A Model for Superplasticity not Controlled By Grain Boundary Sliding

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Foreword

It is a distinct privilege and honor for us to contribute to a volume honoring Professor F.R.N. Nabarro and his work on the occasion of his 90th birthday. Anyone with experience in the field of materials science (called metal physics 50 years ago) will immediately recognize the name F.R.N. Nabarro. His is a household name in our field and his work influences progress in the field on a daily basis. His great contribution, of course, was his recognition that deformation of crystalline solids could occur by the diffusive flow of atoms or vacancies from one place to another in a solid. His diffusional creep stands as one of the great materials science achievements of the 20th century. This was just the first in a long series of major contributions to the field of materials science that have shaped the field for the past 50 years. The present contribution is an attempt to follow the teachings of Nabarro and to show that diffusional processes, together with dislocation processes in crystals, can conspire to produce superplastic deformation properties that others have attributed to grain boundary sliding. It is an attempt to describe superplasticity in a way that Nabarro himself might like, even though he has not seen this meager effort and cannot be held responsible for it.

Abstract

A core-mantle model for superplasticity not controlled by grain boundary sliding is proposed. It is suggested that crystal deformation in the mantle, in the vicinity of grain boundaries, is controlled by the annihilation of oppositely signed dislocations that climb together in the plane of the grain boundary and involve grain boundary diffusion. In the grain interior or core, dislocation climb and power law creep is controlled by lattice diffusion. We use the stress dependent sub-grain size relative to the grain size to describe the transition from grain boundary-diffusion-controlled power law creep at low strain rates to lattice-diffusion-controlled power law creep at high strain rates. We explore the transitions between these limiting behaviours using iso-strain rate and iso-stress models and conclude that a phenomenological model, which limits the predictability of the model, is needed to describe the transitions adequately. The behaviours predicted by the model are reminiscent of the three stages of deformation in superplastic alloys, giving a good account of the temperature and grain size dependence of the strain rate sensitivity for superplastic alloys.

1. Introduction

It is well known that grain boundaries in polycrystalline solids are a source of weakness at elevated temperatures and also that grain boundary sliding can occur on individual grain boundary facets. This has led to the widely held view that grain boundary sliding can be a controlling deformation process in fine-grained solids at elevated temperatures. In particular, a common view is that superplasticity is controlled by grain boundary sliding. As early as 1952 Rachinger [1] suggested that deformation of polycrystalline solids could occur by grain boundary sliding and the movement of grains relative to each other in the course of deformation. This was an attempt to explain how grains in a polycrystalline solid could retain their size and shape after extensive plastic flow at elevated temperatures. Later observations showed that grains in superplastic alloys also retain their size and shape, even after enormous strains. These observations led Ashby and Verrall [2] and others to suggest that superplasticity could be understood as a diffusionally accommodated process in which grains slide relative to each other and switch their neighbors in the course of deformation. This view of superplasticity was supported by observations that little dislocation substructure is typically observed in superplastically deformed solids and that individual grains on the surfaces of deforming tensile samples retain their size and shape and move apart in the course of superplastic flow.

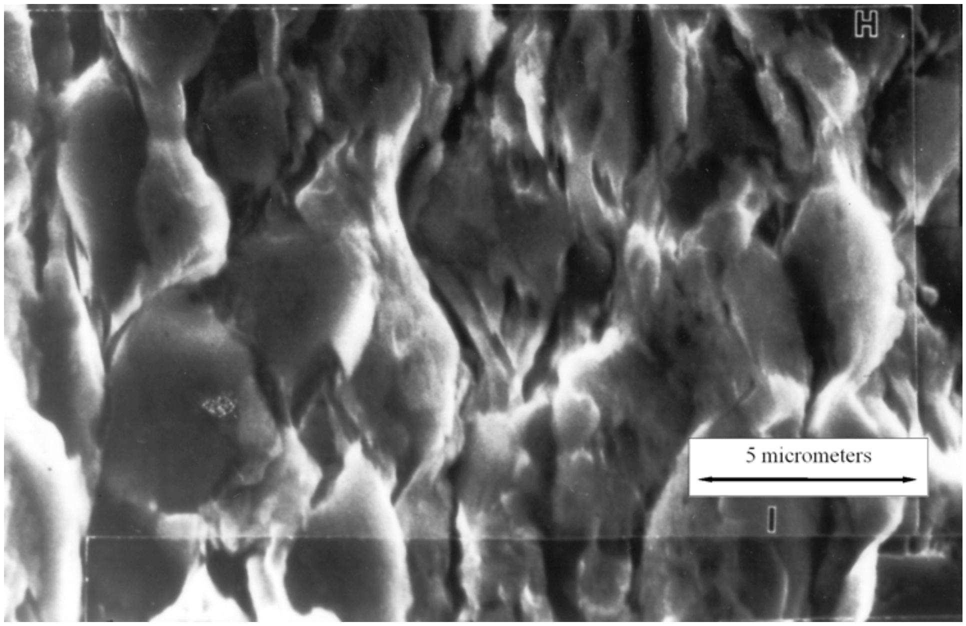

Figure 1. Grain morphologies on the cylindrical surface of a fine-grained Sn-38%Pb alloy after superplastic deformation in torsion to a true strain of more than 100%. Extensive plastic deformation occurs at the grain boundary junctions, or ligaments, between the grains.

A rather different picture of superplastic flow emerges from SEM observations of the surfaces of cylindrical samples deformed in torsion [3]. Because the surface area of a cylindrical sample remains essentially constant in the course of torsional deformation, the number of grains on that surface is fixed and the deformation of each grain can be directly observed. Figure 1 shows the shapes of the surface grains in a fine-grained Sn-38%Pb alloy after superplastic deformation to a true strain of more than 100%. All of the grains appear to be extensively deformed, especially at the grain boundary junctions, or ligaments, between the grains. As described earlier [3], the grains appear to adopt an "hourglass" shape in the course of superplastic flow. This is in contrast to the picture that emerges from SEM observations of the surfaces of deformed tensile samples, where the surface area changes in the course of deformation. There, new material must come from the interior of the sample to the surface during the course of superplastic flow, separating grains that were initially present there and, in some cases, pushing those grains out of the plane of the surface and causing them to act as "floating markers" which do not deform with further straining. We believe that Fig. 1 gives a better view of superplastic flow, one that is applicable to the bulk of the solid. Our approach to superplasticity is based partly on this observation.

Of course, on average, the interior grains of superplastic alloys do remain equiaxed and appear to retain their size and shape after extensive tensile elongation; other mechanisms are needed to explain this. We believe that grain boundary and phase boundary migration are responsible for this, continually reshaping grains in the course of deformation and maintaining an equiaxed grain structure, much in the manner suggested by Lee [4]. Indeed, support for the idea that grain boundary migration accompanies superplastic flow is found in the work of Seidensticker and Mayo [5] who showed that the superplastic strain rate scales almost perfectly with the rate of grain growth for a wide variety of superplastic metals and ceramics.

Even though dislocation substructures are often not seen in superplastically deformed solids, suggesting that dislocation slip might not occur in the grain interiors, the observations of crystallographic texture changes in the course of superplastic flow suggest otherwise. As early as 1974 Cutler et al. [6] observed crystallographic texture changes in superplastically deformed Al-Cu and suggested that dislocation slip must be occurring. This was followed later by the work of Matsuki et al. [7] and Kaibyshev et al. [8] who studied texture changes after superplastic deformation of a number of alloys and concluded that slip in the grain interiors must be occurring. Our approach to superplasticity is also based partly on these observations.

It should not be necessary to remind the reader that grain boundary sliding itself is rarely a rate controlling process in high temperature deformation. As illustrated in Fig. 2 the sliding of grain boundaries in polycrystalline solids needs to be accommodated either by diffusional flow or by dislocation slip in the adjoining grains. Grain boundary sliding accommodated by diffusional flow is usually called Lifshitz sliding [9], to distinguish it from Rachinger sliding as described above. Only for the case of a bicrystal might the deformation be controlled by the rate of sliding itself, and even then local accommodation processes would be required if the boundary is not perfectly flat [10]. We are, of course, not denying that grain boundary sliding occurs in the course of superplastic flow. Instead we are suggesting that the accommodation process and not the sliding itself is rate controlling. Indeed, essentially all previous models of superplastic flow, from Ball and Hutchinson [11] onward, have been based on the idea that the accommodation process controls the rate of deformation.

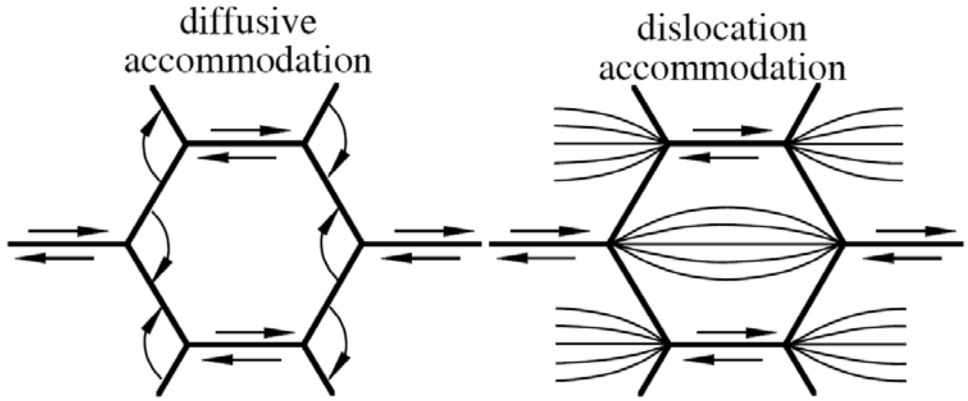

Figure 2. Illustration of both diffusional and dislocation accommodation of grain boundary sliding in a polycrystalline solid.

While there is extensive evidence to support the prevailing view of superplasticity in terms of grain switching, as described above, we believe that many of the characteristics of superplasticity can be explained without considering grain boundary sliding or grain switching as controlling mechanisms. Our approach is based on the idea that crystal deformation by dislocation motion in the vicinity of grain boundaries can be controlled by grain boundary diffusion while deformation by dislocation creep in the grain interiors is controlled by lattice diffusion. Following the approach taken by Spingarn and Nix [12], we assume that crystal deformation in the vicinity of grain boundaries is controlled by the annihilation of oppositely signed dislocations that climb together in the plane of the grain boundary. This naturally involves grain boundary diffusion. In the grain interiors, far from the grain boundaries, dislocation creep is controlled by lattice diffusion. While there are many models of lattice-diffusion-controlled creep that one might use for the grain interior, we use the recent model of Viswanathan et al. [13] involving lattice-diffusion-controlled drag of jogs by moving screw dislocations, as it involves only one adjustable parameter. We further assume that the transition from lattice-diffusion-controlled deformation at high strain rates to grain boundary-diffusion-controlled dislocation creep at low strain rates is controlled by the size of the sub-grains relative to the grain size. At high strain rates the sub-grain size is small relative to the grain size and deformation is controlled completely by creep processes in the grain interior. At low strain rates, the sub-grain size approaches the grain size, with the consequence that little substructure is created in the grain interiors and creep is controlled by grain boundary processes. We use the core-mantle terminology of Gifkins [14] and refer the grain interiors as the core and the material near the grain boundaries as the mantle. The thickness of the grain boundary mantle is assumed to be equal to the sub-grain size so that the volume fraction of the mantle grows with decreasing stress and strain rate. The transition from grain boundary-diffusion-controlled slip creep at low strain rates to lattice-diffusion-controlled dislocation creep at high strain rates leads naturally high strain rate sensitivities in the transition. The behaviours predicted by this model are reminiscent of the three stages of deformation in superplastic alloys.

We start the paper by describing the model in detail and writing the constitutive equations to be used for the core and mantle regions. The derivation of the constitutive law for the mantle follows the development of Spingarn and Nix [12], but is re-derived in a slightly different way in the Appendix. We then consider the problem of predicting the composite response of this two-phase model. We show that the usual iso-strain rate and iso-stress laws for predicting the composite response lead to widely separated bounds, neither of which appears to be realistic. This leads to the introduction of a phenomenological law for describing the transition from core-controlled to mantle-controlled deformation. The model is then used to describe the temperature and grain size dependence of flow in fine-grained polycrystalline solids, using Pb as the basis for the calculations but expressing the results in reduced-dimensional form. Superplastic-like characteristics are revealed by these calculations. We conclude the paper by discussing the strengths and limitations of the present approach and pointing out the need for a more serious treatment of the mechanics of the transition from core-controlled flow at high strain rates to mantle-controlled flow at low strain rates.

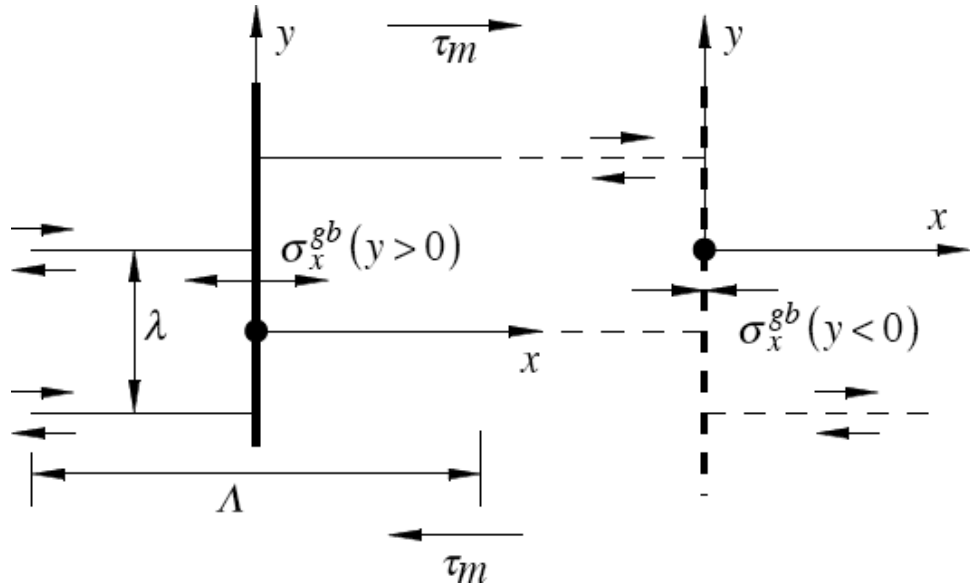

Figure 3. Slip band model for the mantle showing the normal stresses that develop on the intersected grain boundary. The rate of slipping is controlled by grain boundary diffusion from regions of compression to regions of tension. The mantle is extended to an imaginary domain to facilitate a force balance calculation.

2. Dislocation Creep in the Vicinity of Grain Boundaries – The Mantle Flow Law

Consider a grain boundary in a polycrystalline solid having sub-grains of size Λ, subjected to a shear stress, τ_m, as shown in Fig. 3. Following the method of Spingarn and Nix [12], we assume that dislocation slip near the grain boundary is controlled by climb and annihilation of oppositely signed dislocations in the grain boundary. We model slip as freely slipping planes spaced a distance λ apart as shown in the figure. Load transfer from the freely slipping planes leads to normal stresses on the intersecting grain boundary. A simple free body analysis of the forces leads to

$$2\tau_m\lambda = \int_0^{\lambda/2} \sigma_x^{gb} dy + \int_{-\lambda/2}^{0} \sigma_x^{gb} dy, \tag{1}$$

and because symmetry requires

$$\begin{aligned} \int_0^{\lambda/2} \sigma_x^{gb} dy &= 2\int_0^{\lambda/4} \sigma_x^{gb} dy \\ \int_{-\lambda/2}^{0} \sigma_x^{gb} dy &= 2\int_{-\lambda/4}^{0} \sigma_x^{gb} dy \end{aligned}, \tag{2}$$

we have

$$\tau_m \lambda = \int_0^{\lambda/4} \sigma_x^{gb} dy + \int_{-\lambda/4}^{0} \sigma_x^{gb} dy, \tag{3}$$

as expressed by Spingarn and Nix [12]. In the Appendix we show that the normal stresses acting on the grain boundary drive atomic flow along the grain boundary from the regions of compression to the regions of tension and that this process regulates the slipping rate. In steady state, the grain separation (or approach) rate, $\dot{u}$, at the grain boundary is directly related to the overall shear strain rate through

$$\dot{\gamma}_m = \frac{2\dot{u}}{\lambda} \ . \tag{4}$$

In the Appendix we show that the stress-driven diffusion analysis leads to the following constitutive law for grain boundary-diffusion-controlled deformation in the mantle:

$$\dot{\gamma}_m = \frac{192\Lambda}{\lambda^4} \frac{\tau_m \Omega}{kT} \delta_{gb} D_{gb} , \tag{5}$$

where kT has the usual meaning, Ω is the atomic volume and δ_{gb} and D_{gb} are the thickness and atomic diffusivity, respectively, of the grain boundary. This expression is almost identical to the one developed by Spingarn and Nix [12] based on vacancy flow.

Both the slip band spacing and the sub-grain size are expected to depend on stress. Following the observations of Staker and Holt [15] we take the slip band spacing and sub-grain size to be

$$\lambda = \frac{5\mu b}{\tau_m} \tag{6}$$

and

$$\Lambda = \frac{10\mu b}{\tau_m} \tag{7}$$

where μ is the elastic shear modulus and b is the magnitude of the Burgers vector. Using these relations in equation (5) leads to the following law for steady state flow in the mantle region:

$$\dot{\gamma}_m = 3.07\frac{\mu\Omega}{kT}\left(\frac{\tau_m}{\mu}\right)^4\frac{\delta_{gb}D_{gb}}{b^3}. \qquad (8)$$

This law for the mantle is expected to apply when the sub-grain size is smaller than the grain size, L. Below the critical stress

$$\tau_{crit} = \frac{10\mu b}{L}, \qquad (9)$$

where the sub-grain size is equal to the grain size, the sub-grain size in equation (5) should be replaced by the grain size and this leads to

$$\dot{\gamma}_m = 0.307\frac{\mu\Omega}{kT}\frac{L}{b}\left(\frac{\tau_m}{\mu}\right)^5\frac{\delta_{gb}D_{gb}}{b^3}\ (for\,\tau_m < \tau_{crit}). \qquad (10)$$

At very low stresses, where the slip band spacing approaches the grain size, $\lambda = L$, purely diffusional flow in the form of Coble creep would begin to dominate.

3. Dislocation Creep in the Grain Interiors – The Core Flow Law

We adopt the model of Viswanathan et al. [13] to describe power-law creep in the grain interiors. These authors showed that the jogged-screw model of dislocation creep could describe the creep properties of γ-TiAl very well if the stress dependence of the jog height, neglected in earlier versions of this model, is taken into account. The beauty of their model is that only the jog spacing, *s*, is not known with certainty and has to be used as a fitting parameter. Other models of power-law creep could be used in the present analysis but the jogged-screw model of Viswanathan et al. [13] is sufficient for our purposes.

In the power-law creep regime the model of Viswanathan et al. [13] can be expressed as

$$\dot{\gamma}_c = 3.5x10^3\frac{\mu\Omega}{kT}\frac{s}{b}\left(\frac{\tau_c}{\mu}\right)^5\frac{D_L}{b^2}, \qquad (11)$$

where all of the terms have been defined above except for the jog spacing, s, and the lattice diffusivity, D_L. The subscript *c* denotes the core region.

4. The Transion from Core-Controlled to Mantle-Controlled Flow

We now address the problem of the transition from core-controlled flow at high strain rates to mantle-controlled flow at low strain rates. We start by noting that above the critical stress, $\tau_{crit} = 10\mu b / L$, and thinking of spherical grains with spherical cores, the volume fraction of the core and mantle might be expressed as

$$f_c = \left(1 - \frac{\Lambda}{L}\right)^3 = \left(1 - \frac{10\mu b}{\tau L}\right)^3 = \left(1 - \frac{\tau_{crit}}{\tau}\right)^3, \qquad (12)$$
$$f_m = 1 - f_c$$

such that $f_c = 0$ and $f_m = 1$ at $\Lambda = L$ and $\tau = \tau_{crit}$. Next we need to develop a composite law for flow in the transition between mantle-controlled creep and core-controlled creep. Following the method of Tanaka et al. [16], who studied creep of ductile two-phase alloys, we might assume an iso-strain rate condition for the two phases, $\dot{\gamma} = \dot{\gamma}_c = \dot{\gamma}_m$, and compute the composite stress using a rule of mixtures approach:

$$\tau = f_c \tau_c + f_m \tau_m, \qquad (13)$$

which, using equations (8) and (11), leads to

$$\frac{\tau}{\mu} = f_c \left(\frac{\dot{\gamma} b^3 kT}{3.5x10^3 s\mu\Omega D_L} \right)^{1/5} + f_m \left(\frac{\dot{\gamma} b^3 kT}{3.07\mu\Omega\delta_{gb} D_{gb}} \right)^{1/4}. \qquad (14)$$

Alternatively one might use an iso-stress condition, $\tau = \tau_c = \tau_m$, and use a rule of mixtures to obtain the composite strain rate

$$\dot{\gamma} = f_c \dot{\gamma}_c + f_m \dot{\gamma}_m, \qquad (15)$$

which with equations (8) and (11) becomes

$$\dot{\gamma} = f_c \left(3.5x10^3 \frac{\mu\Omega}{kT} \frac{s}{b} \left(\frac{\tau}{\mu}\right)^5 \frac{D_L}{b^2} \right) + f_m \left(3.07 \frac{\mu\Omega}{kT} \left(\frac{\tau}{\mu}\right)^4 \frac{\delta_{gb} D_{gb}}{b^3} \right), \qquad (16)$$

even though this seems less satisfactory on physical grounds. To assess these different treatments of the transition we make explicit calculations of the stress-strain rate relation for a sample of pure Pb with a grain size of 10 μm. The following properties of pure Pb are used for these calculations and for others shown in this paper:

$b = 0.349\,nm$, $D_L = 1.4x10^{-4} \exp(-Q_L / RT)(m^2 / s)$, $Q_L = 109 kJ / mol$,
$D_{gb} = 2.29x10^{-4} \exp(-Q_{gb} / RT)(m^2 / s)$, $Q_{gb} = 66\,kJ / mol$, $\delta_{gb} = b$,

all taken from the book by Frost and Ashby [17]. In addition, we take the jog spacing in the model of Viswanathan et al. [13] to be $s = 200b$. With these material properties the predicted transitions for the iso-strain rate and iso-stress assumptions are as shown in Fig. 4. We see immediately that the bounds represented by these two models for the transition are far apart and neither looks very realistic. The transition for iso-strain rate looks too abrupt while the transition for iso-stress looks too gradual. While the iso-strain rate model might seem more appropriate on physical grounds the sketch shown in Fig. 5 shows that at intermediate volume fractions the core may not deform as much as the mantle. Without a good treatment of the mechanics of this transition we are forced to use a phenomenological treatment to describe the transition from mantle-controlled to core-controlled creep. For the present paper we use the following model, patterned after the iso-strain rate model but adjusted to create gradual transitions:

$$\frac{\tau}{\mu} = \left(1 - \frac{10\mu b}{\tau L}\right)^6 \left(\frac{\tau}{\mu}\right)_c + \left(1 - \left(1 - \frac{10\mu b}{\tau L}\right)^6\right)\left(\frac{\tau}{\mu}\right)_m , \tag{17}$$

where

$$\left(\frac{\tau}{\mu}\right)_c = \left(\frac{\dot{\gamma} b^3 kT}{3.5x10^3 s\mu\Omega D_L}\right)^{1/5} , \tag{18}$$

and

$$\left(\frac{\tau}{\mu}\right)_m = \left(\frac{\dot{\gamma} b^3 kT}{3.07 \mu\Omega\delta_{gb} D_{gb}}\right)^{1/4} . \tag{19}$$

The reader will note that a phenomenological exponent of 6 is used in equation (17) in place of 3 for the iso-strain rate law. The results for this phenomenological treatment of the transition are also shown in Fig. 4. As noted above, equation (10) is used to describe the flow behaviour below the critical stress, τ_{crit}, where the sub-grain size becomes equal to the grain size. Also shown in the figure is the law for purely diffusional creep in the form of the Coble creep equation. This limit will be omitted from subsequent plots, though its position can be determined from the knowledge that the lowest strain rates shown in the subsequent plots are the points where the Coble creep equation produces equal strain rates.

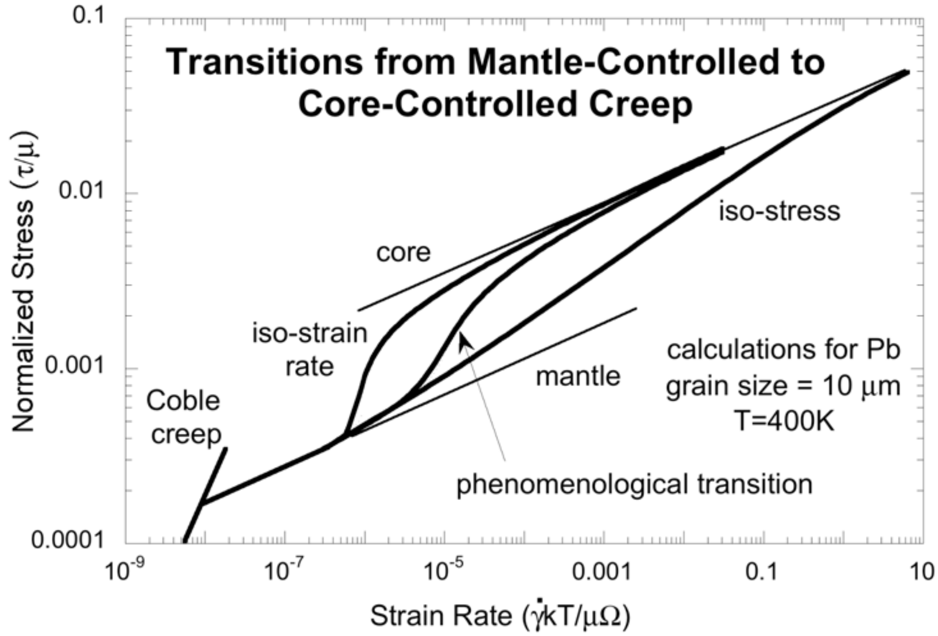

Figure 4. Iso-strain rate and iso-stress predictions of the transition from mantle-controlled creep to core-controlled creep, calculated for Pb with a grain size of 10 μm at T=400K. Also shown is the more gradual transition described by the phenomenological law. The position of the Coble creep law is shown for reference.

5. Superplastic-Like Predictions of the Model

The stress-strain rate relations predicted for Pb with a grain size of 10 μm at three different temperatures are shown in Fig. 6, where the stress and strain rate are expressed in normalized form. The model shows a transition from grain boundary-diffusion-controlled dislocation creep at low strain rates to lattice-diffusion-controlled creep at high strain rates. The separation between the nearly linear portions of the curves reflects the controlling activation energy in those two regimes. The transition from mantle-controlled creep to core-controlled creep leads naturally to a transitional regime where the strain rate sensitivity (the slopes of these curves) reaches a maximum. Figure 7 shows the predicted strain rate sensitivities, again for the three temperatures as a function of the strain rate. We note that the maximum strain rate sensitivities range from about 0.4 to nearly 1 for these conditions. These characteristics bear a striking resemblance to the properties of superplastic alloys. The predicted grain size dependence of deformation at T=450K is shown in Fig. 8. Here one sees the expected result that the transition occurs at higher strain rates for smaller grain sizes. Choosing smaller grain sizes for the modeling, as might be required for some superplastic alloys, would simply shift these transitions to higher reduced strain rates.

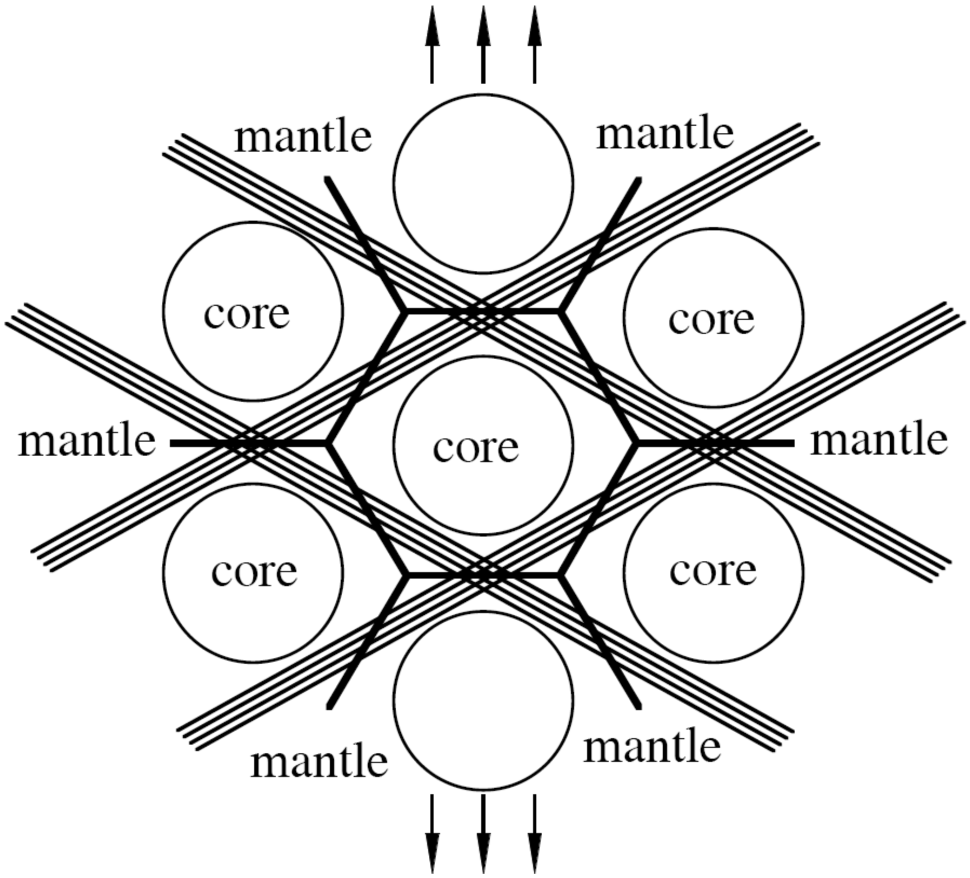

Figure 5. Illustration of the expected inhomogeneous deformation of the core-mantle microstructure, showing how the core need not deform at the same rate as the mantle.

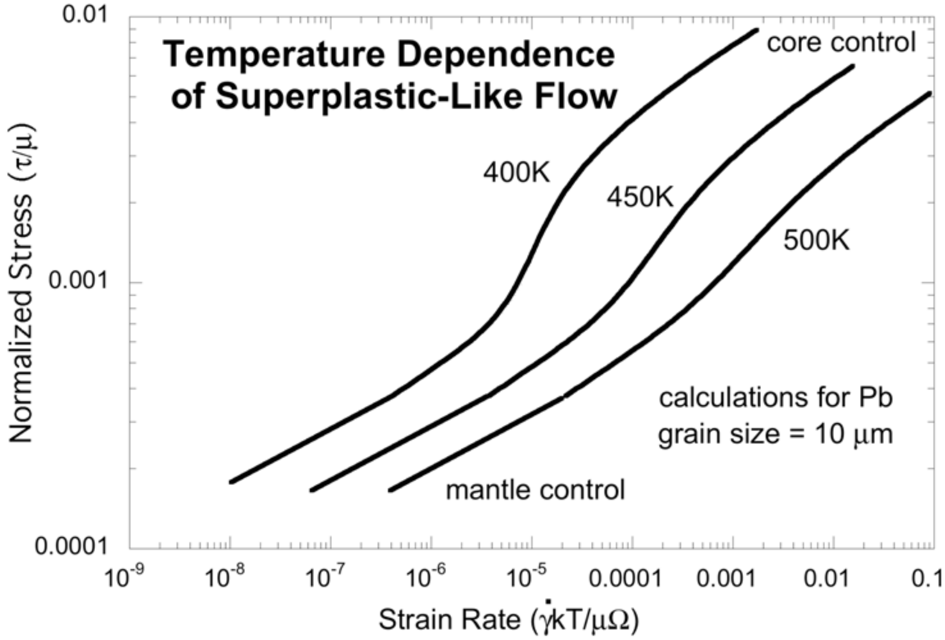

Figure 6. The stress-strain rate relations predicted for Pb with a grain size of 10 μm at three different temperatures, showing superplastic-like properties.

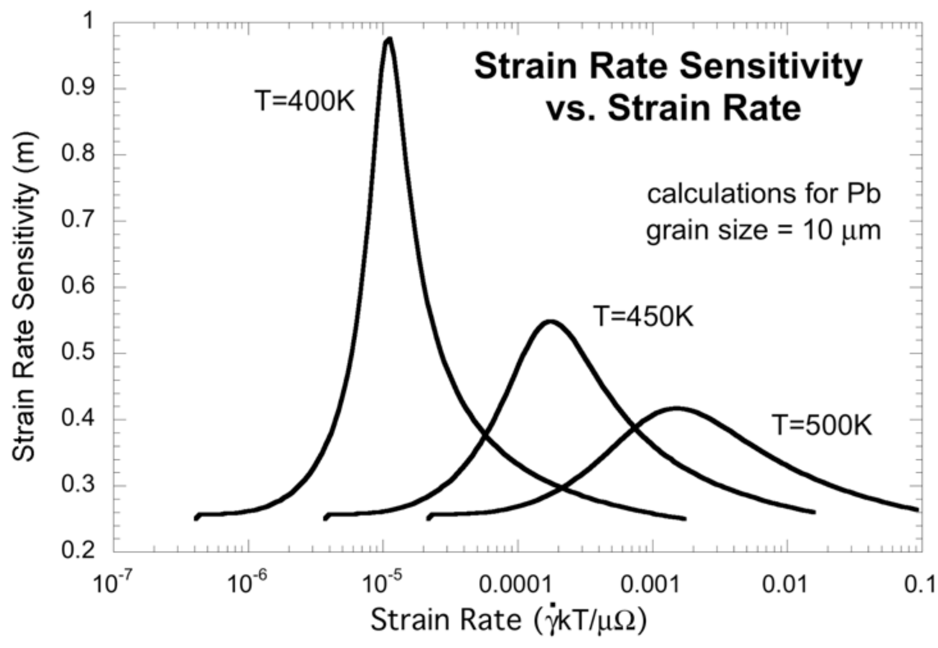

Figure 7. Predicted strain rate sensitivities for Pb with a grain size of 10 μm for three temperatures as a function of the strain rate, again showing superplastic-like behaviour.

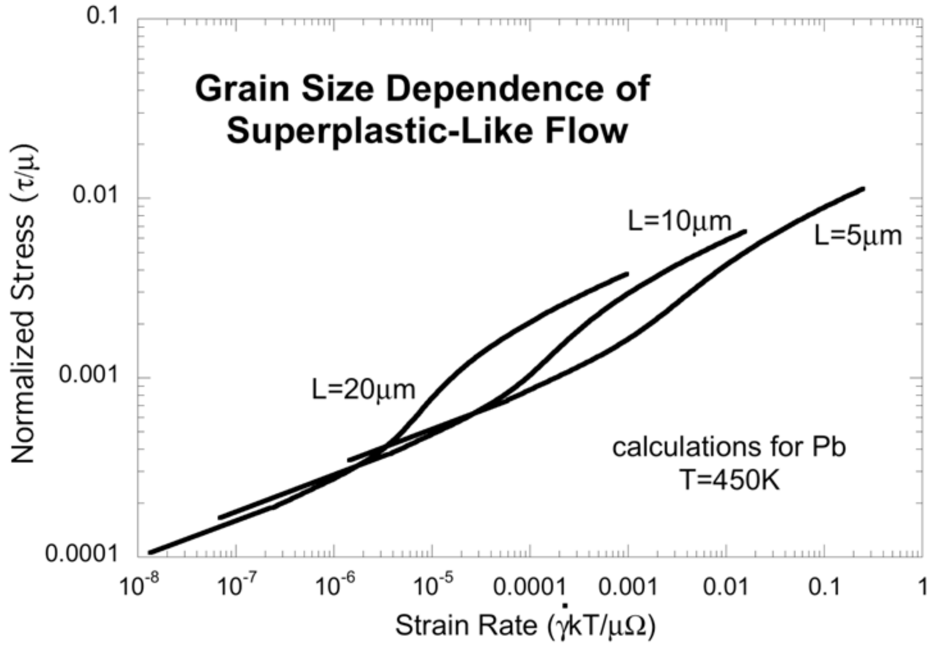

Figure 8. The predicted grain size dependence of deformation at T=450K. The transition occurs at higher strain rates for smaller grain sizes, as expected. The modeling of smaller grain sizes would simply shift these transitions to higher reduced strain rates.

6. Discussion

We have shown that superplastic-like properties can be produced by a model of deformation that makes no specific reference to grain boundary sliding. Instead these properties can arise from the interplay between grain boundary-diffusion-controlled dislocation creep, that operates in the mantle, near grain boundaries, and lattice-diffusion-controlled creep, that operates in the grain interiors, far from the grain boundaries. Such a model is generally consistent with the deformation patterns evident in Fig. 1, where crystal deformation seems to occur preferentially in the ligaments between the grains, where the grain boundaries are located. While we have not made reference to grain boundary sliding in the model, it does, of course, occur. But we believe that the stress redistribution that accompanies sliding on the individual grain boundary facets plays a small role in the overall constitutive response. We remember the work of Crossman and Ashby [18] who showed that power-law creep of polycrystals is hardly affected by whether the grain boundary facets are allowed to slide or not.

While there appear to be some attractive features to the model we have proposed, there are also some glaring weaknesses. The most obvious is that we have had to resort to a phenomenological treatment of the transition between mantle-controlled creep and core-controlled creep. A much better treatment of the mechanics of this transition is needed to fully assess the merit of the present approach. A related point is that the maximum strain rate sensitivity can take on almost any value in this treatment, since it is controlled by the relative positions of the mantle and core creep laws on the stress-strain rate plots. Selecting a different jog spacing in the creep model for the core will cause the core strain rate to change relative to the mantle strain rate and that will directly affect the predicted strain rate sensitivities. Indeed, even for the conditions shown the maximum strain rate sensitivity reaches nearly 1, which is higher that the commonly reported strain rate sensitivity of 0.5. But superplastic Ti alloys are known to have strain rate sensitivities greater than 0.9 [19], so this behaviour is not without some experimental basis.

The model we have proposed is not the first word on this subject and is not likely to be the last. The present treatment bears some likeness to other core-mantle transition models of superplasticity. Gifkins [14] made extensive use of the core-mantle concept, though he did envision grain boundary sliding as a deformation process. Similarly, Baudelet and Lian [20] described superplasticity with a composite model involving the interplay between grain boundary sliding and dislocation creep. Ghosh and Raj [21] pointed out that a distribution of grain sizes in a fine grained solid would lead to superplastic-like transitions similar to those described here. Finally, Ghosh [22] presented a model for superplasticity very similar to the one present here, wherein both dislocation glide and climb are assumed to occur in the mantle and ordinary dislocation flow occurs in the core. Still this treatment makes reference to grain boundary sliding, which is absent in the present model.

6. Summary

Although grain boundaries are a source of weakness in fine-grained polycrystalline solids at high temperatures and grain boundary sliding does occur, we have argued that the boundary sliding process is not a controlling mechanism for deformation. Instead we argue that dislocation slip near grain boundaries is facilitated by grain boundary diffusion and that the interplay between grain boundary-diffusion-controlled dislocation creep near grain boundaries and lattice diffusion controlled dislocation creep in the grain interiors leads to superplastic deformation behaviour that others have attributed to grain boundary sliding. While the model we have proposed gives a good account of the temperature and grain size dependence of the strain rate sensitivity, it is limited by the need to use a phenomenological law to describe the transition from mantle-controlled creep at low strain rates to core-controlled deformation behaviour at high strain rates.

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Appendix

The compressive and tensile stresses, σ_x^{gb}, on the grain boundary intersected by the slip bands in Fig. 2 affect the atomic chemical potential, ψ, on the boundary, as described by

$$\psi = -\sigma_x^{gb}\Omega, \tag{A1}$$

where Ω is the atomic volume. The gradients in chemical potential that develop there drive atomic diffusion from the parts of the boundary under compression to the parts under tension, thus regulating the rate of slip. Eventually a steady state develops where the grain separation rate at the boundary in the domain $0 < y < \lambda / 4$ and the grain approach rate in the domain $-\lambda / 4 < y < 0$ are both constant and equal to $\dot{u}$. Writing the atomic current (per unit thickness) along the grain boundary as

$$q_y = -\delta_{gb}\frac{D_{gb}c}{kT}\frac{\partial\psi}{\partial y} = -\frac{\delta_{gb}}{\Omega}\frac{D_{gb}}{kT}\frac{\partial\psi}{\partial y} = \frac{\delta_{gb}D_{gb}}{kT}\frac{\partial\sigma_x^{gb}}{\partial y}, \tag{A2}$$

where the atomic concentration is taken as $c = 1/\Omega$, the other terms are as defined in the text of the paper and equation (A1) has been used to obtain the last term. At steady state a simple mass balance analysis can be used to relate the grain separation rate in the domain $0 < y < \lambda / 4$ to the divergence of the atomic current,

$$\frac{\partial q_y}{\partial y} = -\frac{\dot{u}}{\Omega}, \tag{A3}$$

which with equation (A2) leads to

$$\frac{\partial^2\sigma_x^{gb}}{\partial y^2} = -\frac{\dot{u}\,kT}{\Omega\delta_{gb}D_{gb}} = -K. \tag{A4}$$

For the domain $0 < y < \lambda / 4$ the corresponding relation is

$$\frac{\partial^2\sigma_x^{gb}}{\partial y^2} = \frac{\dot{u}\,kT}{\Omega\delta_{gb}D_{gb}} = K, \tag{A5}$$

because the grains in this domain are approaching and not separating. Equations (A4) and (A5) can be integrated directly and evaluated using the symmetry boundary conditions

$$\left(\frac{\partial \sigma_x^{gb}}{\partial y}\right)_{y=\lambda/4} = \left(\frac{\partial \sigma_x^{gb}}{\partial y}\right)_{y=-\lambda/4} = 0\,. \tag{A6}$$

The result is

$$\sigma_x^{gb}\left(0 < y < \lambda/4\right) = -\frac{K}{2}y^2 + \frac{K\lambda}{4}y + C_1\,, \tag{A7}$$

and

$$\sigma_x^{gb}\left(-\lambda/4 < y < 0\right) = \frac{K}{2}y^2 + \frac{K\lambda}{4}y + C_2\,. \tag{A8}$$

The requirement of continuous tractions along the grain boundary then leads to $C_1 = C_2$.

When equations (A7) and (A8) are inserted into equation (3),

$$\tau_m \lambda = \int_0^{\lambda/4} \sigma_x^{gb} dy + \int_{-\lambda/4}^{0} \sigma_x^{gb} dy\,, \tag{A9}$$

The constant $C_1 = C_2$ drops out of the analysis and we find

$$\tau_m \Lambda = \frac{K\lambda^3}{96} = \frac{\dot{u}\,kT\,\lambda^3}{96\Omega\delta_{gb}D_{gb}}\,. \tag{A10}$$

Relating the grain separation (approach) rate to the shear strain rate using equation (4) we find

$$\dot{\gamma}_m = \frac{192\Lambda}{\lambda^4}\frac{\tau_m\Omega}{kT}\delta_{gb}D_{gb}\,, \tag{A11}$$

which is equation (5) in the text.