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Grain-boundary sliding controlled creep: its relevance to grain rolling and superplasticity

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A model of a polycrystal is developed which describes creep controlled by the rate of sliding on grain boundaries. Normal boundary stresses are assumed to relax rapidly by a mechanism which transfers material between boundaries to accommodate the sliding displacements. A self-consistent treatment of the shear stresses on the boundaries and the shears between grain centres only arises when the grains are allowed to roll or rotate. The calculated rates of rotation agree with rates observed during Stage II superplastic creep. Many features of the model tie in with the geometrical behaviour of grains deforming superplastically.

1. Introduction

Several papers have appeared recently calculating the creep rate of polycrystals when shear stresses acting on the boundaries are rapidly relaxed by grain-boundary sliding. The resulting inhomogeneous deformation can differ considerably from uniform material deforming homogeneously. Relaxing the boundary shear stresses to zero redistributes the normal boundary stresses. In this case, creep is controlled by the slower relaxation of the redistributed normal stresses [1–4].

The simplifying assumption common to the treatments is that movement of every grain centre corresponds exactly with the bulk strain in the aggregate, implying that the behaviour of one grain is indistinguishable from a neighbour and that co-operative movements of clumps of grains are absent. When a grain centre moves relative to a neighbour a change in distance between the centres can occur through plastic flow within the grain or diffusive plating of material at the boundary. If the grain centres move past each other parallel to their common boundary this can be achieved by shear within the grain or grain-boundary sliding. When sliding is present it must be accommodated by either of the first two processes. Diffusion creep and boundary sliding are mutually accommodating [5, 6].

The present paper also discusses the deformation of a polycrystalline aggregate but differs in treating the case of grain-boundary sliding control. The accommodating mechanism is assumed to be rapid diffusion between grain boundaries. The normal boundary stresses are quickly relaxed leaving the boundary shear stresses to support the aggregate. The much slower relaxation of the shear stresses then controls the creep rate. The physical details of the shear mechanism are not considered, but a phenomenological relationship is assumed between the boundary shear stress and the shear rate. The consequences of these assumptions are developed and it is shown that the shear stresses appearing on a grain are self-consistent only when the grains are allowed to roll over neighbours.

2. The properties of grain models

Real polycrystals are irregular and have a distribution of sizes making analysis difficult. They are often replaced by regular shapes such as hexagons, cubes or tetrakaidecahedra to ease calculations. When strained, the regular shapes deform and become irregular and so creep rates calculated for a particular geometry can be thought of as the instantaneous rate for that configuration.

Hexagonal arrays have strength when either the boundary shear stress or normal stress is relaxed to zero. They are also equally resistant to diffusion creep for all orientations of the hexagon to the applies stress [3]. Cubic grains behave quite differently. If either the normal or shear stress on the boundary is relaxed to zero the array has no strength, and will collapse like a soft plastic solid or a pack of cards for each case respectively. Strength is introduced into the array by mathematically forcing the cube centres to follow the bulk strain [4]. This is justified by saying the aggregate consists of a large number of arrays all at random orientations to the specimen axis. The movement of one array is modified by the movements available to nearby arrays. Since on average the orientations are random the bulk deformation is homogeneous. The stress supported by an array depends on its orientation, some orientations being stronger than others.

Hexagons and cubes have different properties but it is not clear which of these two extremes best represents real grains. It is quite likely that in real crystals, differences in strength do exist between small and large grains, particularly for diffusion creep processes, but the orientation dependence is not known.

Hexagonal grains are only two dimensional and cubic grains have four boundaries meeting at an edge. Despite these limitations, simple shapes are useful in discussing polycrystals. Cubes are the simplest three dimensional shape to analyse especially with regard to shear displacements between grain centres. Shear can be accomplished by sliding along one of the faces and unlike hexagons or tetrakaidecahedra normal stresses are not developed on the other faces. Whilst this may be a disadvantage when modelling a creep process controlled by the relaxation of normal boundary stresses this is not so in the present case. In the situation discussed, normal stresses are relaxed quickly and only the shear stresses need be considered.

3. Analysis

The model considers the shear stresses appearing on the faces of the cubic grains and the associated grain centre motion when the aggregate is deformed in uniaxial tension. The grains are considered to be rigid blocks with all deformation taking place in a

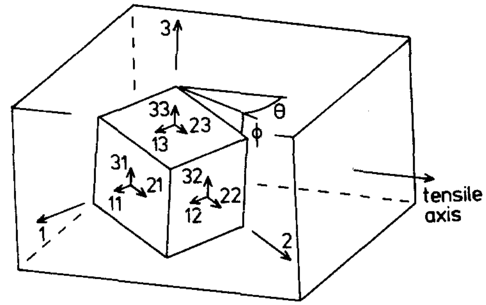

Figure 1 A cubic grain orientated randomly in a tensile specimen.

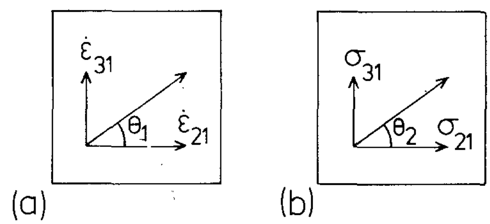

Figure 2 Face 1 of the cubic grain showing the sliding strains (a) and the shear stresses (b) appearing on the surface.

"mantle" on the outside of the grain. Thus, no shear takes place within the grain, and an ideal accommodating process for the boundary shear displacements is rapid diffusion creep. Fig. 1 shows the scheme with the cube orientated at some arbitrary angle to the applied stress; the forces and sliding displacements on face 1 are shown in Fig. 2. If the face is sliding in a particular direction, then the force resulting from the motion must be in the same direction. It follows that the angles θ_1 and θ_2 of Fig. 2 are identical and, if the stress and strain rate are related by a law of the type $\dot{\epsilon} = \lambda\sigma^n$, then the shear strain rate between cube centres is given by

$$\dot{\epsilon}^{s}_{21} = \lambda(\sigma_{31}^2 + \sigma_{21}^2)^{n/2} \cos\theta_2 . \quad (1)$$

Since no shear takes place within the grain, $\dot{\epsilon}^{s}_{21}$ is also the boundary shear velocity on the surface of a unit cube. θ_2 can be obtained from Fig. 2b, and the shear rate is

$$\dot{\epsilon}^{s}_{21} = \lambda\sigma_1^{n-1}\sigma_{21} \quad (2)$$

where

$$\sigma_1^2 = \sigma_{21}^2 + \sigma_{31}^2 , \quad (3)$$

or in general,

$$\dot{\epsilon}^{s}_{ij} = \lambda\sigma_j^{n-1}\sigma_{ij}, i \neq j. \quad (4)$$

Material continuity demands that the cross terms are equal, i.e. $\dot{\epsilon}^s_{12} = \epsilon^s_{21}$ etc. This however can be shown to be inconsistent if $\dot{\epsilon}^s_{12}$ and $\dot{\epsilon}^s_{21}$ are written in terms of the stresses

$$(\sigma_{31}^2 + \sigma_{21}^2)^{(n-1)/2}\sigma_{21} = (\sigma_{12}^2 + \sigma_{32}^2)^{(n-1)/2}\sigma_{12} \tag{5}$$

Since $\sigma_{21} = \sigma_{12}$ it follows $\sigma_{31} = \sigma_{32}$, provided $n = 1$. Repeating the process for faces 2 and 3 leads to the conclusion that all the shear stresses are equal, a situation which is clearly impossible.

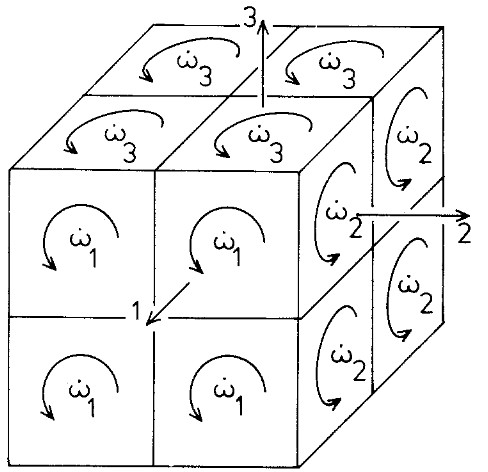

Figure 3 An array of cubic grains showing the system of rotations about the principal axes.

The anomaly is removed when the grains are allowed to rotate (Fig. 3) at angular rates $\dot{\omega}_1$, $\dot{\omega}_2$ and $\dot{\omega}_3$ about the three co-ordinate axis 1, 2 and 3 respectively. If $\dot{\epsilon}_{ij}$ replaces $\dot{\epsilon}^s_{ij}$ as the shear strain between grain centres, and $\dot{\epsilon}^s_{ij}$ is the sliding rate on the cube faces, then rotations and strains are related by

$$\begin{aligned}
\dot{\epsilon}_{12} &= \dot{\epsilon}^s_{12} - \dot{\omega}_3 \\
\dot{\epsilon}_{21} &= \dot{\epsilon}^s_{21} + \dot{\omega}_3 \\
\dot{\epsilon}_{23} &= \dot{\epsilon}^s{}_{23} - \dot{\omega}_1 \\
\dot{\epsilon}_{32} &= \dot{\epsilon}^s_{32} + \omega_1 \\
\dot{\epsilon}_{31} &= \dot{\epsilon}^s_{31} - \omega_2 \\
\dot{\epsilon}_{13} &= \dot{\epsilon}^s_{13} + \omega_2 .
\end{aligned} \tag{6}$$

When the aggregate is deformed, energy is dissipated by sliding on the boundary. The rates of rotation $\dot{\omega}_1$, $\dot{\omega}_2$ and $\dot{\omega}_3$ are chosen to reduce the energy expenditure to a minimum for a given cube-centre strain.

If W_1 is the rate of working on face 1 then

$$W_1 \propto [(\dot{\epsilon}^s_{31})^2 + (\dot{\epsilon}^s_{21})^2]^{1/2}(\sigma_{31}^2 + \sigma_{21}^2)^{1/2}, \tag{7}$$

or in terms of strains and rotations

$$\begin{aligned}
W_1 &\propto [(\dot{\epsilon}_{31} + \dot{\omega}_2)^2 + (\dot{\epsilon}_{21} - \dot{\omega}_3)^2]^{(1+n)/2n} \\
W_2 &\propto [(\dot{\epsilon}_{12} + \dot{\omega}_3)^2 + (\dot{\epsilon}_{32} - \dot{\omega}_1)^2]^{(1+n)/2n} \\
W_3 &\propto [(\dot{\epsilon}_{13} - \dot{\omega}_2)^2 + (\dot{\epsilon}_{23} + \dot{\omega}_1)^2]^{(1+n)/2n}
\end{aligned} \tag{8}$$

where W_2 and W_3 are the rates of working on faces 2 and 3 respectively. The total rate of energy dissipation is given by $W = W_1 + W_2 + W_3$ and the most favourable rotations are found by partially differentiating with respect to the rotations at constants cube-centre strain rate, i.e. $\partial W/\partial\dot{\omega}_1 = \partial W/\partial\dot{\omega}_2 = \partial W/\partial\dot{\omega}_3 = 0$. The derivative with respect to $\dot{\omega}_1$ is

$$\begin{aligned}
\frac{\partial W}{\partial\dot{\omega}_1} \propto {} & [(\dot{\epsilon}_{13} - \dot{\omega}_2)^2 \\
& + (\dot{\epsilon}_{23} + \dot{\omega}_1)^2]^{(1-n)/2n}(\dot{\epsilon}_{23} + \dot{\omega}_1) \\
& - [(\dot{\epsilon}_{12} + \dot{\omega}_3)^2 + (\dot{\epsilon}_{32} - \dot{\omega}_1)^2]^{(1-n)/2n} \\
& (\dot{\epsilon}_{32} - \dot{\omega}_1).
\end{aligned} \tag{9}$$

Next, the shear stresses are written in terms of the strain rates. Since the shear stresses are related to sliding strains by an equation of the type $\sigma = (\dot{\epsilon}^s/\lambda)^{1/n}$, σ_{23} is given by

$$\sigma_{23} = \left(\frac{1}{\lambda}\right)^{1/n} ((\dot{\epsilon}^s_{23})^2 + (\dot{\epsilon}^s_{13})^2)^{1-n/2n} \times \dot{\epsilon}^s_{23} \tag{10}$$

or in terms of grain centre strains and rotations

$$\begin{aligned}
\sigma_{23} = \left(\frac{1}{\lambda}\right)^{1/n} & [(\dot{\epsilon}^2_{13} - \dot{\omega}_2)^2 \\
& + (\dot{\epsilon}_{23} + \dot{\omega}_1)^2]^{(1-n)/2n}(\epsilon_{23} + \dot{\omega}_1),
\end{aligned} \tag{11}$$

and similarly for σ_{32};

$$\begin{aligned}
\sigma_{32} = \left(\frac{1}{\lambda}\right)^{1/n} & [(\dot{\epsilon}_{12} + \dot{\omega}_3)^2 + \\
& + (\dot{\epsilon}_{32} - \dot{\omega}_1)^2]^{(1/n)/2n}(\dot{\epsilon}_{32} - \dot{\omega}_1)
\end{aligned} \tag{12}$$

Equations 9, 11 and 12 show that $\sigma_{23} = \sigma_{32}$ implies that $\partial W/\partial\dot{\omega}_1 = 0$. Similarly, when $\sigma_{12} = \sigma_{21}$, $\partial W/\partial\omega_3 = 0$, and when $\sigma_{13} = \sigma_{31}$, $\partial W/\partial\omega_2 = 0$. Thus, when the cubes deform they follow the path of least energy expenditure, which simultaneously satisfies the balance of shear stresses on the cube faces.

The cubes were considered to be equally resistant to sliding on all faces. If, however, sliding is easier, say, on face 1 than face 2 the material parameter λ takes on different values λ_1, λ_2 and λ_3 for faces 1, 2 and 3 respectively. If the above arguments are repeated with the new values of sliding resistance the same conclusions are reached.

The relationship between the rate of grain rotation and specimen strain rate may be found as follows. The shear rate between cube centres is obtained by putting $\dot{\epsilon}_{ij} = \dot{\epsilon}_{ji}$ and adding the appropriate pairs of equations (Equation 6) to give

$$2\dot{\epsilon}_{ij} = \dot{\epsilon}^{s}_{ij} + \dot{\epsilon}^{s}_{ji} \qquad (13)$$

Subtraction gives the rates of rotation

$$2\dot{\omega}_1 = \dot{\epsilon}^{s}_{23} - \dot{\epsilon}^{s}_{32} \text{ etc.} \qquad (14)$$

Substituting stresses for strain rates from Equation 4 yields

$$2\dot{\epsilon}_{ij} = [\lambda_i \sigma_i^{n-1} + \lambda_j \sigma_j^{n-1}]\,\sigma_{ij},\ i \neq j \qquad (15)$$

for the strains, and for the rotations

$$2\dot{\omega}_j = [\lambda_i \sigma_i^{n-1} - \lambda_k \sigma_k^{n-1}],\ \sigma_{ij} i \neq k \qquad (16)$$

The correct sign is obtained by putting i, j, k equal to 1, 2 and 3 respectively and rotating cyclically. The shear strains between cube centres depend on the cube orientation θ, ϕ, (Fig. 1). When the aggregate deforms uniaxially the strain rates between cube centres are

$$\begin{aligned} \dot{\epsilon}_{12} &= -1.5\dot{\epsilon} \sin\theta \cos\theta \cos\phi \\ \dot{\epsilon}_{23} &= 1.5\dot{\epsilon} \cos^2\theta \sin\phi \cos\phi \\ \dot{\epsilon}_{31} &= -1.5\dot{\epsilon} \sin\theta \cos\theta \sin\phi \end{aligned} \qquad (17)$$

Substituting the trigometrical relationships for the strains (Equations 17) into Equation 15 gives three simultaneous equations with unknowns σ_{ij}, $i \neq j$. These can be solved numerically for particular values of θ and ϕ. The solutions are in terms of $\dot{\epsilon}$ and λ_k and when substituted into Equation 6 give the rotations in terms of the strain $\dot{\epsilon}$.

4. Results and discussion

The rate of grain rotation was first calculated for a cube with all boundaries equally resistance to sliding, i.e. $\lambda_1 = \lambda_2 = \lambda_3$. The rotation about the 3 axis is shown in Fig. 4, for cube orientations within the range $0 < \theta < \pi/2$ and $0 < \phi < \pi/2$ and for a stress exponent n of 2. The rate of rotation is

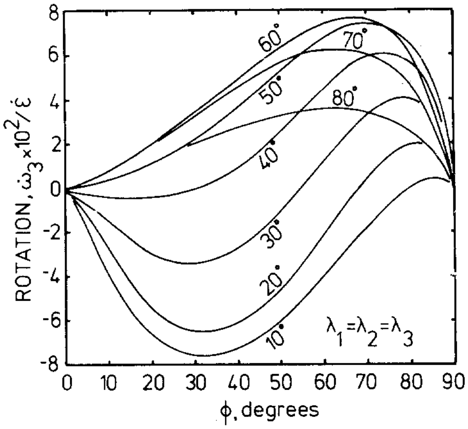

Figure 4 The rate of grain rotation about axis 3, when all grain faces are equally resistance to sliding. The angle specified are values of θ, Fig. 1.

quoted in terms of the strain rate. The relationship between the strain rate and the boundary sliding resistances λ_1, λ_2 and λ_3 is not calculated, but the bulk strain rate will be proportional to the square of the applied stress. As intuitively required, the rotations are zero when $\theta = \phi = 0$ but otherwise depend on the cube orientation. The maximum rate of rotaion is about $0.07\dot{\epsilon}$. Thus, even if a grain is maintained at the optimum angle for a strain of unity the rotation will still only be 0.07 radians or 4°. The rotations about the 1 and 2 axis are similar but with different symmetry.

The effect of stiffening face 1 by a factor of 2 ($\lambda_1 = 0.5\lambda_2^2$, $\lambda_2 = \lambda_3$) is shown in Fig. 5. This increases the rate of rotation about axis 3 and alters the shape of the curves. Rotation about axis 2 is similar but the rate for axis 1 is not increased as much.

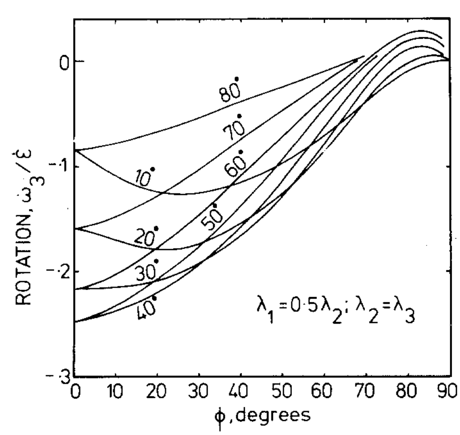

Figure 5 The rate of grain rotation about axis 3, with face 1 of the cube twice as resistant to slip as faces 2 and 3.

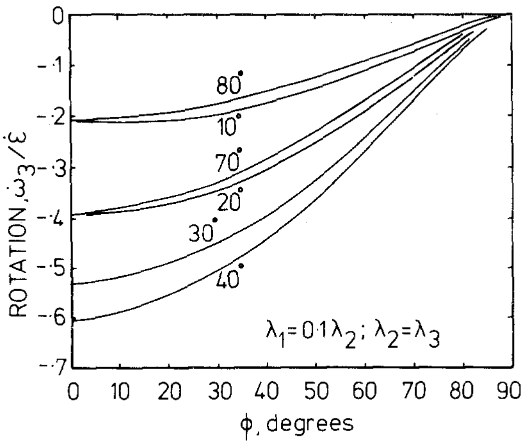

Figure 6 The rate of grain rotation about axis 3, with the face 1 of the cube ten times more resistant to slip as faces 2 and 3.

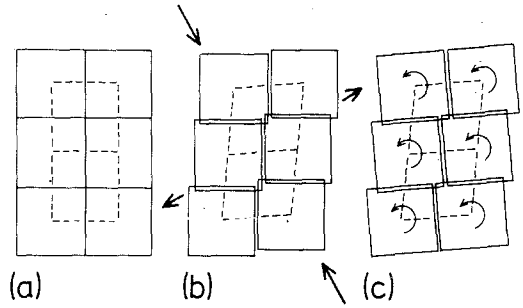

Figure 7 A 2-dimensional section of the cubic grains. The grain centres are joined by dotted lines. The undeformed grains (a) are deformed uniaxially (b) producing sliding on all faces and transfer of material from horizontal to vertical boundaries. If sliding on the vertical faces is difficult this is reduced whilst maintaining the same grain centre positions by rotating the grains (c).

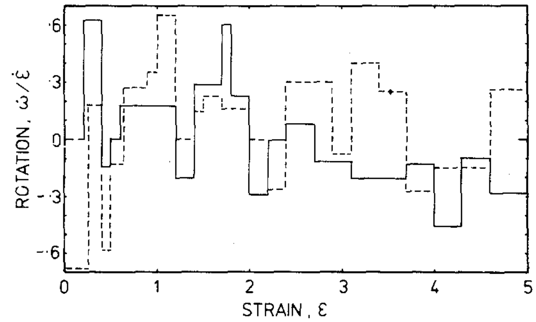

Figure 8 The observed rotations of surface grains on a tensile specimen deformed in superplastic creep *in situ* in a scanning electron microscope [7].

A further increase in sliding resistance to a factor of 10 ($\lambda_1 = 0.1\lambda_2$, $\lambda_2 = \lambda_3$) increases the rates of rotation still further (Fig. 6). Again rotation about axis 2 is similar, whilst rotation axis 1 is much smaller.

Before proceeding with the discussion, it is worth considering a simpler 2-dimensional model to see how the grain rotation arises. Fig. 7a illustrates six cubes with their centres joined by dashed lines. The cubes are deformed uniaxially and the centres move to new positions (Fig. 7b). The accommodating process has to move material from the horizontal to the vertical faces. Sliding takes place on both types of face and the grains are shown without rotation. If, however, sliding is much more difficult on the vertical faces the same grain centre positions can be achieved without sliding along the vertical boundaries. This is illustrated in Fig. 7c. The extra work in the larger sliding displacement on the horizontal boundaries is more than compensated by the reduced sliding on vertical faces resulting from grain rotation.

The rates calculated for the 3-dimensional model can be compared with measurements made in the scanning electron microscope [7]; observations of the surface of creep specimens, deformed superplastically *in situ* showed the grains experienced large rotations. The angular variation with strain has been differentiated, Fig. 8, to give the rate of rotation. The observations do not form smooth curves because the rate is the average value between successive measurements of angle. The rates vary cyclically with a period of about unit strain reaching a maximum of about $0.6\dot{\varepsilon}$. The maximum observed rate and the maximum calculated rate can be compared directly. This suggests that the boundary resistance must vary by a factor of 10 (Fig. 6) to produce the observed maximum rate. Obviously this is a rough comparison, but an assessment of all feasible sliding resistances would be lengthy, and it is fairly clear that grain rotational rates of this order can result from differences in sliding resistance.

It is also worth considering whether the differences in sliding resistance arise from the intrinsic properties of high-angle boundaries, or are caused by a total lack of resistance at the outermost face of a surface grain. If face 1, Fig. 3, is taken to be the exterior face, then it is the average value of λ_1 which will be altered. The analysis showed that altering the sliding resistance on face 1 affects rotations about axis 2 and 3, leaving rotations about 1 little affected. This can be seen intuitively from Fig. 3 by looking down axis 1. Since the outermost grain and the one beneath do not rotate about axis 1 relative to each other, the sliding resistance on face 1 does not directly affect this mode of rotation. Observed rotations are about axis 1, however, and we must conclude that large rotations result from differences in sliding resistance on faces 2 and 3. This is in agreement with the 2-dimensional model which can be considered to be a section of the cubic array viewed along axis 1.

The resistance-to-sliding along boundaries has been measured directly in bi-crystals. The variation with misorientation can be large [8] as can the interspecimen variation between nominally identical bicrystals. A factor of 10 variation between slip resistance is physically reasonable.

Unfortunately theoretical models of corrugated boundaries may not be applicable to the present model. A 10-to-1 variation in boundary viscosity would easily be achieved by varying the corrugation. In the present model, rapid diffusion across the grain has been invoked as the most suitable accommodating mechanism. Since the path difference across the corrugations is much smaller than the grain-size, sliding by this mechanism would be very rapid indeed. Also the shear rate would vary linearly with shear stress.

The creep process developed describes the motion of rigid grains of material which slide past each other. The redistribution of material necessary to accommodate sliding takes place in or near the boundary region leaving the grains undeformed in their interior. When the rate-controlling boundary shear process depends on (shear stress)^2 the grains rotate. The above conditions are often satisfied during stage II superplastic creep (see a recent review, [9]. Stage II is characterized by an apparent stress exponent of 2. Low dislocation density within the grains and an absence of slip bands imply little plastic deformation within the grain. Also surface scratches remain straight and reveal sharp grain-boundary sliding offsets. Superplasticity is observed in materials with a grain size d, usually less than 10 μm. The creep rate varies as $1/d^{1/2}$ to $1/d$ whereas diffusion creep varies as $1/d^2$ or $1/d^3$ for volume and grain-boundary diffusion respectively. Decreasing the grain size increases the rate of a diffusion creep process faster than the observed increase in superplastic creep rate. At a sufficiently small grain size it is reasonable to invoke rapid diffusion creep as an accommodating process. The observed rates of grain rotation are in agreement with the rates calculated for the boundary sliding mechanism. The rotation results in grains rolling over neighbours, and this will facilitate grain switching [10] and the maintenance of a nearly equiaxed structure.

Many rate-controlling mechanisms have been proposed for superplastic creep including various types of dislocation creep, diffusion creep with a threshold stress as well as grain-boundary sliding.

Any theory describing superplastic flow must account for the microstructural changes as well as describing the creep rate. Grain-boudnary sliding is the only rate-controlling process which produces a significant grain rotation. The rotation will not occur when sliding is rapid accommodating mechanism. Consequently sliding appears to be the most likely rate-controlling process during stage II superplastic creep.

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