

Deformation behavior and stress states of a diffusional creeping polycrystal with bimodal grain-size distribution

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DIFFUSIONAL CREEP of a polycrystal with bimodal grain-size distribution is examined with spherical-grain approximation. Deformation behavior and stress states of the polycrystal are formulated when grain-boundary sliding occurs much more rapidly than diffusion. Two distinct effects of the grain-size distribution are discussed; the appearance of an initial transient stage in a creep curve of the polycrystal, and the stress concentration of deviatoric components generated at the center of larger grains.

Key words: diffusional creep, grain-boundary sliding, stress concentration, micro-mechanics.

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1. Introduction

VISCOUS SLIDING AT INTERNAL INTERFACES and stress-directed diffusion are two important fundamental processes in high-temperature deformation of materials. Diffusional creep of polycrystals is a typical example that is caused by the two fundamental processes. We can formulate the processes with an application of micromechanics based on linear elasticity [1]. The formulation method has been shown in our previous papers [2, 3]. In the analyses, combination of both fundamental processes has been considered since occurrence of sliding and diffusion changes both of their driving forces. Some recent studies have also considered the combination of sliding and diffusion to discuss the deformation behavior of composites or nanocrystalline materials [4–6].

In the present paper, using the method of analysis shown in our previous studies [2, 3], we consider a diffusional creeping polycrystal with bimodal grain-size distribution. Uniform grain-size has been often assumed for diffusional creep of polycrystals. However, rates of sliding and diffusion depend on the size of grains, and the grain-size distribution affects deformation behavior of polycrystals. Actually, the effects of the grain-size distribution on the kinetics of creep of materials have been pointed out in recent studies [7, 8]. In the present study, two effects of the grain-size distribution, which have not been reported in ana-

lytical forms as far as we know, will be discussed. One is the appearance of an initial transient stage in a creep curve of the polycrystal, and the other is the stress concentration of deviatoric components generated at the center of larger grains.

2. Grain-boundary sliding and stress-directed diffusion in materials

Here we explain the outline of the present method of analysis. Details of the following discussion were given in previous publications [2, 3].

Considering the generation of Somigliana's dislocations with the Burgers vectors \mathbf{b} on boundaries of the grains, we can describe the occurrence of grain-boundary sliding and diffusion. The tangential and normal components b_T and b_N of \mathbf{b} with respect to the grain boundaries, describe the occurrence of grain-boundary sliding and diffusion, respectively. Since grain-boundary sliding occurs by tangential tractions T_T acting on the grain boundaries, the rate of b_T , db_T/dt is written as a function of T_T . On the other hand, diffusion occurs by gradients of normal tractions T_N along the grain boundaries. The rate of b_N , db_N/dt is written as a function of T_N . Knowing the stresses in the grains σ_{ij}^S due to b_T (sliding) and σ_{ij}^D due to b_N (diffusion), T_T and T_N can be written as functions of both b_T and b_N . To include effects of interactions between grains, we use the average field method [9]. Then we have simultaneous differential equations in the rates db_T/dt and db_N/dt . The generation of b_T and b_N can be transformed into the generation of plastic strains in the grains [2, 3]. Considering the plastic strains ε_{ij}^S by sliding due to b_T and ε_{ij}^D by diffusion due to b_N , we finally obtain simultaneous differential equations in the rates of ε_{ij}^S and ε_{ij}^D [2, 3].

3. Creep behavior and stress states of polycrystal with grain-size distribution

3.1. Polycrystal under a uniaxial stress

Consider a sufficiently large polycrystal consisting of many equiaxed grains. As an example of a polycrystal with grain-size distribution, we consider a polycrystal with bimodal grain-size distribution. Approximating the shape of the equiaxed grains as spherical, we treat the polycrystal as consisting of grains of type 1 with radius a_1 and volume fraction f_1 and of type 2, with radius a_2 , with volume fraction f_2 , where $f_1 + f_2 = 1$. On the $x_1 - x_2 - x_3$ orthogonal coordinate system, we assume that an external stress $\sigma_{33}^A = \sigma^A$ is applied to the polycrystal. Although the effects of grain-boundary junctions where the sliding is suppressed are not included explicitly, the spherical approximation enables us

to treat the present problem in an analytical form. As shown in the previous studies [2, 3], effects of grain-boundary sliding and diffusion on overall deformation behavior of polycrystals have been successfully discussed with the spherical approximation.

For simplicity, we assume that grain-boundary diffusion is the only diffusion mechanism. That is to say, we consider the Coble creep of the polycrystal in the present study. We also assume that grain boundaries in the polycrystal slide in a Newtonian viscous fashion with viscosity η .

3.2. Creep behavior

The macroscopic plastic strain $\varepsilon_{33}^P = \varepsilon^P$ of the polycrystal with bimodal grain-size distribution is given by

$$(3.1) \quad \varepsilon^P = f_1\{\varepsilon^S(1) + \varepsilon^D(1)\} + f_2\{\varepsilon^S(2) + \varepsilon^D(2)\},$$

where $\varepsilon^S(i)$ and $\varepsilon^D(i)$ are the 33 components of the averaged strains in the grains of type i ($i = 1$ or 2) caused by grain-boundary sliding and diffusion, respectively. Using the method of analysis outlined in Section 2, we have simultaneous differential equations in $\varepsilon^S(i)$ and $\varepsilon^D(i)$. The explicit forms of the equations are shown in the Appendix.

In the following discussion, we assume that grain-boundary sliding occurs much more rapidly than diffusion, i.e. $\eta \rightarrow 0$. Then, using the initial conditions $\varepsilon^D(i) = 0$ when $t = 0$, the simultaneous differential equations (A.1) in the Appendix are solved and ε^P of (3.1) is given as a function of time t after loading by

$$(3.2) \quad \varepsilon^P = \frac{35(1-\nu)\sigma^A}{8(7+5\nu)\mu} + \frac{25(1-\nu)(21+\nu)\sigma^A}{8(7+5\nu)(7-5\nu)\mu} \frac{f_1 f_2 (a_1^3 - a_2^3)^2}{\{f_1 a_1^3 + f_2 a_2^3\}^2} \left\{ 1 - \exp\left(\frac{-t}{\tau}\right) \right\} \\ + \frac{20cD\Omega\sigma^A}{kT\{f_1 a_1^3 + f_2 a_2^3\}} t,$$

where μ is the shear modulus, ν the Poisson ratio, $2c$ the grain-boundary thickness, D the grain-boundary diffusion coefficient, Ω the atomic volume, and k and T have their usual meaning. The relaxation time τ in the second term of the right-hand side of (3.2) is given by

$$(3.3) \quad \tau = \frac{5(21+\nu)(1-\nu)kT}{32(49-25\nu^2)\mu c D \Omega} \frac{a_1^3 a_2^3}{\{f_1 a_1^3 + f_2 a_2^3\}}.$$

When $a_1 = a_2$, (3.2) reproduces the result for the polycrystal with uniform grain size [3].

Because of the assumption of the fast grain-boundary sliding ($\eta \rightarrow 0$), η appears in neither (3.2) nor (3.3). The first term of the right-hand side of (3.2) shows

the instantaneous strain caused by fast grain-boundary sliding with $\eta \rightarrow 0$. This term does not have the grain-size dependence. The second term shows transient deformation behavior with relaxation time τ . This term becomes zero when $a_1 = a_2$. During initial deformation after loading, deformation by diffusion in smaller grains occurs faster than in larger grains. The larger grains retard the fast deformation in the smaller grains. As deformation of the polycrystal proceeds, the averaged plastic-strain rates in the smaller and larger grains become the same. This is the reason for the occurrence of the transient behavior caused by the grain-size distribution. The third term of (3.2) gives the rate of steady-state deformation of the polycrystal.

3.3. Stress states in the bimodal grains

The external stress applied to the polycrystal is $\sigma_{33}^A = \sigma^A$. In this case, the stresses $(\sigma_{33} - \sigma_{11})$ and $(\sigma_{33} - \sigma_{22})$ are important components to discuss the deviatoric components. The stress $(\sigma_{33} - \sigma_{22})$ in the spherical grains is essentially the same as $(\sigma_{33} - \sigma_{11})$. We hence consider the variations of the stress $(\sigma_{33} - \sigma_{11})$ in this paper.

By using the average field method [9], the stresses in grains can be written as functions of the averaged strains [10]. The stress $\sigma_{33}(i) - \sigma_{11}(i)$ for the grain of type i ($i = 1$ or 2) is written as a function of time t in the form

$$(3.4) \quad \sigma_{33}(i) - \sigma_{11}(i) = \sigma^A \left[1 + \frac{(21 - 5R^2/a_i^2)}{2(7 + 5\nu)} + \frac{5\{(7 + 2\nu) - R^2/a_i^2\}}{2(7 + 5\nu)} \right. \\ \left. \times \frac{(1 - f_i)(2a_i^3 - a_1^3 - a_2^3)}{\{f_1 a_1^3 + f_2 a_2^3\}} \left\{ 1 - \exp\left(\frac{-t}{\tau}\right) \right\} \right],$$

where

$$(3.5) \quad R^2 = \{(7 - 4\nu)x^2 + 4\nu(x_1^2 + 2x_2^2)\}$$

and $x^2 = x_i x_i = x_1^2 + x_2^2 + x_3^2$ is a function of the position (x_1, x_2, x_3) in the spherical grain having its center at the origin.

From (3.4) and (3.5), the averaged stress $\langle \sigma_{33}(i) - \sigma_{11}(i) \rangle$ in the grain of type i is written as

$$(3.6) \quad \langle \sigma_{33}(i) - \sigma_{11}(i) \rangle = \sigma^A \left[1 + \frac{(1 - f_i)(2a_i^3 - a_1^3 - a_2^3)}{\{f_1 a_1^3 + f_2 a_2^3\}} \left\{ 1 - \exp\left(\frac{-t}{\tau}\right) \right\} \right].$$

Here we have

$$(3.7) \quad \sum_{i=1}^2 f_i \langle \sigma_{33}(i) - \sigma_{11}(i) \rangle = \sigma^A,$$

which means that the sum of the averaged stresses in the grains of types 1 and 2 is equal to the applied uniaxial-stress σ^A as it should be. In the steady state when $t/\tau \gg 1$, the averaged stress in the grain of type i becomes

$$(3.8) \quad \langle \sigma_{33}(i) - \sigma_{11}(i) \rangle (t \gg \tau) = \sigma^A \frac{a_i^3}{\{f_1 a_1^3 + f_2 a_2^3\}}.$$

4. Transient stage of diffusional creep

We have formulated the deformation behavior of diffusional creeping polycrystal with bimodal grain-size distribution. Using (3.2) and (3.3), we can show the time t dependence of the macroscopic strain ε^P of the polycrystal. The curve in Fig. 1 shows the time-dependence of ε^P for the bimodal grain-size distribution with $a_1 = 5 \mu\text{m}$ and $f_1 = 0.8$, and $a_2 = 14.5 \mu\text{m}$ and $f_2 = 0.2$. These values were adopted in a previous study to model the grain-size distribution in an Al alloy [11]. To show the curve in Fig. 1, we have assumed $\sigma^A = 1 \text{ MPa}$, $T = 790 \text{ K}$ and the following parameters appropriate for Al were chosen: $\mu = 1.7 \times 10^{10} \text{ Pa}$, $\nu = 0.34$, $2cD = 3 \times 10^{-19} \text{ m}^3\text{s}^{-1}$, $\Omega = 1.6 \times 10^{29} \text{ m}^3$ [11, 12].

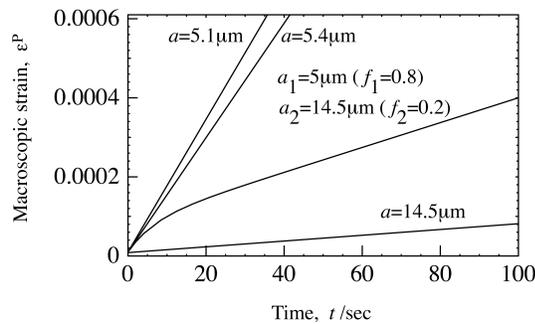


FIG. 1. Theoretically-evaluated creep curves for the polycrystals with bimodal grain-size distribution and three kinds of uniform grain sizes.

For comparison, variations of ε^P for uniform grain-sizes are also indicated in Fig. 1. The three lines are the results for the uniform grain-sizes with 1) $a = 5.1 \mu\text{m}$ (the average grain-size of the bimodal distribution), 2) $a = 5.4 \mu\text{m}$ (the grain-size giving the average grain-volume, $\bar{V} = (\text{total volume})/(\text{number of grains})$) and 3) $a = 14.5 \mu\text{m}$ (the same grain-size with that of a_2). Since the ratio of the numbers of grains of types 1 and 2 for the bimodal grain-size distribution is $(0.8/5^3)/(0.2/14.5^3) \approx 100$, the average values, 5.1 and 5.4 μm , become close to $a_1 = 5 \mu\text{m}$. As shown in Fig. 1, the creep curves obtained by assuming averaged uniform grain-sizes overestimate the deformation rate of the polycrystal with bimodal grain-size distribution. Moreover, an initial transient stage of the creep

curve appears clearly for the bimodal grain-size distribution. The creep curve for the bimodal grain-size distribution is clearly different from those for the uniform grain-sizes shown in Fig. 1. In previous experimental studies on diffusional creep, such transient stages have sometimes been found [13].

As described in Sec. 3.2, the second term of the right-hand side of (3.2) shows the strain $\varepsilon_{\text{tran}}(t)$ of the transient stage, which is written as

$$(4.1) \quad \varepsilon_{\text{tran}}(t) = \frac{25(1-\nu)(21+\nu)\sigma^A}{8(7+5\nu)(7-5\nu)\mu} \frac{f_1 f_2 (a_1^3 - a_2^3)^2}{\{f_1 a_1^3 + f_2 a_2^3\}^2} \left\{ 1 - \exp\left(\frac{-t}{\tau}\right) \right\}.$$

The bimodal-structure dependence of the magnitude of $\varepsilon_{\text{tran}}(t)$ can be evaluated by considering the dimensionless parameter $m(\varepsilon_{\text{tran}})$:

$$(4.2) \quad m(\varepsilon_{\text{tran}}) = \frac{\{\varepsilon_{\text{tran}}(t \rightarrow \infty) - \varepsilon_{\text{tran}}(t = 0)\}}{\left\{ \frac{25(1-\nu)(21+\nu)\sigma^A}{8(7+5\nu)(7-5\nu)\mu} \right\}} = \frac{f_1 f_2 (a_1^3 - a_2^3)^2}{\{f_1 a_1^3 + f_2 a_2^3\}^2}.$$

The maximum of $m(\varepsilon_{\text{tran}})$ is given from (4.2) as

$$(4.3) \quad m(\varepsilon_{\text{tran}})_{\text{max}} = \frac{(a_1^3 - a_2^3)^2}{4a_1^3 a_2^3} \quad \text{when} \quad f_1 = \frac{a_2^3}{a_1^3 + a_2^3} \quad \text{and} \quad f_2 = \frac{a_1^3}{a_1^3 + a_2^3}.$$

From these equations, we know that the transient stage appears most significantly when the bimodal grain-size distribution satisfies the following relation:

$$(4.4) \quad f_1 a_1^3 = f_2 a_2^3.$$

Figure 2 shows the volume-fraction f_1 dependence of $m(\varepsilon_{\text{tran}})$ when $a_1 = 5 \mu\text{m}$ and $a_2 = 14.5 \mu\text{m}$. We have $m(\varepsilon_{\text{tran}})_{\text{max}} \approx 5.6$ when $f_1 \approx 0.96$ and $f_2 = 1 - f_1 \approx 0.04$ as given by (4.3) for $a_1 = 5 \mu\text{m}$ and $a_2 = 14.5 \mu\text{m}$. As shown

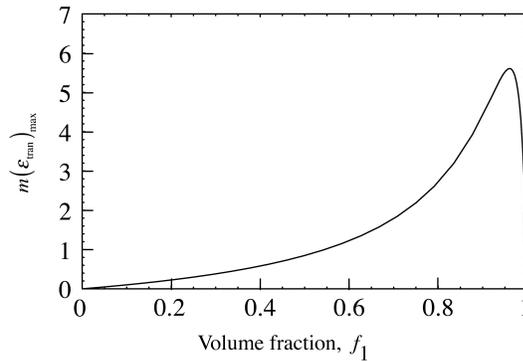


FIG. 2. The volume-fraction f_1 dependence of $m(\varepsilon_{\text{tran}})$ when $a_1 = 5 \mu\text{m}$ and $a_2 = 14.5 \mu\text{m}$.

in Fig. 2, we find that a peak of $m(\varepsilon_{\text{tran}})$ is located at the large value of f_1 . Figure 3 shows the volume-fraction dependence of the creep curve for $a_1 = 5 \mu\text{m}$ and $a_2 = 14.5 \mu\text{m}$. Three solid curves are those for $f_1 = 0.6, 0.8$ and 0.96 . Broken lines are drawn in Fig. 3 to show the rates of steady state deformation of the creep curves. Deviation of the creep curve from the broken line at $t = 0$ shows the magnitude of $\varepsilon_{\text{tran}}(t)$. Although the introduction of the small amount of larger grains does not change the rate of steady-state deformation significantly, it causes a clear transient stage of the creep curve as shown in Fig. 3.

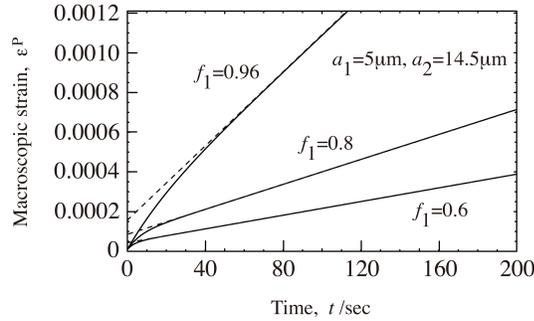


FIG. 3. The volume-fraction dependence of the creep curve when $a_1 = 5 \mu\text{m}$ and $a_2 = 14.5 \mu\text{m}$.

5. Stress concentration in large grains in polycrystals

Using (3.3) and (3.6) and the material parameters shown in Section 4, we show the transitions of the stress states in the polycrystal with the bimodal grain-size distribution $a_1 = 5 \mu\text{m}$ and $f_1 = 0.8$, and $a_2 = 14.5 \mu\text{m}$ and $f_2 = 0.2$. The curves in Fig. 4 show the variations with time t after loading of the normalized

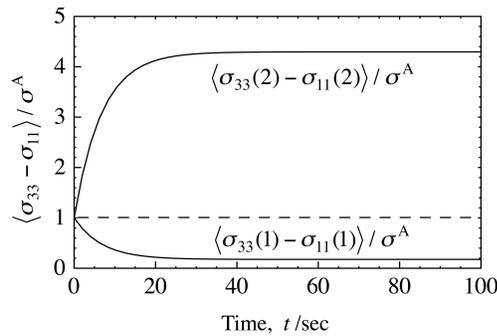


FIG. 4. Relationships between $\langle \sigma_{33}(i) - \sigma_{11}(i) \rangle / \sigma^A$ and t for the grains of types 1 and 2 of the polycrystal, with bimodal grain-size distribution $a_1 = 5 \mu\text{m}$ and $f_1 = 0.8$, and $a_2 = 14.5 \mu\text{m}$ and $f_2 = 0.2$. σ^A is the applied uniaxial stress.

averages of the stresses $\langle \sigma_{33}(i) - \sigma_{11}(i) \rangle / \sigma^A$ in the grains of types 1 and 2. Since the rate of diffusional creep is faster for smaller grains, the stresses become lower in the smaller grains of type 1. On the other hand, the higher stresses are generated in the larger grains of type 2. The generation of higher stresses in the larger grains is not surprising, since the sum of the averaged stresses in the smaller and larger grains should be equal to the applied stress as shown by (3.7).

In the larger grains, the stress $(\sigma_{33}(i) - \sigma_{11}(i))$ becomes the largest at the center of the grains. This is understood by substituting $x^2 = x_i x_i = x_1^2 + x_2^2 + x_3^2 = 0$ into (3.4) and (3.5). The maximum of $(\sigma_{33}(2) - \sigma_{11}(2))$ in the grains of type 2 for $t/\tau \gg 1$ is written as

$$(5.1) \quad (\sigma_{33}(2) - \sigma_{11}(2))_{\max}(t \gg \tau) = \frac{5(7 + 2\nu)\sigma^A}{2(7 + 5\nu)} \frac{a_2^3}{\{f_1 a_1^3 + f_2 a_2^3\}}.$$

We have $(\sigma_{33}(2) - \sigma_{11}(2))_{\max}(t \gg \tau) \approx 9.5\sigma^A$ when $\nu = 0.34$ for the bimodal grain-size distribution with $a_1 = 5 \mu\text{m}$ and $f_1 = 0.8$, and $a_2 = 14.5 \mu\text{m}$ and $f_2 = 0.2$. From (3.4) and (3.5), the contour lines of $(\sigma_{33}(2) - \sigma_{11}(2))(t \gg \tau)$ on the $x_1 - x_3$ cross-section of the larger grain are obtained as shown in Fig. 5. Figure 5 shows that the stress concentration is generated extensively in the larger grain. The grain boundaries in polycrystals cause the stress relaxation and the locations at the center of the larger grains are those farthest from the grain boundaries. These are the reasons why the stress concentration occurs at the center of the larger grains, in the diffusional creeping polycrystal with a bimodal grain-size distribution.

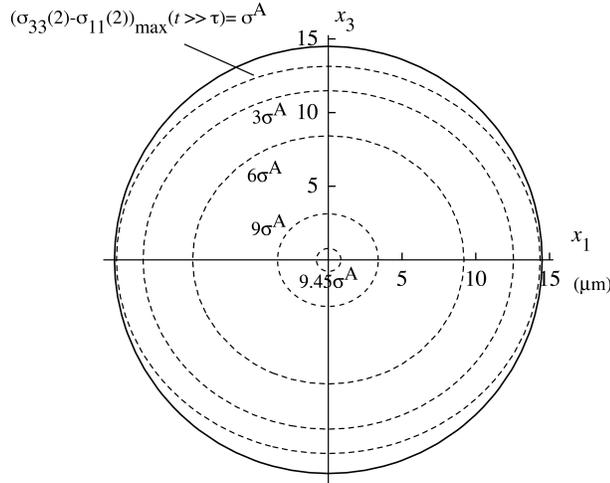


FIG. 5. Contour lines of $(\sigma_{33}(i) - \sigma_{11}(i))(t \gg \tau)$ on the $x_1 - x_3$ cross-section of the larger spherical grain of type of 2 in the polycrystal with bimodal grain-size distribution $a_1 = 5 \mu\text{m}$ and $f_1 = 0.8$, and $a_2 = 14.5 \mu\text{m}$ and $f_2 = 0.2$. σ^A is the applied uniaxial stress.

6. Application to nano-structured materials

We have shown the effects of the grain-size distribution on the creep rates and stress states in the creeping polycrystals. The calculations to evaluate the effects have been made by using grain sizes reported in a previous study for a usual Al alloy [11]. This is to show that the effects cannot be neglected even in conventional materials. However, since both the rates of diffusion and sliding increase with decreasing the grain size, the effects may appear more significantly in deformation of fine- or nano-grained materials [6, 14]. Coexistence of high strength and high ductility has been reported for nano-structured metals with bimodal grain-size distributions [15]. Large stress-relaxation or high strain-rate dependence of flow stress is a characteristic of the fine- or nano-grained materials [16]. Analysis of such deformation behavior is a possible application of the results shown in the present paper.

7. Conclusions

We have discussed deformation behavior and stress states of a diffusional creeping polycrystal with a bimodal grain-size distribution. Using the spherical-grain approximation, the creep rates and stress states of the polycrystal have been formulated when grain-boundary sliding is much faster than diffusion. The results obtained in the present study are summarized as follows.

1. The rates of diffusional creep given from averaged grain-sizes overestimate the creep rate of a polycrystal with bimodal grain-size distribution.
2. An initial transient stage appears in the creep curve of a polycrystal with a distribution of grain-sizes.
3. Larger deviatoric stresses generate in larger grains and the stresses become largest at the centers of the grains.

Appendix

Using a method of analysis shown in our previous papers [2, 3], the simultaneous differential equations in the rates of ε^S and ε^D for the bimodal grain-size distribution are written as

$$\begin{aligned}
 (A.1) \quad & d\varepsilon^S(1)/dt = (A/a_1)[\beta - P_1(f_1)\varepsilon^S(1) + P_2(f_1)\varepsilon^D(1) + Q(f_2)\{\varepsilon^S(2) + \varepsilon^D(2)\}], \\
 & d\varepsilon^D(1)/dt = (B/a_1^3)[\beta + P_2(f_1)\varepsilon^S(1) - P_3(f_1)\varepsilon^D(1) + Q(f_2)\{\varepsilon^S(2) + \varepsilon^D(2)\}], \\
 & d\varepsilon^S(2)/dt = (A/a_2)[\beta - P_1(f_2)\varepsilon^S(2) + P_2(f_2)\varepsilon^D(2) + Q(f_1)\{\varepsilon^S(1) + \varepsilon^D(1)\}], \\
 & d\varepsilon^D(2)/dt = (B/a_2^3)[\beta + P_2(f_2)\varepsilon^S(2) - P_3(f_2)\varepsilon^D(2) + Q(f_1)\{\varepsilon^S(1) + \varepsilon^D(1)\}],
 \end{aligned}$$

where

$$(A.2) \quad \begin{aligned} A &= \frac{4c\mu}{175(1-\nu)\eta}, \quad B = \frac{16cD\Omega\mu}{175(1-\nu)kT}, \quad \beta = \frac{35(1-\nu)\sigma^A}{\mu}, \\ P_1(f) &= \{5(21+\nu) - 7(7-5\nu)f\}, \\ P_2(f) &= \{5(7+19\nu) + 7(7-5\nu)f\}, \\ P_3(f) &= \{5(35+11\nu) - 7(7-5\nu)f\}, \\ Q(f) &= 7(7-5\nu)f. \end{aligned}$$

The variables shown in (A.1) and (A.2) are explained in the main text. For diffusional creep of polycrystal with uniform grain-size distribution, simultaneous differential equations similar to the above equations have been derived [3]. When $a_1 = a_2$, (A.1) and (A.2) become identical to the results in the paper by ONAKA *et al.* [3].

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