The effect of grain size distribution on the rheological behavior of polycrystalline materials

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Abstract—This paper investigates the possible effect of grain size distribution on the rheological behavior of polycrystalline materials, specifically on the stress exponent n, activation energy Q, and grain size exponent p in the steady-state deformation. All grains in a specimen are assumed to deform simultaneously by power-law creep and grain boundary diffusion (Coble) creep. It is shown that the overall values of n, Q and p are affected by the sizes of grains and their volume fractions in the specimen. In the case that grains of different sizes deform at the same stress, but at different rates, a small number of fine grains in a coarse polycrystal may initiate an overall Newtonian creep behavior. In the case that grains of different sizes deform at the same strain rate, but support different stresses, a small number of coarse grains in a fine polycrystal may induce an overall power-law creep behavior. When a diverse grain size distribution exists, but only the average grain size is considered, the conclusion about the dominant mechanism operating is misleading. Care should be taken when inferring the overall deformational behavior of rocks containing grains of widely differing sizes based on the microstructures preserved.

INTRODUCTION

For single-phase polycrystalline materials deformed at high temperatures, the steady-state creep rate is often described by (e.g. Chokshi & Langdon 1991)

$$\dot{\varepsilon} = A\sigma^n \, d^{-p} \exp - \frac{Q}{RT}, \qquad (1)$$

where $\dot{\varepsilon}$ is the normal strain rate, σ is the normal stress, d is grain size, T is temperature, R is the gas constant, A is the material constant, n is the stress exponent, p is the grain size exponent and Q is the activation energy for creep. The creep parameters, n, p and Q may be derived from equation (1) as:

at constant T and d, $\qquad n = \dfrac{\sigma}{\dot{\varepsilon}} \dfrac{\partial \dot{\varepsilon}}{\partial \sigma}$ $\qquad (2)$

at constant T and σ, $\qquad p = - \dfrac{d}{\dot{\varepsilon}} \dfrac{\partial \dot{\varepsilon}}{\partial d}$ $\qquad (3)$

at constant σ and d, $\qquad Q = \dfrac{1}{\dot{\varepsilon}} \dfrac{\partial \dot{\varepsilon}}{\partial \left(-\dfrac{1}{RT} \right)}$ $\qquad (4)$

and determined from experimental data. The experimentally determined n, p and Q may be used to infer the operating deformation mechanism(s). Theoretically, for dislocation creep, $p = 0$, $Q = Q_v$, the activation energy for lattice diffusion, and $n = 3–5$ (power-law creep) or $n = 1$ (Harper–Dorn creep). For diffusional creep, however, $n = 1$, $Q = Q_v$ and $p = 2$ in the case of lattice diffusional (Nabarro–Herring) creep, but $Q = Q_b$, the activation energy for grain boundary diffusion, and

$p = 3$ in the case of grain boundary diffusional (Coble) creep. For grain boundary sliding creep, generally, $n = 1 \sim 2$, $Q = Q_b \sim Q_v$ and $p = 1 \sim 3$. Dislocation creep does not depend on grain size, but diffusional and grain boundary sliding creep are sensitive to grain size. See Poirier (1985) and Chokshi & Langdon (1991) for an exhaustive review of creep mechanisms.

These specific values of n, Q and p have theoretical validity when only one creep mechanism is operative. In other words, all constituent grains in the material deform by an identical mechanism. To meet this requirement at a given temperature and stress, the grain size must be: (1) very large or very small so that any individual grain deforms by only one mechanism (dislocation glide or climb creep for the case of very large grain size, diffusional or sliding creep for the case of very small grain size); and (2) be sufficiently uniform over the whole specimen so that all grains deform by the same mechanism.

Such a strict requirement is scarcely met in real polycrystalline materials. The grain sizes in metals, ceramics and rocks are often not uniform, but vary from grain to grain. Besides, grain sizes may also change during deformation (e.g. by dynamic recrystallization or grain growth). In these cases, more than one mechanism (grain size sensitive and insensitive) may operate in individual grains, or different mechanisms in different grains, or both. With the presence or development of grain size distribution in the material, the observed rheological behavior may be significantly different from the theoretical prediction for a single-valued grain size.

Effects of grain size distribution on deformation have been considered to account for the wide strain-rate transition (over several orders of magnitude) from power-law creep to diffusional creep (Raj & Ghosh

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1981), to simulate the steady-state, loading and load relaxation behaviors of superplasticity (Ghosh & Raj 1981), to explain the oscillating shape of the stress–strain curves of aluminium alloys during superplastic deformation (Ghosh & Raj 1986). Freeman & Ferguson (1986) studied the effect of grain size distribution using deformation mechanism maps. They illustrated that at a given average grain size, the stress and temperature ranges in which one creep mechanism is dominant over others change with a change in grain size distribution. However, they did not show how, with changing grain size distribution, the creep parameters might change, whether or under what conditions there could be a switch from power-law creep to diffusional creep or vice versa, or what would be the microstructural evidence for such switching. The specific purpose of this paper is to seek possible answers to these questions.

By considering a material deforming *in part* by a grain-size sensitive process, it will be shown that the overall values of n, Q and p are affected by the sizes of grains and their volume fractions in the specimen. In the case that grains of different sizes deform at the same stress, but at different strain rates, a small number of fine grains in a coarse polycrystal may initiate an overall linear creep behavior. In the case that grains of different sizes deform at the same strain rate, but support different stresses, a small number of coarse grains in a fine polycrystal may induce an overall power-law creep behavior. These results have important implications for interpreting the experimentally determined creep parameters and for inferring aggregate properties from observations of deformation microstructures.

MODELS

To illustrate the effect of grain size distribution, only power-law creep and Coble creep are chosen for the investigation here (Nabarro–Herring creep, or grain boundary sliding, or pressure-solution creep can be similarly combined with power-law creep). The coupling of Coble creep with power-law creep will be studied for two cases:

(1) the grain size is single-valued, and thus has a unimodal distribution;

(2) the grain size is multiple-valued, and thus has a diverse distribution.

Unimodal grain size distribution

In an ideal single phase material with a unimodal grain size distribution, all grains have the same size d, and hence deform by the same mechanism(s). Two questions may be posed: under what conditions will more than one mechanism operate simultaneously and what effect will this have on the values of n, p and Q?

For convenience, by simplifying equation (1), rate equations for power-law creep and Coble creep are expressed as:

$$\dot{\varepsilon}_p = A_p \sigma^{n_0} \exp - \frac{Q_v}{RT} \qquad (5)$$

$$\dot{\varepsilon}_d = A_d \frac{\sigma}{d^3} \exp - \frac{Q_b}{RT}, \qquad (6)$$

respectively, where n_0 is the stress exponent for power-law creep, and A_p and A_d are pre-exponential factors.

When power-law creep and Coble creep operate concomitantly, the overall strain rate of each grain is the summation of equations (5) and (6):

$$\dot{\varepsilon} = \dot{\varepsilon}_p + \dot{\varepsilon}_d \qquad (7)$$

as they are two independent and thus additive mechanisms (Frost & Ashby 1982). The relative contributions of $\dot{\varepsilon}_p$ and $\dot{\varepsilon}_d$ to $\dot{\varepsilon}$ depends on the grain size.

A critical size d_c can be found by equating (5) and (6) as:

$$d_c = \left\{ \frac{E_{dd}}{\dot{\varepsilon}_p} \right\}^{1/3} \qquad (8)$$

with $E_{dd} = A_d \sigma \exp(-Q_b/RT)$. At this size, power-law creep and Coble creep contribute equally to the overall strain rate. At a size $d > d_c$, power-law creep dominates, whereas at a size $d < d_c$, Coble creep dominates. d can be related to d_c by:

$$d = u d_c, \qquad (9)$$

where u is a constant describing the deviation of d from d_c.

Suppose the ratio of the strain rate of diffusional creep to the total strain rate is ϕ, then

$$(1 - \phi) \dot{\varepsilon} = \dot{\varepsilon}_p \qquad (10)$$

$$\phi \dot{\varepsilon} = \dot{\varepsilon}_d. \qquad (11)$$

By combining equations (2)–(4) and (5)–(11), the following relations can be derived:

$$n = \frac{n_0 \dot{\varepsilon}_p + \dot{\varepsilon}_d}{\dot{\varepsilon}_p + \dot{\varepsilon}_d}, \qquad (12)$$

$$Q = \frac{Q_v \dot{\varepsilon}_p + Q_b \dot{\varepsilon}_d}{\dot{\varepsilon}_p + \dot{\varepsilon}_d} \qquad (13)$$

$$p = \frac{3 \dot{\varepsilon}_d}{\dot{\varepsilon}_p + \dot{\varepsilon}_d} \qquad (14)$$

$$\phi = \frac{\dot{\varepsilon}_d}{\dot{\varepsilon}_p + \dot{\varepsilon}_d}. \qquad (15)$$

For numerical calculations, the power-law creep parameters and diffusion coefficients for pure nickel are selected and listed in Table 1 (the following calculations can be made for any other crystalline materials). Computation is performed at a temperature of 1100 K and stress of 10 MPa. The variation of ϕ, n, Q and p with u are discussed as follows.

The variation of ϕ with grain-size is shown in Fig. 1. By definition when $u = 1$ ($d = d_c$), then $\phi = 50\%$ (equation 8). In this case, dislocation and Coble creep contribute equally, and the overall stress exponent,

Table 1. Material data used for equations (5) and (6) (after Frost & Ashby 1982)

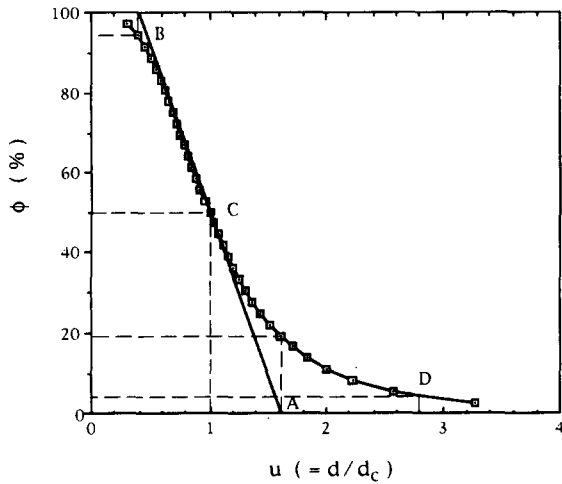| Material	Temp (K)	σ (MPa)	A_p (MPa)$^{-n_o}$ s^{-1}	n_o	Q_v (kJ mol)$^{-1}$	A_d (MPa^{-1} m^3 s^{-1})	Q_b (kJ mol)$^{-1}$
Pure Ni	1100	10	78.0	4.6	284.0	1.24×10^{-11}	115

Fig. 1. Variation of the ratio of the diffusional creep rate to the total creep rate for each grain with the deviation of grain size from d_c. $u = 1.0$ (C), $\phi = 50\%$, power-law creep and diffusional creep contribute equally; $u > 2.8$ (D), $\phi < 5\%$, less than 5% of the total creep rate is contributed by diffusional creep; $u < 0.4$ (B), $\phi > 95\%$, more than 95% of the total creep rate is contributed by diffusional creep.
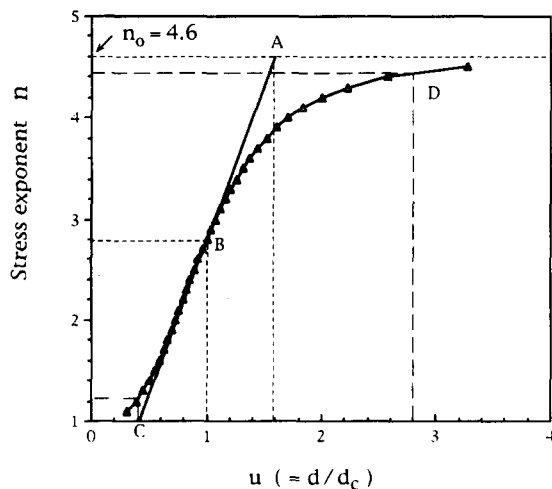

Fig. 2. Variation of stress exponent with the deviation of grain size d from d_c. $u = 1.0$ (B), $n = 2.8$; $u > 2.8$ (D), $n > 4.4$, close to $n_o = 4.6$ for power-law creep; $u < 0.4$ (C), $n < 1.2$, close to unity for diffusional creep.

activation energy and grain size exponent are 2.8 (Fig. 2), 200 kJ mol^{-1} and 1.5, respectively. When $u > 1$, $\phi < 50\%$, power-law creep dominates over Coble creep. For $u > 2.8$, $\phi < 5\%$, power-law creep acts almost solely, and thus n, Q and p approach n_0 (Fig. 2), Q_v and zero. When $u < 1$, $\phi > 50\%$, Coble creep dominates over power-law creep. For $u < 0.4$, $\phi > 95\%$, Coble creep operates almost exclusively, and thus n, Q and p approach 1 (Fig. 2), Q_b and 3.
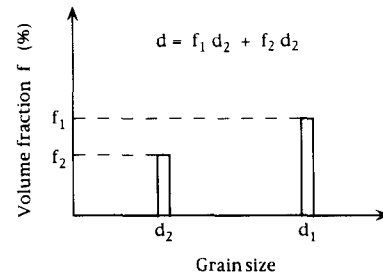
Thus, it follows that if the size of a grain is around the

Fig. 3. Schematic diagram showing bimodal grain size distribution with two modal values d_1 and d_2, and an average size d.

critical size d_c at a given temperature and stress, the grain deforms by more than one mechanism, and the overall n, Q and p could have values intermediate between those for the individual mechanisms.

Bimodal grain size distribution

Suppose the grain size distribution in a single phase polycrystal is not unimodal, but bimodal (Fig. 3) with d_1 and d_2 being the two modal values ($d_1 > d_2$) (the following discussions can be easily extended to distributions of higher orders). The volume fractions of grains with size d_1 (group 1) and of those with size d_2 (group 2) are represented by f_1 and f_2, respectively. Then the grain size distribution is determined by d_1, d_2, f_1 and f_2. The grains of the two groups support stresses of σ_1 and σ_2, and deform at strain rates of $\dot{\varepsilon}_1$ and $\dot{\varepsilon}_2$, respectively.

According to equations (5), (6) and (7), the strain rate equations for the two groups can be expressed by:

$$\dot{\varepsilon}_1 = \dot{\varepsilon}_{p1} + \dot{\varepsilon}_{d1} = A_p \sigma_1^{n_o} \exp\left(-\frac{Q_v}{RT}\right) + A_d \frac{\sigma_1}{d_1^3} \exp\left(-\frac{Q_b}{RT}\right)$$

(16)

$$\dot{\varepsilon}_2 = \dot{\varepsilon}_{p2} + \dot{\varepsilon}_{d2} = A_p \sigma_2^{n_o} \exp\left(-\frac{Q_v}{RT}\right) + A_d \frac{\sigma_2}{d_2^3} \exp\left(-\frac{Q_b}{RT}\right)$$

(17)

which can be simplified to the form of equation (1)

$$\dot{\varepsilon}_1 = A_1 \sigma_1^{n_1} d_1^{-p_1} \exp\left(-\frac{Q_1}{RT}\right)$$

(18)

$$\dot{\varepsilon}_2 = A_2 \sigma_2^{n_2} d_2^{-p_2} \exp\left(-\frac{Q_2}{RT}\right)$$

(19)

where A_i, n_i, p_i and Q_i ($i = 1$ or 2) are the pre-exponential factor, stress exponent, grain size exponent and activation energy for the creep of group 1 and group 2, respectively. The overall strain rate equation is expressed by equation (1).

The grain sizes d_1 of group 1 and d_2 of group 2 are related to d_c by:

$$d_1 = id_c \tag{20}$$

$$d_2 = jd_c \tag{21}$$

with i and j being two constants determining the deviation of d_1 and d_2 from d_c. The average grain size d of the whole material is expressed as:

$$d = f_1 d_1 + f_2 d_2. \tag{22}$$

For convenience, f_2 is equated with f and f_1 with $(1-f)$ in which

$$f = \frac{(u - i)}{(j - i)} \tag{23}$$

with u determining the deviation of the average grain size from d_c as in equation (9).

The real relationships between the overall strain rate $\dot{\varepsilon}$ and $\dot{\varepsilon}_1$, $\dot{\varepsilon}_2$ and between the overall stress σ and σ_1, σ_2 depend not only on the volume fractions f_1 and f_2, but also on the real morphologies (Raj & Ghosh 1981) and the spatial distribution of group 1 and group 2 grains. That is, the distribution of the two groups of differing grain sizes through the aggregate (e.g. their continuity or contiguity) also influences their loading configuration and hence the partitioning of the stress and strain between them (Freeman & Ferguson 1986). If a full precise solution were required, it would be necessary to carry out finite element calculations as made by Jinoch et al. (1978) and Tullis et al. (1991). Such a solution is so complicated that it would obscure the problem at hand. However, simple geometrical and morphological considerations can provide approximate solutions.

Uniform stress model. If the two groups of different grain size are assumed to be arranged in a series manner, then

$$\dot{\varepsilon} = f_1 \dot{\varepsilon}_1 + f_2 \dot{\varepsilon}_2 \tag{24}$$

$$\sigma = \sigma_1 = \sigma_2. \tag{25}$$

In this case, grains of different sizes deform at different strain rates, but support the same stress as does the overall specimen; a uniform stress is assumed. By combining equations of (2)–(4), (16), (17), (24) and (25), the following relations can be obtained:

$$n = \frac{n_o \dot{\varepsilon}_p + f_1 \dot{\varepsilon}_{d1} + f_2 \dot{\varepsilon}_{d2}}{\dot{\varepsilon}_p + f_1 \dot{\varepsilon}_{d1} + f_2 \dot{\varepsilon}_{d2}} \tag{26}$$

$$Q = \frac{Q_v \dot{\varepsilon}_p + Q_b f_1 \dot{\varepsilon}_{d1} + Q_b f_2 \dot{\varepsilon}_{d2}}{\dot{\varepsilon}_p + f_1 \dot{\varepsilon}_{d1} + f_2 \dot{\varepsilon}_{d2}} \tag{27}$$

$$p = 3 \frac{f_1 \dot{\varepsilon}_{d1} + f_2 \dot{\varepsilon}_{d2}}{\dot{\varepsilon}_p + f_1 \dot{\varepsilon}_{d1} + f_2 \dot{\varepsilon}_{d2}}. \tag{28}$$

Uniform strain rate model. If the two groups are assumed to be arranged in a parallel manner, then

$$\dot{\varepsilon} = \dot{\varepsilon}_1 = \dot{\varepsilon}_2 \tag{29}$$

$$\sigma = f_1 \sigma_1 + f_2 \sigma_2. \tag{30}$$

In this case, grains of different sizes deform at the same

Table 2. Bimodal grain size distribution details designed for numerical calculations

	$d_1 = i\,d_c$ i	$d_2 = j\,d_c$ j	Group 1 $\dot{\varepsilon}_{p1}/\dot{\varepsilon}_1$	Group 2 $\dot{\varepsilon}_{d2}/\dot{\varepsilon}_2$
Case 1	5.0	1.0–2.5	>95%	50–7%
Case 2	5.0	0.1–0.8	>95%	95–65%
Case 3	1.4	0.1–1.3	≈75%	95–40%
Case 4	0.5	0.1–0.4	≈5%	>95%

strain rate as does the overall specimen, but support different stresses; a uniform strain (rate) is assumed. An iterative method needs to be applied for actual computation.

Two expressions for n can be found from equations (2), (16)–(19) which contain the derivatives of $\partial\sigma_1/\partial\sigma$ and $\partial\sigma_2/\partial\sigma$, respectively. Another equation containing these two derivatives can be obtained from equation (30). An expression for n can thus be established as

$$n = \frac{\sigma n_1 n_2}{f_1 \sigma_1 n_2 + f_2 \sigma_2 n_1}. \tag{31}$$

Two expressions for Q can be found from (4), (18)–(21) which contain the derivatives of $\partial\sigma_1/\partial(-1/RT)$ and $\partial\sigma_2/\partial(-1/RT)$, respectively. Another equation containing these two derivatives can be obtained from equation (30). An expression for Q can thus be found as

$$Q = \frac{1}{\dot{\varepsilon}_2} \left\{ (Q_v \dot{\varepsilon}_{p2} + Q_b \dot{\varepsilon}_{d2}) + \left(\frac{n_o}{\sigma_2} \dot{\varepsilon}_{p2} + \frac{\dot{\varepsilon}_{d2}}{\sigma_2} \right) \frac{\partial\sigma_2}{\partial\left(-\frac{1}{RT}\right)} \right\}, \tag{32}$$

where

$$\frac{\partial\sigma_2}{\partial\left(-\frac{1}{RT}\right)} = \frac{(Q_v \dot{\varepsilon}_{p1} + Q_b \dot{\varepsilon}_{d1}) - (Q_v \dot{\varepsilon}_{p2} + Q_b \dot{\varepsilon}_{d2})}{\left(\frac{n_o}{\sigma_2} \dot{\varepsilon}_{p2} + \frac{\dot{\varepsilon}_{d2}}{\sigma_2} \right) + \frac{f_2}{f_1} \left(\frac{n_o}{\sigma_1} \dot{\varepsilon}_{p1} + \frac{\dot{\varepsilon}_{d1}}{\sigma_1} \right)}.$$

Similar procedures can be applied to find an expression for p. Due to its complexity, it is not included here.

RESULTS

With reference to Fig. 1, and according to the contribution of power-law creep and diffusional creep to the total rate of one group, four distinct cases are considered (Table 2). In case 1 ($i = 5$, $j = 1$–2.5), grains of both groups deform mainly by power-law creep. In case 2 ($i = 5$, $j = 0.1$–0.8), grains of group 1 deform mainly by power-law creep, but grains of group 2 mainly by diffusional creep. In case 3 ($i = 1.4$, $j = 0.1$–0.8), grains of group 1 deform partly by power-law creep and partly by diffusional creep, while grains of group 2 mainly by diffusional creep. In case 4 ($i = 0.5$, $j = 0.1$–0.4), grains of both groups deform mainly by diffusional creep. Focus will be placed on case 2. Pure nickel is taken as the material for numerical calculations.
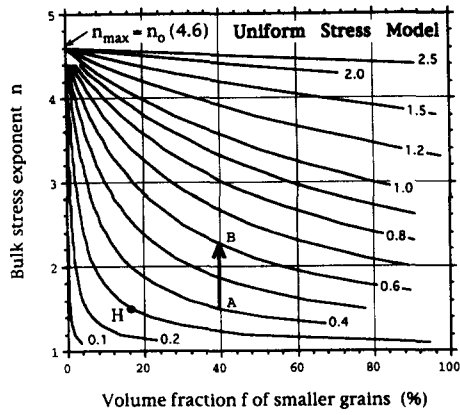
Fig. 4. Uniform stress model: variation of stress exponent n with the volume fraction f of smaller grains at $i = 5, j = 0.1$–2.5.
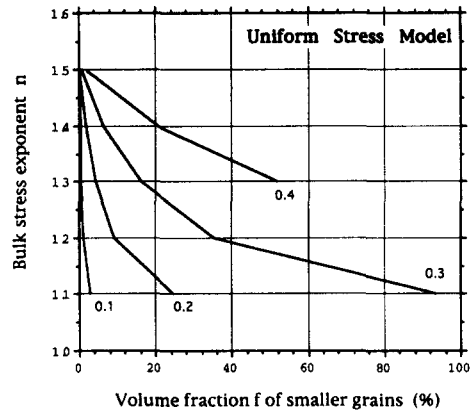

Fig. 6. Uniform stress model: variation of stress exponent n with the volume fraction f of smaller grains at $i = 0.55, j = 0.1$–0.4.
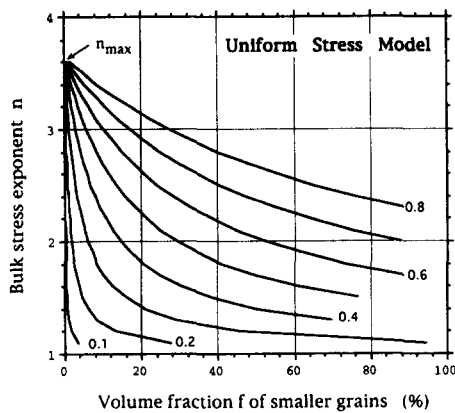

Fig. 5. Uniform stress model: variation of stress exponent n with the volume fraction f of smaller grains at $i = 1.4, j = 0.1$–0.8.
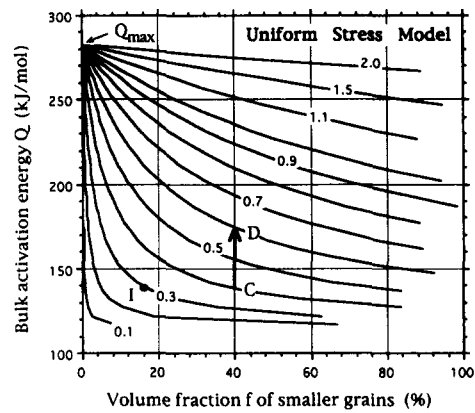

Fig. 7. Uniform stress model: variation of activation energy Q with the volume fraction f of smaller grains at $i = 5, j = 0.1$–2.5.

For the uniform stress model

Results for the uniform stress model are presented in Figs. 4–8. In these figures, it is clearly shown that the overall n, Q and p depend strongly on the grain size distribution (the sizes and volume fractions of the two groups). The following points need be noted.

(1) *At constant* i *and* f, *but variable* j. When the size of big grains of group 1 and the volume fraction of small grains of group 2 are given, rheological parameters are affected by the size of the small grains. As j increases, n and Q also increase, but p decreases. For example, at $i = 5$ and $f = 40\%$, for $j = 0.4$–0.6, $n = 1.25$–2.15 (A → B, Fig. 4); $Q = 140$–175 kJ mol^{-1} (C → D, Fig. 7); $p = 2.7$–1.95 (E → F, Fig. 8). This is because as the size of small grains increases, the contribution of Coble creep to the overall creep decreases.

(2) *At constant* i, j, *but variable* f. When the sizes of the grains of both groups are given, the rheological parameters are affected by the volume fraction of the small grains. As f increases from 0 to 100%, n and Q decrease, but p increases. This is because, as the fraction of small grains increases, the contribution of Coble creep to the overall creep increases.
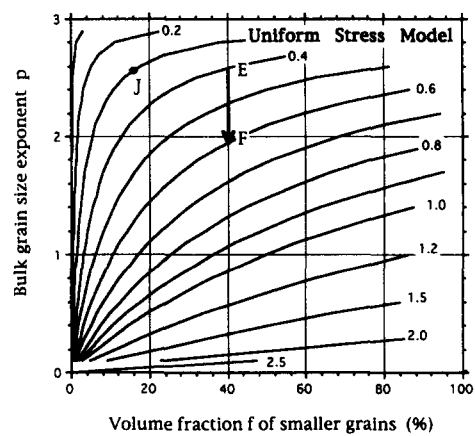

Fig. 8. Uniform stress model: variation of grain size exponent p with the volume fraction of smaller grains at $i = 5, j = 0.1$–2.5.

(3) *At constant* j *and* f, *but variable* i. When the size and volume fraction of grains of group 2 are given, the rheological parameters are affected by the size of grains of group 1. As i increases from 0.5 to 5, n and Q increase, but p decreases. This is because, as the size of big grains increases, the contribution of Coble creep to the overall creep decreases.
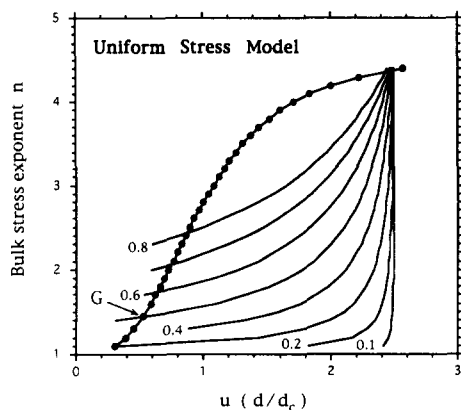
Fig. 9. Uniform stress model: comparison in variation of stress exponent n with the deviation u of the average grain size d from d_c between unimodal (dotted) and bimodal (fine lines) at $i = 5$, $j = 0.1$–0.8 size distributions.

Fig. 10. Uniform strain model: variation of stress exponent n with the volume fraction of smaller grains at $i = 5$. $j = 0.1$–0.8.

(4) *In different cases of grain size distribution* (Table 2), *the ranges in which the overall creep parameters vary are different*. In case 1, where d_1 and $d_2 > d_c$ ($i = 5$, $j = 1$–2.5), they vary between those for pure power-law creep and about half of each of these values (Figs. 4, 7 and 8). The slight deviation from pure power-law creep is due to the minor contribution of Coble creep to the total strain rate as the size of the smaller grains decreases. In case 4, where d_1 and $d_2 < d_c$ ($i = 0.5$, $j = 0.1$–0.4), the creep parameters vary within only limited ranges which are close to those for pure Coble creep (Fig. 6). This is because grains of both groups deform mainly by Coble creep. The minor contribution of power law creep causes the overall behavior to deviate slightly from that of pure Coble creep. In case 3 ($i = 1.4$, $j = 0.1$–0.8), a pure power-law creep behavior cannot be approached because of the operation of Coble creep also in grains of group 1 with larger grain sizes (Fig. 5). However, in case 2 where $d_1 > d_c$, but $d_1 > d_c$ ($i = 5$, $j = 0.1$–0.8), n, p and Q could have any values between those for pure power-law creep and those for pure Coble creep depending on the detail of grain size distribution (Figs. 4, 7 and 8).

Variation of n with the deviation of the average grain size d from d_c (at $i = 5$, $j = 0.1$–0.8) is presented in Fig. 9. Such a variation in the case that the grain size distribution is unimodal, as presented in Fig. 2, is superposed. In the unimodal case (represented by circles) where all grains have the same size, n varies with u only. But in the bimodal case (represented by fine lines) where the average grain size is determined by the sizes of the two groups and their volume fractions (equation 22), n varies not only with u, but also with j at constant i. The larger the j and u, the larger the n. Only at specific j values (e.g. at $j = 0.5$ when $u = 0.5$, point G in Fig. 9), can n in the unimodal case be identical to those in the bimodal case.

A specific case of interest is discussed in detail. Group 1 is supposed to deform by power-law creep only, and group 2 by diffusion creep only. With reference to Fig. 1, this is true for $i > 2.8$ and $j < 0.4$. $i = 5$ and $j = 0.3$ are selected.
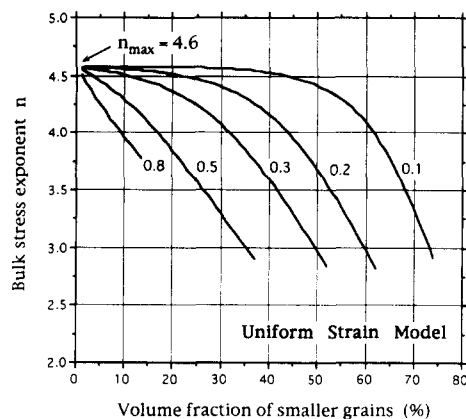
Under this condition, n, Q and p vary with f only; that is, they are determined by the volume fractions of group 1 and group 2 only. When $f = 16\%$, $n = 1.5$ (point H in Fig. 4), $Q = 140\,kJ\,mol^{-1}$ (point I in Fig. 7), and $p = 2.6$ (point J in Fig. 8), respectively, which are close to 1115 $kJ\,mol^{-1}$ and 3 for pure diffusion creep. This means that at 1100 K and 10 MPa stress, a pure nickel polycrystal will deform dominantly by diffusion (Coble) creep if 84% of the grains are of a size $d_1 = 5\,d_c = 174.25\,\mu m$ and 16% are of a size $d_2 = 0.3\,d_c = 10.46\,\mu m$. Obviously here, most of the grains are very coarse and only a very small number of grains are very fine. But such a polycrystal shows diffusional creep behavior rather than power-law creep behavior!

However, if the bimodal grain size distribution is not taken into account and only the average grain size d is considered, the conclusion will be different. When $f_1 = 84\%$, $i = 5$ and $f_2 = 16\%$, $j = 0.3$, the average grain size $d = 148.04\,\mu m$ (equation 22), corresponding to $u = 4.25$, the deviation of d from d_c (equation 9). If the grain size distribution of the polycrystal is considered as unimodal, then, $n \approx 4.5$, $Q \approx 280\,kJ\,mol^{-1}$ and $p \approx 0.02$ (calculated from equations 12–14), which are very close to $n_0 = 4.6$, $Q_v = 284\,kJ\,mol^{-1}$ and $p = 0$, respectively, for pure power-law creep. That is, if all grains are assumed to have an identical size d, the polycrystal is expected to show power-law creep behavior rather than diffusional creep behavior.

Therefore, a small number of fine grains in an overall coarse polycrystal influences the deformation behavior dramatically for the uniform stress case. Neglecting to consider the grain size distribution would lead to erroneous conclusions about the dominating deformation mechanism.

For the uniform strain model

Results for the uniform strain (rate) model are shown in Figs. 10 and 11. Calculations are made only at $i = 5$, $j = 0.1$–0.8.

In such a uniform strain case, the bulk n, Q and p values are much less sensitive to changes in the volume fraction f and the size d_2 of the smaller grains than in the uniform stress case. It appears that the smaller the size of
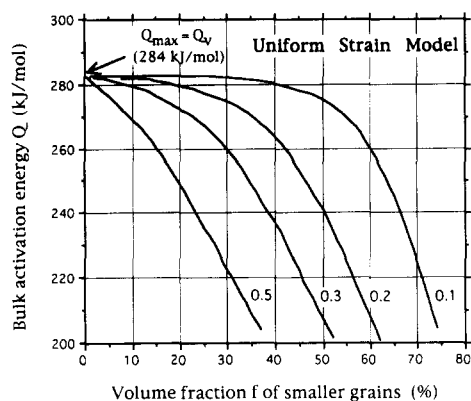
Fig. 11. Uniform strain model: variation of activation energy Q with the volume fraction of smaller grains at $i = 5$, $j = 0.1$–0.5.

Fig. 12. Dependence of the specimen strain rate and the strain rate of the small and large grains on the size of the small grains d_2. Uniform stress in a sample composed of 25% small grains.

Fig. 13. Dependence of the specimen stress and the stress in the small and large grains on the size of the small grains. Uniform strain in a sample composed of 25% large grains.

the small grains, the less sensitive they are to changes in f and d_2. For example, at $i = 5$ and $j = 0.1$, when the volume fraction of the small grains is 75%, $n = 2.8$ (Fig. 10), $Q = 200$ kJ mol^{-1} (Fig. 11). This means that for the uniform strain model, a pure Ni polycrystal composed of mainly very small grains will show power-law creep behavior rather than diffusional creep behavior.

DISCUSSION

The important feature of the above results is that the overall rheological behavior of a polycrystalline solid is affected by grain size distribution (the size of grains in each group and their volume fractions). The effect is most prominent when the smaller grains in the material deform mainly or completely by a grain size sensitive process such as diffusional creep, while large grains deform by a grain size insensitive process such as power-law dislocation creep. Under this circumstance, a small number of fine grains may invoke an overall diffusional creep behavior if the distribution of stress is uniform between grains of different sizes, but a small number of coarse grains may prompt an overall power-law creep behavior if the distribution of strain in the material is uniform.

The cause for the above observations is that in the uniform stress case, because all grains are assumed to support the same stress as the whole material, the smaller grains deform at a strain rate faster, but the larger ones deform at a strain rate much smaller, than that the bulk specimen (Fig. 12). As the size of the small grains becomes smaller and smaller, their contribution in the form of diffusion creep becomes larger and larger. However, the contribution by the big grains in the form of power-law creep remains unchanged. The consequence is that smaller and smaller numbers of fine grains are required to induce an overall diffusion creep behavior. Hence a small number of fine grains can invoke an overall behavior similar to that of diffusional creep.

By contrast, in the uniform strain rate case, because all grains are assumed to deform at the same strain rate as the whole specimen, the stress supported by big grains σ_1 must be much larger than that supported by small
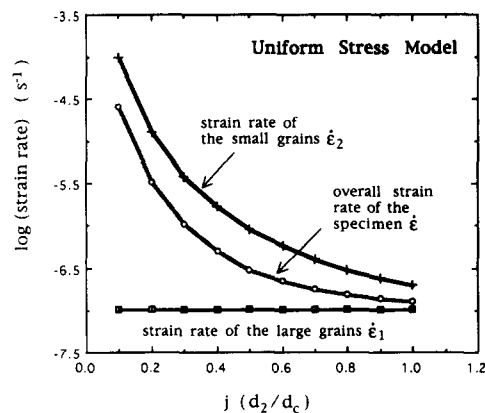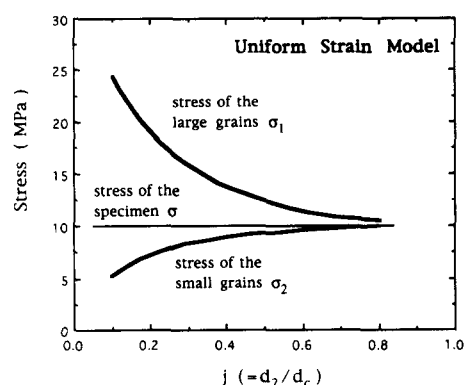
grains σ_2. As the size of the small grains decreases, σ_1 must increase (Fig. 13) so as to increase the strain rate of the big grains by power-law creep. The consequence is that smaller and smaller numbers of big grains are required to produce an overall power-law creep behavior. Hence a small number of coarse grains may cause the overall behavior to be similar to that of power-law creep.

The uniform stress and uniform strain rate models represent two extreme situations of distribution of stress and strain rate between small and big grains in a material. The uniform stress models tends to overestimate the role of small grains, whereas the uniform strain rate model tends to overestimate the role of big ones. The real rheological behavior of the material with a diverse grain size distribution may be determined by the uniform stress model as the lower bound and by the uniform strain rate model as the upper bound. This is shown in Fig. 14. As the size of small grains (j) increases, the gap between the upper and lower bounds diminishes.

Which of the two models is more likely in a material depends on the microstructures developed during deformation. If the distribution of stress is uniform, because small grains deform at a strain rate faster, but big grains deform at a strain rate much slower, than that of the bulk
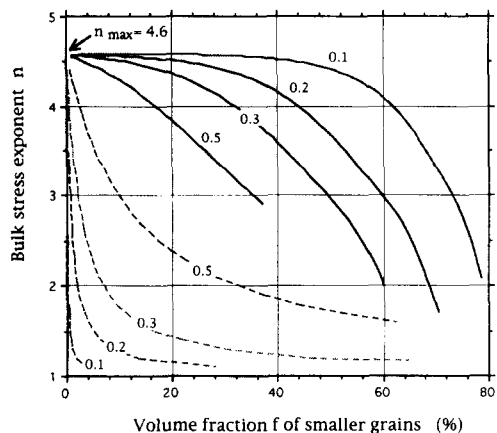
Volume fraction f of smaller grains (%)

Fig. 14. Upper bound (uniform strain, solid lines) and lower bound (uniform stress, dashed lines) for $i = 5, j = 0.1$–0.5.

(a)

(b)

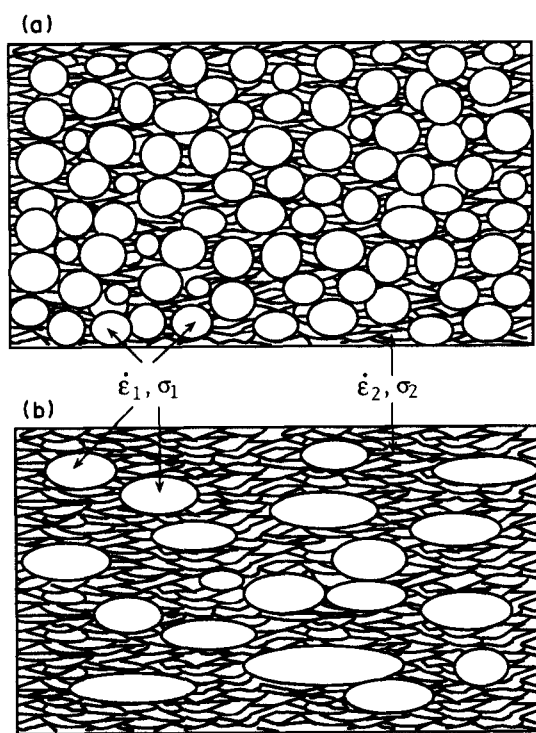$\dot{\varepsilon}_1, \sigma_1$ $\dot{\varepsilon}_2, \sigma_2$

Fig. 15. Schematic deformation microstructures of materials with grains of widely differing sizes in which the deformation has been in part by a grain size sensitive mechanism. (a) The uniform stress case ($\sigma = \sigma_1 = \sigma_2$). A small fraction of fine grains may induce an overall diffusional creep behavior. Fine grains are greatly flattened, whereas coarse ones show little deformation. (b) The uniform strain case ($\varepsilon = \varepsilon_1 = \varepsilon_2$). A small fraction of coarse grains may result in an overall power-law creep behavior. Both fine and coarse grains show equal flattening.

specimen, microstructurally, fine grains are expected to show great flattening, whereas coarse ones are expected to exhibit little deformation (Fig. 15a). In contrast, if the distribution of strain is uniform, microstructurally, fine and coarse grains should show equal flattening (Fig. 15b).

Since grain size distributions have not been reported along with the rheological data in the literature, it is premature to make a quantitative comparison between experimental results and this theoretical work. Nevertheless, a qualitative account is beneficial to interpret experimentally determined values of n, p and Q and to

deduce bulk mechanical properties from microstructural observations for materials containing grains of distributed sizes.

Different creep mechanisms control the deformation of a material only at specific experimental conditions. The theoretical values of n, p and Q for a deformation mechanism can be experimentally observed only when this mechanism is operative exclusively. However, the observed parameters may be different from theoretical values for any creep models. At a given stress and temperature, this difference may just be a result of operation of more than one mechanism due to the presence of a diverse grain size distribution. Take grain boundary sliding as an example. There are wide variations in the dependence of sliding rate on stress (generally from 1 to 3), temperature (Q from $0.2\,Q_v$ to Q_v) and grain size (p from 1 to 3). Various models have been developed to predict the experimental observations (see Langdon & Vastava 1982 for a review). However, all models and experimental measurements have ignored the possible presence of grain size distribution in the material. Since the steady state, loading and load relaxation behavior and the oscillating shape of the stress–strain curves during superplastic deformation can be explained in terms of the effect of grain size distribution (Ghosh & Raj 1986), the various experimentally observed n, p and Q may result from the coupling of dislocation creep with diffusional creep in different ways under different conditions. According to this study, it appears necessary to consider whether or not there is a grain size distribution in the material used for studying grain boundary sliding.

Dynamic recrystallization induces the development of a diverse grain size distribution. Grain growth increases the size of fine grains, but subgrain rotation reduces the size of relatively large grains. Therefore, there might be a switch in overall deformation behavior from power-law creep to diffusional or grain boundary sliding creep in the case of subgrain rotation or vice versa in the case of grain growth. Such a switch may occur when the volume fraction of the new grains is still small. Mechanical data are essential for determining whether or not this change occurs during experiments.

Determination of deformation mechanism of rocks based on the microstructures preserved may be dubious if the rocks contain grains of largely different sizes. The reason is that the distribution of stress and/or strain between grains of different sizes is often not easy to determine. For example, if the rock consists of a large number of big grains which show dislocation creep, but only a small number of grains which show diffusional creep, the overall deformation behavior of the rock might be similar to that of diffusional creep rather than dislocation creep if the distribution of stress across the big and small grains is uniform. In contrast, if the rock consists of a large number of small grains, but a small number of big ones, the overall deformation behavior of the rock might be similar to that of dislocation creep rather than to that of diffusional creep if the distribution of strain across all grains is uniform. In these cases, it is

critical to examine whether or not the big grains have been deformed significantly. If they have, the distribution of strain is likely to be uniform, otherwise, the distribution of stress may be considered to be uniform.

Recently, there have been a number of attempts to estimate the rheological behavior of two-phase aggregates in terms of the flow laws, volume proportions and configurations of the constituent phases (Tharp 1983, Jordan 1988, Handy 1990, 1994, Tullis et al. 1991). The results obtained here may be applicable to two-phase aggregates if the group of small grains and that of big grains are considered as two different phases: weak and strong, respectively.

Handy (1990) suggested three basic classes of approximation for polyphase aggregates.

(1) A load-bearing framework of a strong phase with a relatively small volume proportion of weak phase (<25%); in this case, the strength of the aggregate approaches that of the strong phase. According to the present study, this is true only if the distribution of strain rate is uniform between the weak and strong phases, and thus the bulk rheology of such a structure tends to be closer to the uniform strain rate bound. Instead, if the distribution of stress is uniform, then the strength of the aggregate will approach that of the weak phase, and the bulk rheology will be closer to the uniform stress bound.

(2) Isolated clasts of a strong phase dispersed in a much weaker matrix (strength contrast >10/1); in this case, the strength of the aggregate approaches that of the weak phase. This is true only if the distribution of stress is uniform. If the distribution of strain rate is uniform, then the strength of the aggregate will approach that of the strong phase, and the bulk rheology will be close to the uniform strain rate bound.

(3) Two phases which have a relatively low strength contrast (<10/1), in which case both will undergo extensive flow and the strength of the aggregate will lie between those of the two individual phases. According to this study, the bulk rheology will lie in the middle between the uniform stress and uniform strain bounds.

It has been shown in Wang (1992) that Heavitree quartzite deforms at high temperatures by power-law creep ($n = 2.4$) at high stresses, and by Newtonian creep ($n = 1$) at low stresses (papers in preparation). In the latter case, dynamic recrystallization and melting occurred. Whether or not the Newtonian behavior at low stresses is related to the existence of a grain size distribution in the specimens is discussed as follows.

Eighty percent of grains in the starting material have sizes between 150 and 200 μm, about 10% smaller than 100 μm, and the rest larger than 200 μm. During deformation, dynamic recrystallization resulted in the formation of more small grains. Melts, often together with new fine grains (crystallized or recrystallized) are distributed mainly at triple grain junctions and at boundaries between grains oriented parallel to the loading direction. Both the original and the newly formed small grains might deform by grain boundary diffusion and/or sliding creep enhanced by the presence of melts at low stresses, while big grains deform by power-law creep.

According to the numerical modeling here, the overall creep behavior of the specimens might be Newtonian if the distribution of stress across grains of all sizes is uniform. If this is the reason why the stress exponent n is lowered from 2.4 at high stresses to 1 at low stresses, then:

(1) the activation energy Q should also be lowered from that for creep at high stresses to a value presumably equal to that for grain boundary diffusion;

(2) the Q for creep of Ta buffered specimens should be higher than that for creep of Mn buffered specimens because the Ta buffered specimens contain much smaller fractions of recrystallized grains and melts than the Mn buffered ones;

(3) bigger grains should show little deformation and no crystallographic preferred orientations.

However, these are not observed. It is observed that the Q for power-law creep at high stresses is about the same as that for Newtonian creep at low stresses, and that the Q for Newtonian creep in the Mn buffered environment is the same as that for Newtonian creep in the Ta buffered environment. Besides, it is shown that bigger grains were greatly flattened during deformation and that c-axis preferred orientations developed. These experimental observations indicate that the distribution of stress across bigger and smaller grains are not uniform, and oppose the suggestion that the Newtonian creep behavior at low stresses is caused by the operation of grain boundary diffusion and/or sliding creep enhanced by the presence of melt. The Newtonian behavior is attributed to be induced by a dislocation process operating in Harper–Dorn creep (Wang 1992).

CONCLUSIONS

At a constant temperature and stress, the rheological parameters, n (stress exponent), p (grain size exponent) and Q (activation energy) are influenced by the grain size distribution in a polycrystal. If the grain size is single-valued, these are affected by the grain size only. When the grain size is so large or so small that only one mechanism functions, the rheological parameters are equal to those for the single mechanism operating. If the distribution is diverse, these parameters are affected by the sizes of grains, their volume fractions and the loading configuration. In the case that grains of different sizes deform at the same stress, but at different rates, a small number of fine grains in a coarse polycrystal may initiate an overall Newtonian creep behavior. In the case that grains of different sizes deform at the same strain rate, but support different stresses, a small number of coarse grains in a fine polycrystal may induce an overall power-law creep behavior. The wide ranges of n, Q and p values in the literature might be (at least partly) attributed to the simultaneous operation of more than one mechanism. When a wide range of grain sizes exists, but is neglected, any conclusion about the dominant mechanism operating would be misleading if only the average

grain size is considered. It is recommended that increased attention be given to the grain size and its distribution in reporting and analyzing experimental data. Care should be taken when using microstructures to infer the overall rheology of rocks containing grains of widely differing sizes.

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