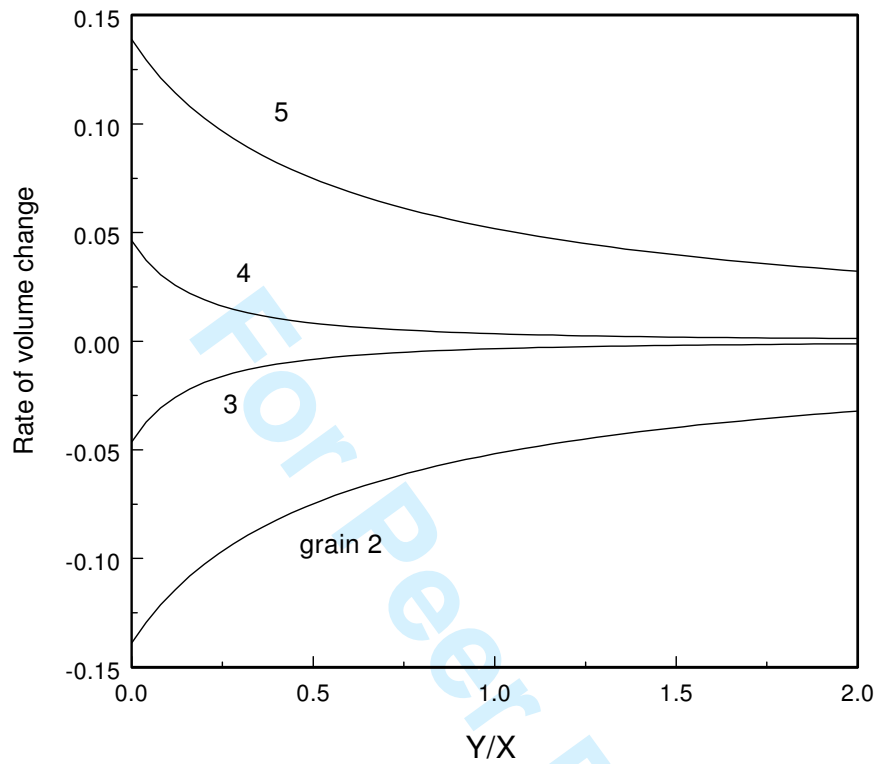


Fig.3 The rate of grain volume change, represented in the normalised form

$\dot{V}Y^3kT / M\Omega\omega D_g$, as a function of aspect ratio Y/X for grains 2-5 in a beam with $N = 6$.

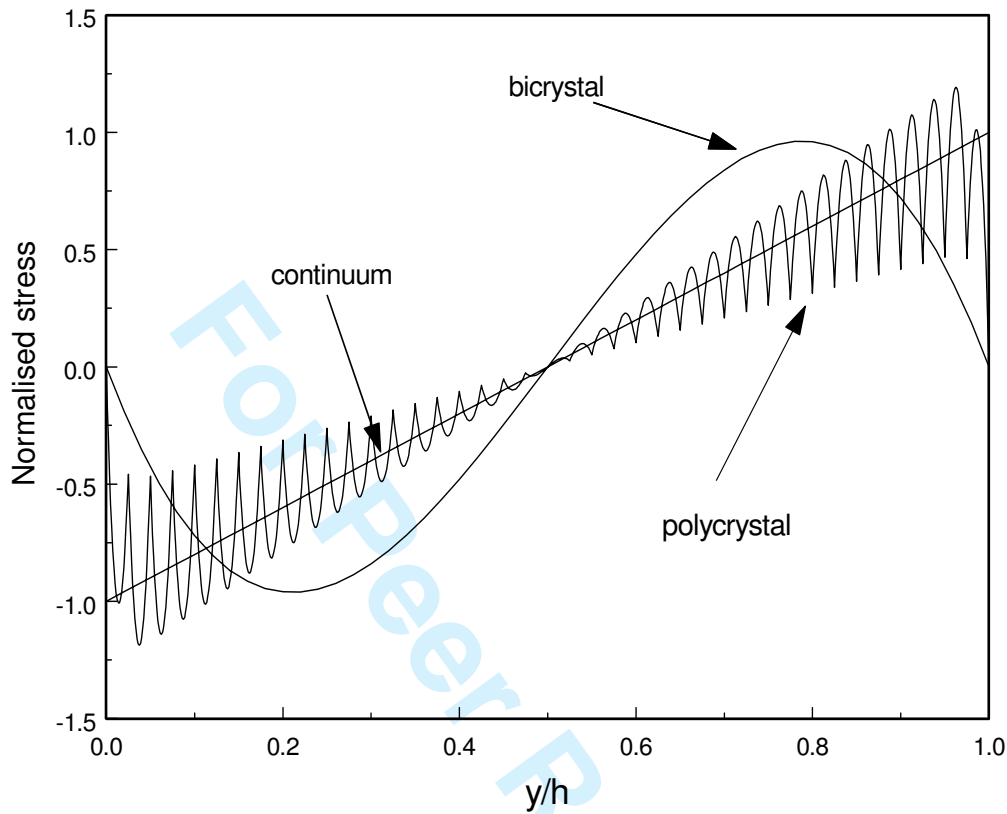


Fig.A.1 Variation of the local stress $\sigma(y)$ along the boundary AB as a function of the fractional distance y/h , for a beam with $N = 40$ and $Y/X = 1$. The stress is represented in the normalised form $\sigma(y)Zh^2/M$. The equivalent curves are shown for a bicrystal and a material undergoing continuum creep.