ON THE THEORY OF DIFFUSION-VISCOUS FLOW OF POLYCRYSTALLINE BODIES

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The mechanism is analyzed and a quantitative theory is developed for the high-temperature diffusion viscous flow of polycrystalline bodies at low stresses. The role of slip along grain boundaries during their motion and diffusion deformation is explained. The viscosity coefficient tensor, which depends on the structural anisotropy of the substance (grain shapes and sizes) and on the magnitude of resistance to slip along grain boundaries, is derived. In addition to the exact value of this tensor, simple interpolation formulas are given which permit investigation of the general flow equations. By way of example the kinetics of the filling-up of a spherical pore under pressure is considered. A study was made of the effects accompanying the process of diffusion-viscous flow: the appearance of nonuniform stress fluctuations in a single grain (stresses of the second kind), variation of the macroscopic elastic moduli during flow, etc. The limits of applicability of the theory are discussed.

1. MECHANISM OF DIFFUSION-VISCOUS FLOW. STATEMENT OF THE PROBLEM

IT is known that, apart from the plastic flow of crystals, which is a threshold effect and occurs under sufficiently high loads, there is also a diffusion-viscous flow in solids at arbitrarily low stresses. The latter process is due to the diffusion of vacancies and is important only at high temperatures when this diffusion is sufficiently intensive. Strictly speaking, this process is dominant only at low stresses when all the other mechanisms of a threshold nature (in particular the formation and motion of dislocations) are inactive.

The basic idea of the mechanism of diffusion-viscous flow was first put forward in the work of Nabarro [1] and Herring; [2] the latter work gives calculations and estimates for some typical cases of such flow. However, neither Nabarro nor Herring allowed for some important factors. Consequently there were many obscurities in their picture of the process as a whole and in the conditions for its appearance, their estimates were not always valid. In the present work this mechanism is analyzed from a somewhat different point of view and a derivation is given of a complete system of equations describing the process of diffusion-viscous flow in the general case. At the same time the concomitant phenomena, typical of the mechanism of diffusion-viscous flow, become clear.

The first assumption in the mechanism of diffusion-viscous flow is that the surfaces bounding structural units in a real crystalline body (separate grains in a polycrystal or separate blocks in a coarse-mosaic single crystal) are virtual sources and sinks for vacancies. In a perfect crystalline lattice a vacancy cannot be generated or annihilated by itself but a sufficiently defective surface represents, as it were, an "amorphous" layer which is capable of reversible rearrangement when some vacancies reach it: it becomes as it were "compressed" to its initial density and vacancies disappear. [1)]

On the basis of this assumption the mechanism of flow is as follows: in a body subjected to a macroscopically uniform but anisotropic stress σ_{ik}, various normal stresses $\sigma_{ik}n_in_k$ (n is the vector normal to the surface) act on various portions of crystallite surfaces. Consequently near these surfaces the extent of saturation with vacancies varies: the chemical potential μ of a vacancy at the surface (which is a virtual source of vacancies) will, by virtue of the equilibrium between the annihilation and generation of vacancies, be equal to

$$\mu = \mu_0 + \sigma_{nn}\omega_0, \qquad \mu - \mu_0 = kT \ln (c/c_0) \qquad (1)$$

(c_0 is the equilibrium concentration of vacancies at $p = 0$; μ_0 is the chemical potential for the concentration c_0; ω_0 is the volume per unit vacancy);

[1)] An analysis of the conditions under which a block boundary can be considered as a surface with virtual sources is given in Appendix 1.

hence the value of the vacancy excess $\Delta_c = c - c_0$ is determined by the relationship

$$\Delta c = c_0\omega_0\sigma_{nn}/kT. \qquad (2)$$

The resultant concentration gradients within a grain give rise to diffusion currents of vacancies (or equivalent currents of atoms in the opposite direction). These currents produce a change of the grain shape without a change of its volume. The characteristic feature of this process is the absence of macroscopic diffusion currents in the body as a whole and the presence only of complex microscopically nonuniform currents within each grain.

Deformation of the whole crystalline body consisting of a very large number of grains is a self-consistent process in the sense that discontinuities are not produced at the grain boundaries and the diffusion-viscous deformation of a particular grain depends on the deformations of the grains which surround it. The analysis given below shows that this necessarily produces stress fluctuations within each grain (stresses of the second kind) in spite of a macroscopically uniform stress state of the whole sample.

The self-consistent change in the shape of the grains is the result of the directional motion of their centers of gravity which produces macroscopic changes in the shape of the body (flow). This displacement of the centers of gravity of the grains in diffusion-viscous flow is similar to the displacement of molecules in the process of the viscous flow of liquids, and is necessarily accompanied by slip along grain boundaries.

If we introduce an average value of the stress tensor $p_{ik} = \bar{\sigma}_{ik}$ in a small macroscopic element of volume containing a large number of grains, and also an average value of the velocities of displacement of particles in this element $V_i = \bar{v}_i$, then a macroscopic description of the process of flow is equivalent to the establishment of a relationship between the tensor p_{ik} and the rate-of-deformation tensor $V_{ik} = \frac{1}{2}(\partial V_i/\partial x_k + \partial V_k/\partial x_i)$. In the general case of quasi-steady-state flow such a relationship should have the form

$$p_{ik} = p_0\,\delta_{ik} + \alpha_{iklm}V_{lm}, \qquad V_{ii} = 0, \qquad (3)$$

where the viscosity tensor α_{iklm} is governed by the sizes and shapes of the grains, i.e., by the "structural anisotropy" of the polycrystal.

The equation of continuity $V_{ii} = 0$ characterizes the aforementioned constancy of the grain volume and the absence of discontinuities. In the simplest case of structural isotropy α_{iklm} reduces to a scalar η and Eq. (3) becomes

$$p_{ik} = -p\delta_{ik} + \eta V_{ik}, \qquad -p = p_{ll}/3. \qquad (3a)$$

According to Eq. (2) the variation of the vacancy concentration δc on the grain surface is governed by the non-spherical (shear) part $p'_{ik} = p_{ik} + p\delta_{ik}$ of the stress tensor: $\delta c = c_0\omega_0 p'/kT$. Therefore, the rate of deformation related to the diffusion currents $j_i = D_0\partial c/\partial x_i$ should be of the order of magnitude of

$$V_{ik} \sim D_0\partial^2 c/\partial x_i\partial x_k \sim D_0\delta c/L^2 \sim p'D_0c_0\omega_0/L^2kT$$

(L is the grain size). This gives an estimate of the expected magnitude of the viscosity tensor α_{iklm}:

$$\alpha_{iklm} \sim \eta \sim kTL^2/D\omega_0, \qquad D = D_0c_0$$

(D_0 is the vacancy diffusion coefficient and D is the atomic self-diffusion coefficient). We shall see, however, that this estimate is valid only in the case of free slip along grain boundaries.

The macroscopic coordinate dependence of the tensors p_{ik} and V_{ik} is determined by the equilibrium equation

$$\partial p_{ik}/\partial x_k = 0, \qquad (4)$$

which, together with Eq. (3), forms a complete system for the determination of the four quantities V_i and p_0:

$$\frac{\partial p_0}{\partial x_i} + \frac{\partial}{\partial x_k}\alpha_{iklm}\frac{\partial V_l}{\partial x_m} = 0, \qquad \operatorname{div}\mathbf{V} = 0. \qquad (4a)$$

Thus our problem reduces to the derivation of Eq. (3) and the determination of α_{iklm} in terms of the structural anisotropy of the polycrystal and the properties of the grain boundaries.

2. SELF-CONSISTENT DISPLACEMENT AND DEFORMATION OF GRAINS. ALIGNMENT OF STRESSES. ROLE OF SLIP ALONG GRAIN BOUNDARIES.

We shall consider a macroscopically uniform portion of the polycrystal (large compared with the grain dimensions) with given constant values of the average quantities p_{ik} and V_{ik} ($V_{ii} = 0$). We shall select a microscopic element of volume (small compared with the grain dimensions) and follow its motion. The mass-current density, or in other words the average velocity $\mathbf{v}$ of this element, consists of a part $\mathbf{v}^\alpha$, related to the motion of the grain as a whole, and a part related to the vacancy-diffusion current $\mathbf{j} = -D_0\nabla c$; since the current of atoms is equal to the current of vacancies in the opposite direction, then [2)]

[2)]Hereafter we shall assume that the diffusion coefficient is isotropic.

$$\mathbf{v} = \mathbf{v}^{\alpha} + D_0 \nabla c. \tag{5}$$

From the continuity condition it follows that at the boundary of two grains denoted by α and β the normal components of the velocity v_n should be equal. According to Eq. (5) this gives the expression

$$D_0 \frac{\partial c}{\partial n}\Big|_{\alpha} - D_0 \frac{\partial c}{\partial n}\Big|_{\beta} = v_n^{\beta} - v_n^{\alpha}, \tag{6}$$

which represents the conditions for self-consistent motion of the grains and diffusion currents.

Since the concentration of vacancies is very small, only a negligibly small deformation ($\sim c_0$) can take place during the time necessary to establish a quasi-steady-state diffusion current, and consequently during the whole process the distribution of vacancies is given by $\Delta c = 0$ (according to Eq. (5) this means div $\mathbf{v} = 0$).

For convenience in later treatment, instead of the concentration of vacancies we shall use a potential proportional to it

$$\varphi = \mu - \mu_0/\omega_0 = (kT/c_0\omega_0)(c - c_0). \tag{7}$$

As mentioned above, the potential φ is governed by the equation

$$\Delta\varphi = 0 \tag{8}$$

and by the boundary conditions at the surfaces of separation of the grains

$$\delta\left(\frac{\partial\varphi}{\partial n}\right)\Big|_S = \frac{\partial\varphi}{\partial n}\Big|_{\alpha} - \frac{\partial\varphi}{\partial n}\Big|_{\beta} = \varkappa(v_n^{\beta} - v_n^{\alpha}), \quad \varkappa = \frac{kT}{D\omega_0}. \tag{9}$$

Moreover, according to the equilibrium condition of Eq. (1) the value of φ at each point on a grain boundary represents the normal stress at that surface

$$\varphi|_S = \sigma_{nn}. \tag{10}$$

Strictly speaking, the equilibrium condition of Eq. (10) in the presence of currents $\approx \nabla\varphi$ should be replaced by the dynamic condition $\varphi|_S - \sigma_{nn} = \lambda\partial\varphi/\partial n$. However, if the natural assumption is made that $\lambda \approx a$ (a is the lattice constant), the term $\lambda\partial\varphi/\partial n$ may be neglected.

An important conclusion follows from the conditions formulated above: since the conditions of Eqs. (9) and (10) cannot be satisfied independently, then for the quasi-steady-state flow to appear, a preliminary alignment of the stresses near a grain boundary should occur, making Eqs. (9) and (10) compatible. This can easily be explained by a simple example: let us consider the diffusion-viscous compression of a single-crystal cube under the pressure p of a perfectly hard piston (Fig. 1). Obviously the upper face of the cube can be displaced only as a whole. Initially the normal stress σ_{nn} at all points of this face is constant and equal to $-p$; consequently $\varphi = -p$ at the upper face and $\varphi = 0$ at the lateral faces. This means that very strong diffusion currents appear near the corners and weak diffusion currents in the center. Since the rate of displacement of the boundary cannot match these currents at each point, elastic deformations appear on the surface due to the redistribution of atoms when the boundary position is fixed.

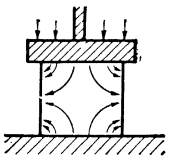

FIG. 1

Then σ_{nn} is no longer constant in the boundary and only $\overline{\sigma_{nn}} = -p$; in particular the pressure decreases near the corners, becoming zero at the corner. Steady-state motion of the piston is achieved when the pressure distribution over the surface is such that the diffusion current is constant at all points on the upper face. [3)]

Thus the initial elastically uniform state of the body is destroyed in the process of establishing diffusion-viscous flow and is replaced by a complex distribution of stresses inside each grain (stresses of the second kind). It is necessary to emphasize particularly that the stresses of the second kind appearing in diffusion-viscous flow are not identical to the stress fluctuations in polycrystals due to the elastic anisotropy [3] of the separate crystallites, and may even occur in the isotropic model. The actual distribution of these stresses will be considered below.

A second important point in the characteristics of the stressed state is related to the role of slip along "amorphous" layers at grain boundaries. It follows from Eq. (10) that the potential φ and consequently also its tangential derivative are continuous at the grain boundary. This means, according to Eq. (5), that the tangential components of the velocity v_t have a discontinuity at the boundary $\delta v_t|_S = v_t^{\beta} - v_t^{\alpha}$ (here $\delta v_t|_S$ is the velocity of slip along the boundary). Thus the self-consistent change of the shape of blocks and their displacement in the process of diffusion-viscous flow are necessarily accompanied by slip along boundaries. (Obviously for an arbitrary grain shape the vanishing values of all $v_t^{\beta} - v_t^{\alpha}$

[3)] An analysis of the process of stress "alignment" and of the concomitant phenomena will be given in a separate communication.

mean that for all grains $v^\alpha = 0$ and nothing can occur except a directional diffusion current in the body as a whole.)

An estimate of the tangential stresses σ_{tn} at the boundary due to flow can be obtained from the following considerations: we shall represent the viscosity of the "amorphous" layer at the boundary by a coefficient η_S and relate it to the resistance to slip by the self-evident equality

$$\sigma_{tn}|_S = \eta_S (v_t^\beta - v_t^\alpha)/a \qquad (11)$$

(a is the lattice constant). Obviously $v_t^\beta - v_t^\alpha \approx LV_{ik} \approx L\delta\sigma_{nn}/\eta^0 a$, $\eta^0 \approx \kappa L^2$ (L is the grain size, $\delta\sigma_{nn}$ is the variation of σ_{nn} along the boundary) consequently

$$\sigma_{tn} \sim \eta_S \delta\sigma_{nn}/\varkappa aL, \qquad \varkappa = kT/D\omega_0. \qquad (11a)$$

The viscosity of the amorphous layer is clearly independent of the grain size and for a sufficiently defective boundary (at high temperatures) its order of magnitude is $\eta_S \approx \kappa a^2 \approx kT/Da$. This gives us an estimate $\sigma_{tn}|_S \approx a\delta\sigma_{nn}/L$, i.e., in practice $\sigma_{tn}|_S = 0$. Thus in this case the distribution of stresses is given by the condition (10) for the normal stresses, and by zero values of the tangential stresses at the surfaces of separation between the grains.

However, if the surface of separation between the grains is insufficiently amorphous, then slip may be greatly impeded and the estimate $\eta_S \approx \kappa a^2$ is no longer valid. If η_S is so large that $\eta_S L/a\eta^0 \gg 1$, then according to Eq. (11a) the tangential stresses are very large:

$$\sigma_{th} \sim \eta_S LV_{ik}/a \gg \eta^0 V_{ik}.$$

In this case the rate of deformation is limited by slip. A simple estimate of the non-spherical part of p'_{ik} gives

$$p'_{ik} = \overline{\sigma'_{ik}} \sim \sigma_{tn} \sim \eta^* V_{ik}, \qquad \eta^* = \eta_S L/a,$$

i.e., the effective viscosity of the polycrystal η^* is considerably greater than the expected value $\eta = \eta^0$. The estimate (11a) shows that in this case the normal stresses are practically constant at the boundary

$$\delta\sigma_{nn} \sim \frac{\eta_0}{\eta_S}\frac{a}{L}\sigma_{tn} \sim \frac{\eta_a}{\eta_S}\frac{a}{L}p' \ll p'.$$

Therefore, the diffusion currents are much smaller than the estimate in the preceding case and "align" themselves automatically with the deformation rate governed by the possibility of slip.

3. SOLUTION OF THE DIFFUSION PROBLEM. CALCULATION OF THE VISCOSITY TENSOR

Let us return now to the diffusion problem. Equation (8) with the condition (9) corresponds to the electrostatic problem of the potential distribution in the presence of a network of surface charges with density $4\pi q = -\kappa(v_n^\beta - v_n^\alpha)$. Its solution has the well-known form

$$\varphi(\mathbf{r}) = \varphi_0 + \int \frac{q\,dS}{R'}, \qquad \mathbf{R}' = \mathbf{R} - \mathbf{r},$$

where integration is carried out over the whole network of surfaces of separation ($\mathbf{R}$ is the integration variable, and φ_0 is constant because of the macroscopic uniformity and is determined below).

The basis of the derivation (given below) of a relationship between V_{ik} and p_{ik} is that, by selecting fixed values of V_{ik}, we can find the average stresses in the medium during flow. Consequently before proceeding further it is necessary to relate the velocities of motion of individual grains to the macroscopic deformation-rate tensor $\hat{V} = V_{ik}$.

When the deformation is completely uniform the velocity at the point $\mathbf{R}$ is $\mathbf{V} = \hat{V}\mathbf{R}$, where $V_i = V_{ik}X_k$, taking account of the rotation of the medium as a whole; consequently if R^α is the coordinate of the center of gravity of the α-th grain, then

$$v_i^\alpha = V_{ik}X_k^\alpha + u_i^\alpha, \qquad (12)$$

where u^α are the random deviations of the velocity of motion of the α-th grain from the average value of the velocity of matter at this point ($\overline{u} = 0$).

Taking into account the fact that vector normals to the surface of each of neighboring grains have different signs at the surface and using Eq. (12), we transform the expressions for $q^{\alpha\beta}$ into the form

$$q^{\alpha\beta} \equiv q^\alpha + q^\beta = -(\varkappa/4\pi)(\mathbf{v}^\alpha\mathbf{n}^\alpha + \mathbf{v}^\beta\mathbf{n}^\beta)$$

$$= -(\varkappa/4\pi)[(\mathbf{v}^\alpha - \hat{V}\mathbf{R})\mathbf{n}^\alpha + (\mathbf{v}^\beta - \hat{V}\mathbf{R})\mathbf{n}^\beta],$$

$$4\pi q^\alpha = \varkappa V_{ik}\xi_k^\alpha n_i - \varkappa u_i^\alpha n_i^\alpha, \qquad \xi^\alpha = \mathbf{R} - \mathbf{R}^\alpha. \qquad (13)$$

Here $\xi^\alpha = \mathbf{R} - \mathbf{R}^\alpha$ are the coordinates of a point on the surface of separation, reckoned from the center of gravity of the corresponding grain. Therefore

$$\int \frac{qdS}{R'} = \sum_\alpha \int \frac{q^\alpha dS^\alpha}{R'_\alpha} = \frac{\varkappa}{4\pi}\sum_\alpha \left\{V_{ik}\int \frac{n_i\xi_k\,dS^\alpha}{R'_\alpha} - \int \frac{u_i^\alpha n_i^\alpha\,dS^\alpha}{R'_\alpha}\right\}$$

$$= \frac{\varkappa}{4\pi}V_{ik}\sum_\alpha \int_{\Omega_\alpha} \frac{\partial}{\partial\xi_i}\left(\frac{\xi_k}{R'_\alpha}\right)d\xi - \frac{\varkappa}{4\pi}\sum_\alpha \int \frac{u_i^\alpha n_i^\alpha\,dS^\alpha}{R'_\alpha},$$

$$\mathbf{R}'_\alpha = \mathbf{R}^\alpha + \boldsymbol{\xi} - \mathbf{r}, \qquad (14)$$

where dS_α is an element of area on the surface of the α-th grain, and Ω_α is the volume of this grain.

For an arbitrary scatter of the shape and dimensions of the grains, the random deviations of the grain velocities u^α are, in general, not equal to zero and should be determined from the requirement that the total force and momentum acting on each grain separately should vanish. [4] In order to eliminate the quantity u^α, we shall consider first a portion of the medium consisting of equivalent grains (cf. the plane model in Fig. 2). In spite of some elements of artificiality in this model, it allows us to introduce a description of the structural anisotropy in terms which are related to the shape and dimensions of the grains and the nature of the grain packing. Obviously, because of the equivalence of the grains, there are no random deviations of the velocity ($u^\alpha = 0$).

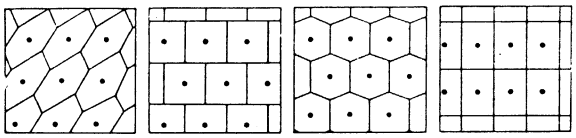

FIG. 2

This means that, in particular, the discontinuity $\partial\varphi/\partial n$ at the boundary between the grains α and β has the simple form

$$\delta\,(\partial\varphi/\partial n)\,|_S = V_{ik} R_k^{\alpha\beta} n_i; \qquad (15)$$

$\mathbf{R}^{\alpha\beta} = \mathbf{R}^\alpha - \mathbf{R}^\beta$ is the distance between the centers of gravity of the neighboring grains. Consequently, according to Eq. (14), we have the following exact formula for the potential:

$$\varphi\,(\mathbf{r}) = \varphi_0 + \varkappa V_{ik}\psi_{ik}\,(\mathbf{r}) \qquad (V_{ii} = 0),$$
$$\psi_{ik}\,(\mathbf{r}) = \frac{1}{4\pi}\sum_\alpha \int \xi_k \frac{\partial}{\partial \xi_i}\left(\frac{1}{R'_\alpha}\right) d\xi. \qquad (16)$$

Integration in Eq. (16) is carried out over the volume of one grain. If the origin of coordinates $\mathbf{r} = 0$ is taken at the center of gravity, then $\mathbf{R}_\alpha$ represents the vector in a lattice based on centers of gravity of the grains.

To obtain the required relationship (3) we have to express the magnitude of the average stresses in a grain p_{ik} in terms of the potential φ and the deformation velocity V_{ik}, taking into account the equalities (10) and (11). It is known that the average value $p_{ik} = \overline{\sigma_{ik}}$ is expressed in terms of surface forces f_i by the formula

$$p_{ik} = \frac{1}{\Omega_0}\int x_i f_k\, dS.$$

The normal component, $f_n = \sigma_{nn}|_S$, and the tangential component, $f_t = \sigma_{tn}|_S$, of the force are given by Eqs. (10) and (11), and hence

$$f_k = \varphi n_k + g_k \eta_S/a, \qquad g_k = V_{kl} R_l^\beta - n_k n_l V_{lm} R_m^\beta,$$
$$p_{ik} = p_0\delta_{ik} + \frac{1}{\Omega_0}\int x_i \frac{\partial\varphi}{\partial x_k}\, d\mathbf{r} + \frac{\eta_S}{a\Omega_0}\int x_i g_k\, dS, \quad p_0 = \frac{1}{\Omega_0}\int_{\Omega_0} \varphi\, d\mathbf{r}$$

(Ω_0 is the grain volume, and $\mathbf{R}^\beta$ is the distance between the centers of gravity of adjoining grains).

Finally, allowing for Eq. (16), we obtain

$$p_{ik} = p_0\delta_{ik} + \alpha_{iklm}V_{lm}, \qquad \alpha_{iklm} = \alpha^0_{iklm} + \alpha^*_{iklm},$$
$$\alpha^0_{iklm} = \frac{\varkappa}{\Omega_0}\int_{\Omega_0} x_i \frac{\partial\psi_{lm}}{\partial x_k}\, d\mathbf{r},$$
$$\alpha^*_{iklm} = \frac{\eta_S}{a\Omega_0}\int (x_i R_l^\beta \delta_{km} - x_i n_k n_l R_m^\beta)\, dS. \qquad (17)$$

Thus the viscosity tensor consists of two components, one of which represents diffusional viscosity in the case of zero resistance to slip, and the second is entirely due to this resistance. In order of magnitude

$$\alpha^0_{iklm} \sim \eta^0 \sim \varkappa L^2, \qquad \alpha^*_{iklm} \sim \eta^* \sim \eta_S L/a.$$

We have seen that in the case of easy slip (amorphous surface of separation) $\eta_S \approx \kappa a^2$ and $\eta^*/\eta^0 \approx a/L \ll 1$; then $\alpha_{iklm} = \alpha^0_{iklm}$. In the case of strong resistance to slip $\eta^*/\eta^0 \gg 1$ and $\alpha_{iklm} = \alpha^*_{iklm}$.

The expression for α^*_{iklm} can be simplified by an approximation (averaging process) consisting of replacing the vector $\mathbf{R}^\beta$, which connects the centers of gravity of adjoining grains to the point $\mathbf{r}$, by double the distance to the point of contact: $\mathbf{R}^\beta(\mathbf{r}) \approx 2\,\mathbf{r}$. This gives [5]

$$\alpha^*_{iklm} = \frac{2\eta_S}{a\Omega_0}\int (x_i x_l \delta_{km} - x_i x_m n_k n_l)\, dS. \qquad (17a)$$

Thus, for a spherical grain of radius R the tensor α^*_{iklm} reduces to the scalar $\eta^* = 2\eta_S R/5\pi a$.

Let us now analyze the diffusion component α^0_{iklm}. In the present work we shall consider mainly the case of easy slip (reasonably defective boundary) and, therefore, subsequently, unless

[4] Each quantity u^α is specified by two constant vectors u_0^α and ω^α: $u^\alpha = u_0^\alpha + [\omega^\alpha \times \xi^\alpha]$, representing the relative velocity of the center of gravity of the grain and the angular velocity of the grain. Thus the number of conditions for mechanical equilibrium is the same as the number of unknowns.

[5] Here and subsequently the quantity α_{iklm} should be made symmetrical for each pair of the indices i,k and l, m, if this symmetry is lost in the approximate formulas (17a), (18a), etc.

otherwise specified, we shall assume $\alpha_{ik\,lm} = \alpha^0_{ik\,lm}$. It follows from Eqs. (16) and (17) that in this case

$$\alpha_{iklm} = \frac{\varkappa}{4\pi\Omega_0}\sum_\alpha \int_{\Omega_0}\int_{\Omega_0} x_i\,\xi_m \frac{\partial^2}{\partial x_k\,\partial\xi_l}\left(\frac{1}{R'_\alpha}\right) dx\,d\xi;$$

$$\mathbf{R}'_\alpha = \mathbf{R}^\alpha + \xi - \mathbf{x}. \qquad (18)$$

It should be noted that since the coordinates $\mathbf{x}$ and ξ in the integral (18) are reckoned from the center of gravity of a grain ($\int \Omega_0 \mathbf{x}\,d\mathbf{x} = \int \Omega_0 \xi\,d\xi = 0$), the terms of the series (18) decrease as R^{-5} and the series converges very rapidly. Therefore, in the majority of cases, satisfactory accuracy is obtained by taking from the exact formula (18) one term of the series with $\mathbf{R}^\alpha$ (cf. footnote [5]):

$$\alpha_{iklm} = \frac{\varkappa}{4\pi\Omega_0}\int_{\Omega_0}\int_{\Omega_0} x_i\,\xi_m \frac{\partial^2}{\partial x_k\partial\xi_l}\frac{1}{|\mathbf{x}-\xi|}\,dx\,d\xi. \qquad (18a)$$

Transforming to the nondimensional coordinates $x_i \to x_i\Omega_0^{1/3}$, $\xi_i \to \xi_i\Omega_0^{1/3}$, we obtain

$$\alpha_{iklm} = \eta\gamma_{iklm}, \qquad \eta = kT\Omega_0^{5/3}/D\omega_0,$$

$$\gamma_{iklm} = \frac{1}{4\pi}\int_\omega\int_\omega x_i\,\xi_m \frac{\partial^2}{\partial x_k\partial\xi_l}\frac{1}{|\mathbf{x}-\xi|}\,dx\,d\xi, \qquad (19)$$

where the integrals $\gamma_{ik\,lm}$ are taken over a nondimensional portion ω of a grain of unit volume and represent numbers which depend only on the grain shape.

An interpolation formula, which makes it possible to generalize the expression for the viscosity tensor to the case of an arbitrary distribution of grain shapes and dimensions, is obtained by averaging the expression (18a) over this distribution. The meaning of such averaging may be obtained from two points of view. On the one hand, such averaging is exact for a packing model with grains varying in size and shape slowly from point to point (the changes being random). On the other hand, in the exact formula obtained from Eq. (14) for the general case, averaging involves neglecting the grain velocity fluctuations u^α. Thus, for example, if we represent the grain distribution by the probability $W(\mathbf{x}, \xi)\,d\mathbf{x}\,d\xi$ that two points, separated by the distances $\mathbf{x}$ and ξ from the center of gravity of the grain, belong to this grain, then the tensor $\alpha_{ik\,lm}$ can be written in the form

$$\alpha_{iklm} = \frac{\varkappa}{4\pi\bar{\Omega}}\iiint_{-\infty}^{\infty} W(\mathbf{x}, \xi)\,x_i\,\xi_m \frac{\partial^2}{\partial x_k\,\partial\xi_l}\frac{1}{|\mathbf{x}-\xi|}\,dx\,d\xi,$$

$$\bar{\Omega} = \iiint_{-\infty}^{\infty} W(\mathbf{x}, \xi)\,dx\,d\xi. \qquad (20)$$

It should be noted that the tensor $\alpha_{ik\,lm}$ is specified, correct to terms of the type $A_{ik}\delta_{lm}$ and $\delta_{ik}B_{lm}$, since $A_{ik}V_{ll}$ disappears because of the condition $V_{ll} = 0$ and $\delta_{ik}(B_{lm}V_{lm})$ can be taken back to the first term in Eq. (3). Therefore Eq. (18a) can be written in another form:

$$\alpha_{iklm} = \frac{\varkappa}{4\pi\Omega_0}\int_{S_0}\int_{S_0} \frac{x_i\,x'_m\,dS_k\,dS'_l}{|\mathbf{x}-\mathbf{x}'|}, \qquad (18b)$$

where the integral is taken over the grain surface, and $dS_k = n_k dS$.

A convenient method of investigating the anisotropy of $\alpha_{ik\,lm}$ is based on the Fourier representation of the integrand in Eq. (18a). Simple transformations, using the equality

$$\frac{1}{r} = \frac{1}{2\pi^2}\int e^{i\mathbf{k}\mathbf{r}}\frac{d\mathbf{k}}{k^2},$$

give [6]

$$\alpha_{iklm} = \frac{\varkappa}{8\pi^3\Omega_0}\int_{-\infty}^{\infty} k_l k_k \frac{\partial Q}{\partial k_i}\frac{\partial Q^*}{\partial k_m}\frac{d\mathbf{k}}{k^2},$$

$$Q = \int_{\Omega_0} e^{i\mathbf{k}\mathbf{x}}\,d\mathbf{x}. \qquad (18c)$$

Thus, for spherical grains, Q depends only on the modulus of $\mathbf{k}$ and the tensor $\alpha_{ik\,lm}$, being isotropic, reduces to the scalar of Eq. (3a).

For very strong grain-shape anisotropy, for example in the case when the grains are greatly elongated along one direction ($C/A \gg 1$, where C is the length of the grain and A represents its transverse dimensions), it is insufficient to use in Eq. (18) only the term with $\mathbf{R}^\alpha = 0$: it is necessary also to retain the terms with $R^\alpha \approx C$ in the transverse direction.

On the basis of the equality $V_{ll} = 0$ it can be easily shown that in the case of axial symmetry there are only three independent components of $\alpha_{ik\,lm}$. If x_3 is the selected axis, then

$$p_{\alpha\beta} = p_0\delta_{\alpha\beta} + \eta_1 V_{\alpha\beta}, \qquad \alpha, \beta = 1, 2,$$

$$p_{33} = p_0 + \eta_3 V_{33};\quad p_{\alpha 3} = \eta_2 V_{\alpha 3},\quad -p = p_0 + \tfrac{1}{3}(\eta_3 - \eta_1)V_{33}. \qquad (21)$$

A simple analysis of the expressions in Eq. (18) shows that when $C \gg A$ the orders of magnitude are given by $\eta_1 \sim \kappa A^2$, $\eta_2 \sim \kappa AC$, $\eta_3 \sim \kappa C^2$.

4. EXAMPLE: THE CASE OF A PARALLELEPIPEDAL STRUCTURE

In spite of the relatively compact form of Eqs. (18a)—(18c) for the tensor $\alpha_{ik\,lm}$, these formulas

[6] It should be noted that a similar representation of the exact formula (18) reduces to a substitution of integration over the space $\mathbf{k}$ in Eq. (18c) with summation over the points $\mathbf{H}$, where $\mathbf{H}$ are vectors of the reciprocal lattice with respect to $\mathbf{R}^\alpha$.

are far too complicated for practical applications. Therefore, we shall consider here one case which can be solved exactly, giving the simplest expressions for the viscosity tensor. We refer to the rectangular parallelepiped grain shape and packing of the type shown in Fig. 2c.

If the edges of the parallepiped are of lengths $2A_1$, $2A_2$, $2A_3$, then, according to Eq. (15), the discontinuity of the derivative $\partial\varphi/\partial n$ at the grain boundaries is given by

$$\delta\partial\varphi/\partial n\,|_{x_i=A_i(1+2N)} = 2\varkappa V_{il}A_i^2, \qquad i = 1, 2, 3 \qquad (22)$$

where N is an integer.

It is easily seen that the periodic harmonic function satisfying the conditions of Eq. (22) (in each grain the coordinates x_i are reckoned from its center of gravity) is

$$\varphi(r) = \varphi_0 + \tfrac{1}{2}\varkappa(V_{11}x_1^2 + V_{22}x_2^2 + V_{33}x_3^2), \qquad V_{ii} = 0. \quad (23)$$

For p_{ik} the formula (17) gives

$$p_{ik} = p_0\delta_{ik} + \tfrac{1}{3}\varkappa\,\delta_{ik}V_{kk}A_k^2;$$

$$-p = p_{ll}/3 = p_0 + \theta, \qquad \theta = \frac{\varkappa}{3}\sum_k V_{kk}A_k^2, \qquad p_0 = \varphi_0 + \theta/2, \quad (24)$$

and, therefore, the nonspherical part of the stress tensor $p'_{ik} = p_{ik} + p\delta_{ik}$ is

$$p'_{il} = p_{il} + p = -\tfrac{1}{2}\varkappa\theta + \tfrac{1}{3}\varkappa V_{il}A_i^2, \qquad i = 1, 2, 3,$$
$$V_{il} = p'_{il} + \sum_k p'_{kk}A_k^{-2} \Big/ \sum_k A_k^{-2}. \qquad (24a)$$

The relationships in Eq. (24) express the relationship being sought between the stresses and the deformation rate V_{ik}. We shall consider especially the case $A_1 = A_2 = A$, $A_3 = C$:

$$p_{33} = p_0 + \frac{\varkappa}{3}V_{33}C^2, \qquad p_{11} + p_{22} = 2p_0 - \frac{\varkappa}{3}V_{33}C^2.$$

Then

$$p'_{33} = p_{33} + p = \frac{\varkappa}{3}V_{33}\frac{2C^2 + A^2}{3},$$

$$p'_{11} + p'_{22} = -p'_{33} = -\frac{\varkappa}{3}V_{33}\frac{2C^2 + A^2}{3}. \qquad (24b)$$

For C = A all the axes are equivalent and $p'_{ii} = (1/3)\varkappa A^2 V_{ii}$ (i = 1, 2, 3). Finally, in the planar case ($V_{33} = 0$, $V_{11} = -V_{22}$) $p_{11} = p_0 + (1/3)\varkappa A^2 V_{11}$, $p_{22} = p_0 - (1/3)\varkappa B^2 V_{11}$, or

$$p_{11} + p = -p_{22} - p = \tfrac{1}{3}\varkappa V_{11}(A^2 + B^2),$$

$$V_{11} = \tfrac{3}{2}(p_{11} - p_{22})/\varkappa(A^2 + B^2). \qquad (24c)$$

It is clear from Eq. (24) that in the case considered the nondiagonal components p_{ik} vanish. This is related to some degeneracy, due to the model of grain packing which has been assumed: on this model, corresponding to Fig. 2c, the points of contact between the grains are degenerate (the general nondegenerate case of contact is shown in Figs. 2a and 2b). A simple analysis shows that in this case there is instability with respect to any nondiagonal component of p_{ik}. Figure 3 shows, by way of example, the deformations for this model under the action of forces applied along the diagonals of the squares. Consequently the model gives reasonable results only in the case when the load conditions are such that the nondiagonal components of p_{ik} are absent.

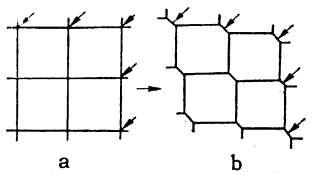

FIG. 3

Another characteristic of this model is related to the fact that the diagonal components of the deformation velocities V_{11}, V_{22}, V_{33} produce no slip along grain boundaries, while the nondiagonal components produce slip only, without the need for diffusion currents. When forced slip is allowed, the formulas (24a)—(24c) for the diagonal components of p_{ik} remain unaltered, while for the nondiagonal components the general formula (17) gives a simple equality $p_{ik} = \eta_S(A_i + A_k)V_{ik}/a$, $i \neq k$.

We shall now deal with the problem of the stress distribution in the case considered. According to Eq. (10) the stresses are strongly inhomogeneous at the boundary:

$$\sigma_{nn}\,|_{x_i=\pm A_i} = \varphi_0 + \tfrac{1}{2}\varkappa A_1^2 V_{11} + \tfrac{1}{2}\varkappa(x_2^2 V_{22} + x_3^2 V_{33}). \quad (25)$$

For simplicity we shall consider only the planar case ($V_{33} = 0$). Expressing φ_0 and $V_{11} = -V_{22}$ in Eq. (25) in terms of average stresses p_{11} and p_{22}, we shall write the boundary conditions in the form

$$\sigma_{xx}\,|_{x=\pm A} = -p + (B^2/3 - y^2)M,$$

$$\sigma_{yy}\,|_{y=\pm B} = -p + (x^2 - A^2/3)M,$$

$$\sigma_{xy}\,|_{x=\pm A} = \sigma_{xy}\,|_{y=\pm B} = 0, \qquad M = \tfrac{3}{4}(p_{11} - p_{22})/(A^2 + B^2). \quad (26)$$

From the theory developed above it is clear that the results obtained so far are completely unrelated to the elastic properties of the medium; in particular the distribution of stresses at a grain boundary, given by Eqs. (25) and (26), is independent of these properties. However, in general, the stress distribution in the interior of a grain

depends strongly on the elastic moduli. In our example the elastic moduli disappear from the final formulas only in the case of an elastically isotropic medium. In that case it can easily be shown that σ_{xx}, σ_{yy} and σ_{xy} have, over the whole volume of the grain, the same distribution as at the boundary:

$$\sigma_{xx} = p_{11} + \frac{p_{11} - p_{22}}{4} \frac{1 - 3(x/A)^2}{1 + (B/A)^2},$$
$$\sigma_{yy} = p_{22} + \frac{p_{22} - p_{11}}{4} \frac{1 - 3(y/B)^2}{1 + (A/B)^2}, \qquad (27)$$
$$\sigma_{xy} = 0, \qquad \sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

where ν is Poisson's ratio.

This result is naturally affected by the presence of elastic anisotropy. It should be noted that the appearance of inhomogeneous stresses as a result of alignment and the distribution of these stresses should be one of the more important criteria in an experimental verification of the theory of the flow process given here. Obviously in the limiting case of a single crystal the equivalent boundary conditions can be modeled by a system of rigid pistons at the faces of the crystal.

5. ELASTIC ENERGY AND MACROSCOPIC ELASTIC MODULI OF A POLYCRYSTAL IN THE PROCESS OF DIFFUSION-VISCOUS FLOW

We shall consider the macroscopic elastic properties of a polycrystal during the process of diffusion-viscous flow.

The elastic energy of a macroscopic element of volume consists of two parts: E_0, related to the average stresses p_{ik}, and a fluctuation part E^*, related to the deviations $\sigma^*_{ik} = \sigma_{ik} - p_{ik}$ from these average values. In particular if the crystallites forming the system are elastically isotropic, the elastic energy per macroscopic unit of volume is

$$E = E_0 + E^*,$$
$$E_0 = p^2/2K + p'^2_{ik}/4\mu, \qquad p'_{ik} = p_{ik} + p\delta_{ik},$$
$$E^* = \sigma^{*2}_{ik}/4\mu, \qquad \sigma^*_{ik} = \sigma_{ik} - p_{ik} \qquad (28)$$

where K is the hydrostatic bulk modulus and μ is the shear modulus. As shown above, σ^*_{ik} is linearly related to V_{ik} and consequently to the nonspherical part of the stress tensor p'_{ik}. Thus the fluctuation part of the elastic energy has the form

$$E^* = E^*(p_{ik}) = \nu_{iklm} p'_{ik} p'_{lm}/4\mu, \qquad (29)$$

where the numerical values of ν_{iklm} are determined by the structural anisotropy of the crystal. Thus, for example, in the planar flow considered at the end of the preceding section this energy is

$$E^* = \frac{1 + \nu^2}{5\mu} \left(\frac{p_{11} - p_{22}}{4} \right)^2$$

where ν is Poisson's ratio.

Thus the elastic energy for given stresses p_{ik} acquires an additional term during flow which is of the same order as the main part of the energy related to uniform homogeneous stresses. (The expression "of the same order" implies the absence of a small physical parameter, although the numerical value of the ratio of the energies may be quite small for grains of near-spherical shape.)

The relationship between the macroscopic (average) values of the elastic deformation ϵ_{ik} and the stresses p_{lm} is obtained by differentiating the elastic energy E with respect to the stresses p_{ik}:

$$\varepsilon_{ik} = c_{iklm} p_{lm}, \qquad c_{iklm} = c^0_{iklm} + c^*_{iklm},$$
$$c^0_{iklm} = \frac{\partial^2 E^0}{\partial p_{ik} \partial p_{lm}}, \qquad c^*_{iklm} = \frac{\partial^2 E^*}{\partial p_{ik} \partial p_{lm}}. \qquad (30)$$

The above equation shows that the tensor c^*_{iklm} is anisotropic. This means that during flow the anisotropy of the macroscopic moduli changes and even a medium consisting initially of elastically isotropic crystallites becomes, in general, elastically anisotropic.

There is another important point as follows. Because of the positive quadratic form of $E^*(p_{ik})$ the eigenvalues of the matrix c_{iklm}, arranged in increasing order, are larger than the eigenvalues of the matrix c^0_{iklm}. The reciprocals of these eigenvalues are the basic elastic moduli of the polycrystal. This means that as a result of diffusional flow the elastic moduli of a polycrystal become smaller. For an elastically isotropic medium this means a reduction of the Lamé coefficients.

6. VARIATION OF THE GRAIN SHAPE AND OF THE VISCOSITY TENSOR DURING FLOW

The flow changes the grain shape and the structural anisotropy. This alters the viscosity tensor α_{iklm}. A microscopic deformation of a single grain is described by the velocity of displacement of the points $\mathbf{x}^S$ on its boundary due to the diffusion current:

$$\frac{d\mathbf{x}^S}{dt} = \frac{1}{\varkappa} \nabla\varphi|_S,$$

where φ is given by Eq. (16). However, qualitatively or "on the average," we may assume that

the grain shape varies as if it were deformed uniformly together with the whole medium. This means that

$$dx_i^S/dt = V_{ik}x_k^S. \tag{31}$$

Correspondingly the derivative $d\alpha_{ikl m}/dt$ is determined by varying $\alpha_{ikl m}$ with the shape of the surface. Using the general formula for the change in an integral when the integration region is varied

$$\delta \int_{\Omega_0} \Psi d\mathbf{x} = \int_S \Psi \delta x_i^S dS_i,$$

we can easily obtain the detailed microscopic formulas by means of equalities (18) and (31). These formulas are, however, complicated and of little interest, and it is more helpful to use the approximate approach developed below.

If the final deformation of the medium at a time t is represented by the matrix $\hat{\lambda} = \lambda_{ik}$, in the sense that any small vector with initial coordinates x_i^0 transforms into the vector $x_i = \lambda_{ik}x_k^0$, it follows from Eq. (31) that

$$d\hat{\lambda}/dt = \hat{V}\hat{\lambda}. \tag{32}$$

In view of the condition $V_{ii} = 0$ (conservation of volume) the determinant $D(\lambda_{ik}) = 1$. V_{ik} is taken at the point of location of the grain at the time t and, in general, depends on time and coordinates. Initially $\lambda_{ik}(0) = 1$. If the "average" shape of the grains is initially spherical [$(\mathbf{x}^0\mathbf{x}^0) = 1$], then the value of $\lambda_{ik}(t)$ is given by the ellipsoid $(\hat{\lambda}^{-1}\mathbf{x}, \hat{\lambda}^{-1}\mathbf{x}) = 1$ with semiaxes λ_i (λ_i are the principal values of $\hat{\lambda}$; $\lambda_1\lambda_2\lambda_3 = 1$). Therefore, it is natural to represent the structural anisotropy by the ellipsoid λ_{ik}. If the initial anisotropy is given by the matrix $\hat{\lambda}^0$, and the deformation at time t is $\hat{\lambda}(t)$, then the anisotropy at the time t is $\hat{\lambda}(t)\hat{\lambda}^0$ [obviously $D(\hat{\lambda}\hat{\lambda}^0) = D(\hat{\lambda})D(\hat{\lambda}^0) = 1$]. Thus, for example, if $\hat{V}$ is independent of the coordinates and of time, we obtain from Eq. (32)

$$\hat{\lambda} = e^{t\hat{V}}\hat{\lambda}^0.$$

If, on the contrary, $\hat{V} = \hat{V}(s)$ depends on the point s on the trajectory of the grain, and $v(s) = ds/dt$ is the grain velocity, then $d\hat{\lambda}/ds = \hat{V}(s)\hat{\lambda}/v(s)$. If $\hat{V}(s)$ remains diagonal along the trajectory, then

$$\frac{d\lambda_i}{ds} = V_{ii}(s)\lambda_i/v(s), \qquad \lambda_i(s) = \exp\int_{s_0}^{s} V_{ii}(s)\frac{ds}{v(s)}.$$

To obtain a complete solution of the problem of flow it remains to select a reasonable approximation for $\alpha_{ikl m}$ in a medium with structural anisotropy given by the ellipsoid λ_{ik}. For this purpose we can use the formulas (18) and (18a), where the region of integration Ω_0 is the ellipsoid $\hat{\lambda}$ or the approximate estimates given in formulas of the type of (21) or (24). It follows from these formulas that good interpolation is obtained on the assumption [7]

$$p_{ik} = p_0\delta_{ik} + \eta\lambda_i\lambda_k V_{ik}, \qquad \lambda_1\lambda_2\lambda_3 = 1, \tag{33}$$

or, for the nonspherical part,

$$p'_{ik} = p_{ik} - p_{ll}\delta_{ik}/3 = p_{ik} + p\delta_{ik},$$

$$p'_{ik} = \eta\lambda_i\lambda_k V_{ik} - \eta\delta_{ik}\sum_l \lambda_l^2 V_{ll}/3,$$

$$\eta V_{ik} = \lambda_i^{-1}\lambda_k^{-1}p'_{ik} - \delta_{ik}\lambda_i^{-2}\sum_l \lambda_l^{-2}p'_{ll}/\sum_l \lambda_l^{-2}, \tag{33a}$$

where $\eta \approx \kappa\Omega_0^{2/3} = kT\Omega_0^{2/3}/Dc_0\omega_0$ is the isotropic viscosity when $\lambda_i = 1$.

Thus, for example, for the axially symmetric structure $\lambda_3 = \lambda$, $\lambda_1 = \lambda_2 = \lambda^{-1/2}$, taking into account the equality $V_{11} + V_{12} = -V_{33}$ we obtain

$$p'_{33} = p_{33} + p = \tfrac{1}{3}(2\lambda^2 + \lambda^{-1})V_{33}, \qquad p'_{\alpha 3} = p_{\alpha 3} = \eta\lambda^{1/2}V_{\alpha 3},$$

$$p'_{\alpha\beta} = p_{\alpha\beta} + p\delta_{\alpha\beta} = \tfrac{1}{3}\eta(\lambda^2 - \lambda^{-1})V_{33} + \eta\lambda^{-1}V_{\alpha\beta},$$

$$\alpha, \beta = 1,2. \tag{34}$$

If we use the relationships (33) and (32), then the equilibrium conditions of Eq. (4) lead to a nonlinear system

$$\frac{\partial p_0}{\partial x_i} + \eta\frac{\partial}{\partial x_k}\lambda_{il}\lambda_{km}\frac{\partial V_l}{\partial x_m} = 0, \qquad \operatorname{div}\mathbf{V} = 0,$$

$$\frac{d\lambda_{ik}}{dt} = V_{il}\lambda_{lk}. \tag{35}$$

As an example of such a calculation, the filling-up of an isolated spherical pore under the action of hydrostatic pressure is considered in Appendix 2.

The whole analysis in this section is based on the assumption that the diffusion-viscous mechanism is the only cause of the displacement of grain boundaries and the change of their shape. However, the presence of inhomogeneous stresses inside the grains and the related fluctuation energy E* increase the probability of processes of boundary displacement by recrystallization. Such processes may be particularly important in the case of strong structural anisotropy (for example, greatly elongated grains), when the fluctuation energy and the

[7] In the invariant matrix form the relationships (33) and (33a) have the form

$$\hat{d} = p_0 + \eta\hat{\lambda}\hat{V}\hat{\lambda}, \quad \hat{p}' = \eta\hat{\lambda}\hat{V}\hat{\lambda} - \eta/3\,(\mathrm{Sp}\hat{\lambda}^2\hat{V}),$$

$$\eta\hat{V} = \hat{\lambda}^{-1}\hat{p}'\hat{\lambda}^{-1} - \hat{\lambda}^{-2}(\mathrm{Sp}\hat{\lambda}^{-2}p'/\mathrm{Sp}\hat{\lambda}^{-2}).$$

excess surface energy are relatively large. Since, however, the characteristic velocities of the process of recrystallization are governed by quite different parameters, there is one region where practically the only process is the diffusion-viscous flow, and another where the change in the shape and dimensions of the grains is governed by recrystallization processes. In the latter region the variation of the viscosity tensor α_{iklm} with time is naturally independent of that in the former region, although the basic equations (3) and (4a) are retained.

In some cases the diffusion of vacancies along grain boundaries, where the diffusion coefficient D_S is considerably greater, may be important in the mechanism of diffusion-viscous flow. This type of vacancy diffusion is a small effect if $D_S a/L \approx D_S(\omega_0/\Omega_0)^{1/3} \ll D$ (a is the atomic spacing and L represents the grain dimensions). In the opposite limit when $D_S a/L \gg D$ the whole process is governed by surface and not by volume diffusion. This obviously may occur in sufficiently small grains. Finally, on increase of p_{ik} the low-threshold processes of diffusion-viscous flow (for example, the generation and motion of dislocations) may be important. An analysis of some of these processes will be given in a separate paper.

APPENDIX 1

BOUNDARY CONDITIONS ON THE SURFACES OF BLOCKS IN A MOSAIC CRYSTAL

An analysis of the conditions under which mosaic block boundaries are capable of absorbing and emitting vacancies has been given by Herring [2], but not all the arguments and results of his analysis seem to be justified. Here we shall investigate the behavior of such boundaries from another point of view.

A boundary between blocks with a low tilt angle θ can be considered as an array of dislocations lying in the plane of this boundary separated by a mean distance d, so that $\theta \approx a/d$, where a is the atomic spacing. The absorption or emission of Δn vacancies, uniformly distributed between dislocations in an element of area of the boundary (dimensions $\Delta L \gg d$), produces motion of the dislocation network to the right or left, and this involves performing an amount of work $\pm\sigma_{nn}\omega_0\Delta n$. Therefore, if we consider uniform "consistent" average motion of dislocations along the boundary then in such motion each dislocation represents a virtual source or sink of vacancies.

From this point of view the absence of complete freedom of arbitrary displacement of a single dislocation when the other dislocations are fixed is not very important and does not alter the condition (2) for equilibrium vacancy concentration at a single dislocation.

In the electrostatic analogy each dislocation is represented by a wire of radius a (a is the atomic spacing) at a potential $\varphi_0 = \sigma_{nn}$. The problem consequently reduces first to the question of under what conditions a grid of such wires, separated by a distance d from each another, can be considered as a uniform plane with a potential $\varphi = \varphi_0$. For this to be so it is obviously necessary for the potential dip between the wires, $\delta\varphi \approx e\,ln(d/a)$, where e is the "charge," to be considerably smaller than the change in the potential along the surface $\delta\varphi \approx p'$ (p' is the nonspherical part of the stress tensor). The average density of "charge" on the surface (i.e., the discontinuity $\partial\varphi/\partial n$) is obviously $q^* \approx p'/L$ (L is the grain dimension), i.e., the charge is $e \approx q^*d \approx p'd/L$. Thus the condition $\delta\varphi \ll \delta\varphi_0 \approx p'$ gives

$$(d/L)\ln(d/a) \ll 1 \quad \text{or} \quad \theta/\ln\theta \gg a/L.$$

However, much more important is the second limitation. As shown at the end of Sec. 2, for the flow mechanism described to be realized it is necessary to have the possibility of slip along the grain boundaries. The estimate of the tangential stresses at the boundary, given in Sec. 2, leads to an additional condition for the effective viscosity η_S of the boundary layer (the surface of separation between blocks): $\sigma_{tn}/p' \approx \eta_S/\kappa aL \ll 1$. For sufficiently large tilt angles θ a reasonable estimate of η_S is $\eta_S \approx \kappa d^2$. This gives $d^2/aL \ll 1$, and hence we have a restriction on the magnitude of the tilt angle: $\theta^2 \gg a/L$. However, if θ is sufficiently small then the crystal between dislocations is in general perfect, and diffusional slip along the boundary is excluded practically completely. Therefore, for sufficiently small θ the mechanism described could apply only in those exceptional cases when, due to the symmetry of the block structure and the applied stress, flow occurs without slip at the boundaries (for example as in the case of rectangular parallelepipeds along the direction of the applied forces, discussed in Sec. 4).

APPENDIX 2

KINETICS OF THE FILLING-UP OF A SPHERICAL PORE UNDER PRESSURE

The problem of the kinetics of the filling-up of an isolated spherical pore in a polycrystalline body at various stages of this process has been

considered in [4]. Here we shall consider the influence of the change in the grain shape on this process.

Initially an infinite sample contains a spherical pore of radius $R_0 \gg L$, where L is the dimension of the grains. An external hydrostatic pressure p_0 produces a diffusion-viscous flow toward the center of the pore. The equation of equilibrium in spherical coordinates has the form

$$\frac{1}{r^3}\frac{\partial}{\partial r} r^3 (p_{rr} + p) + \frac{\partial p}{\partial r} = 0 \qquad (p = -p_{ll}/3). \quad (2.1)$$

From the equation of continuity it follows that

$$r^2 V_r = R^2 \dot{R}, \quad (2.2)$$

where $R = R(t)$ is the radius of the pore at a time t. Hence

$$V_{rr} = \frac{\partial V_r}{\partial r} = -\frac{2V_r}{r} = \frac{R^3}{r^3} V_{RR},$$

$$V_{RR} = V_{rr}|_{r=R} = -\frac{2\dot{R}}{R}. \quad (2.3)$$

From the symmetry of the problem it is clear that the structural anisotropy due to flow has, at each point, axial symmetry connected to the elongation of the grains in the radial direction. According to Eq. (35) this leads to a relationship between $(p_{rr} + p)$ and V_{rr}:

$$p_{rr} + p = \eta(\lambda) V_{rr}, \qquad \eta(\lambda) = \tfrac{1}{3}\eta(2\lambda^2 + 1/\lambda), \quad (2.4)$$

$$V_{RR}\frac{R^3}{r^3}\frac{\partial \eta(\lambda)}{\partial r} + \frac{\partial p}{\partial r} = 0. \quad (2.5)$$

The grain deformation parameter λ (the major semiaxis of the deformation ellipsoid) and also the pressure are functions of r and t [or of r and R(t)].

The boundary conditions for Eq. (2.5) (taking into account that $p_{rr}|_{r=k} = 2\gamma/R$, where γ is the surface tension) are

$$p|_{r=\infty} = p_0, \qquad p(R) + \frac{\gamma}{R} = \eta(\lambda_R) V_{RR},$$

$$\lambda|_{r=\infty} = 1, \qquad \lambda|_{r=R} = \lambda_R. \quad (2.6)$$

From Eqs. (2.3), (2.5) and (2.6) we find

$$p(R) - p_0 = -\int_{\infty}^{R} \frac{R^3}{r^3}\frac{\partial \eta(\lambda)}{\partial r} dr \cdot V_{RR} = \eta(\lambda_R) V_{RR} - p_0 - \frac{\gamma}{R}$$

or

$$p_0 + \frac{\gamma}{R} = V_{RR}\left\{\eta(\lambda_R) + \int_{\infty}^{R} \frac{R^3}{r^3}\eta'(\lambda)\frac{d\lambda}{dr} dr\right\}$$

$$= \eta V_{RR}\left\{1 + \frac{1}{3}\int_1^{\lambda_R}\left(1 + \frac{R^3}{r^3}\right)\left(4\lambda - \frac{1}{\lambda^2}\right) d\lambda\right\}.$$

If a grain with an initial coordinate r_0 is at $r = r(t, r_0)$ at a time t, it follows from the conservation of volume that $\lambda = (r_0/r)^2$; on the other hand from Eq. (2.2) we have $r^3 - R^3 = r_0^3 - R_0^3$.

Eliminating r_0 from these two equations we obtain a relationship between r, R and λ:

$$\frac{R^3}{r^3} = \frac{\lambda^{3/2} - 1}{\lambda_R^{3/2} - 1}, \qquad \lambda_R = (R_0/R)^2.$$

Hence

$$2\eta \dot{R}/R = (p_0 + \gamma/R)/[1 + f(R_0/R)],$$

$$f(z) = \frac{2}{3}\int_1^z \left[1 + \frac{x^3 - 1}{z^3 - 1}\right]\left(4x^2 - \frac{1}{x^4}\right) x dx.$$

In the initial stage $R \approx R_0$, and $f(1) = 0$, and we obtain the formula given in [4]: $p_0 + \gamma/R = -2\eta\dot{R}/R$. The velocity $\dot{R}/R$ then decreases due to grain growth in the radial direction. However, due to fluctuations of the initial shape and dimensions of the grains the formulas cease to be valid when the transverse grain dimensions at the boundary of the pore become of the order of the scatter of the initial dimensions, i.e., when $\lambda_R \approx (L/\delta L)^2$. The axial symmetry in the neighborhood of the pore is then lost and the transverse dimensions of the grains at the pore boundary cease to decrease: the grains "drift" on top of each other until the whole pore is found within the limits of one or two grains. According to [4] this gives a dependence of $\dot{R}/R$ on R of the type shown in Fig. 4.

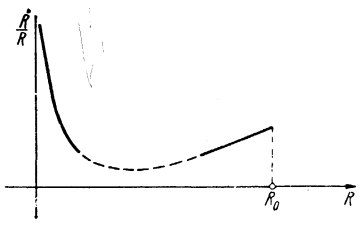

FIG. 4

APPENDIX 3

THE CASE OF INTENSE SURFACE DIFFUSION ALONG GRAIN BOUNDARIES

If the process of surface diffusion along grain boundaries is intense, it may govern the mechanism of diffusion-viscous flow. Variation of $\varphi = \sigma_{nn}$ along the grain boundary gives rise to a volume diffusion current, as well as surface currents

$$j_S = (D_S \omega_0 a/kT)\nabla_S \varphi$$

where D_S is the surface self-diffusion coefficient referring to a monatomic layer, $\nabla_S \varphi$ is the sur-

face gradient of the potential φ, and a is the atomic spacing. On allowing for these currents the conditions (6) and (9), which relate the velocity of the relative motion of the grains $\delta v_n = v_n^\alpha - v_n^\beta$ to the diffusional inflow of additional matter to a given part of the boundary, are altered: together with the volume term

$$\left(\frac{\partial\varphi}{\partial n}\Big|_\alpha - \frac{\partial\varphi}{\partial n}\Big|_\beta\right)\frac{1}{\varkappa}$$

there are sources on the surface due to the surface diffusion:

$$q_S = \operatorname{div} j_S = \frac{a}{\varkappa_S}\Delta_S\varphi, \qquad \varkappa_S = kT/D_S\omega_0.$$

Thus the condition replacing Eq. (9) becomes

$$\varkappa(v_n^\beta - v_n^\alpha) = \frac{\partial\varphi}{\partial n}\Big|_\alpha - \frac{\partial\varphi}{\partial n}\Big|_\beta + \frac{\varkappa a}{\varkappa_S}\Delta_S\varphi, \quad \frac{\varkappa}{\varkappa_S} = \frac{D_S}{D} \qquad (3.1)$$

If the surface self-diffusion coefficient is so large that $D_S/D \gg L/a$, then surface diffusion plays the dominant role and the main contribution to the right-hand part of Eq. (3.1) is given by the term $\approx \Delta_S\varphi$, i.e.,

$$\Delta_S\varphi = \varkappa_S(v_n^\beta - v_n^\alpha)/a. \qquad (3.2)$$

Equation (3.2) replaces Eqs. (8) and (9) and its solution determines the quasi-steady-state distribution of the normal stresses $\sigma_{nn} = \varphi$; the tangential stresses are, as before, governed by the resistance to slip and are expressed by the conditions (11).

The order of magnitude of the variation of σ_{nn} along the grain surface follows from Eq. (3.2):

$$\delta\sigma_{nn} \sim L^2\varkappa_S(v_n^\alpha - v_n^\beta)/a \sim L^3\varkappa_S V_{ik}/a.$$

For free slip the nonspherical part of the stress tensor is

$$p' \sim \delta\sigma_{nn} \sim L^3\varkappa_S V_{ik}/a \sim \eta_0 V_{ik} LD/aD_S,$$

i.e., the effective viscosity η becomes

$$\eta \sim L^3\varkappa_S/a = \eta_0 LD/aD_S \qquad (LD/aD_S \ll 1). \qquad (3.3)$$

We shall give concrete expressions for the tensor α_{iklm} in the case of surface diffusion only for the parallelepiped packing model considered in Sec. 2, para. 4. In that case Eq. (3.2) becomes

$$\Delta_S\varphi|_{x_i=\pm A_i} = -2\varkappa_S\frac{A_i}{a}V_{ii}, \qquad i = 1, 2, 3.$$

It can easily be shown that the solution of the above equations, continuous at all lines of contact (parallelepiped edges), can be represented by values of the function

$$\varphi = \varphi_0 + \frac{\varkappa_S}{2}\sum_i \Lambda_i x_i^2, \qquad \Lambda_i = 2\frac{A_i V_{ii}}{a} - \sum_l \frac{A_l V_{ll}}{a},$$

on the surfaces $x_i = \pm A_i$:

$$\sigma_{nn} = \varphi_S = \varphi|_{x_i=\pm A_i}.$$

Consequently, as before [Eqs. (17), (23), (24)], we obtain the relationship sought between p_{ik} and V_{ik}:

$$p_{ik} = p_0\delta_{ik} + \frac{\varkappa_S}{3}\delta_{ik}\Lambda_i A_i^2,$$

i.e.,

$$p_{ii} = p_0 + \frac{\varkappa_S}{3a}\left\{2A_i^3 V_{ii} - \sum_l A_l^2 A_l V_{ll}\right\}.$$

In the case of cubic packing ($A_1 = A_2 = A_3 = A$):

$$p_{ii} = p_0 + \frac{2}{3}\varkappa_S\frac{A^3}{a}V_{ii}.$$

In the planar case ($V_{33} = 0$):

$$p_{22} - p_{11} = \frac{\varkappa_S}{3}\frac{A_1 + A_2}{a}(A_1^2 + A_2^2)V_{11}.$$

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