MICROMECHANICS OF DIFFUSIONAL CREEP

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Abstract—In polycrystalline materials at high temperatures and low stresses, creep occurs mostly by the diffusion of vacancies through the grain bodies and over the grain boundaries. A continuum theory of vacancy motion is considered to analyze diffusional creep on a microscopical level. A linear version of such a theory was formulated by Nabarro, Herring, Coble and Lifshitz. We revise this theory from the perspectives of continuum mechanics and present it in a thermodynamically consistent nonlinear form. A certain difficulty, which one has to overcome in this endeavor, is the absence of Lagrangian coordinates in diffusional creep, the major building block of any theory in continuum mechanics. A linearized version of the theory is studied for the case of bulk diffusion. We consider the derivation of macro constitutive equations using the homogenization technique. It is shown that macroequations are nonlocal in time and nonlocality is essential in primary creep. For secondary creep polycrystals behave as a viscoelastic body. For secondary creep, a variational principle is found which determines microfields and macromoduli in stress-strain rate constitutive equations. A two-dimensional honeycomb microstructure and single crystal deformation are studied numerically by a finite element method. © Elsevier Science Ltd. All rights reserved. © 1997 Elsevier Science Ltd.

1. INTRODUCTION

Predictions of the mechanical behavior of solids can be roughly classified as short-term and long-term predictions. In short-term prediction, the behavior can be elastic or plastic, depending on the level of stress. For sufficiently low stresses, solids behave elastically. However, over long time periods, even under very low stresses, solids develop irreversible deformations. This phenomenon is called creep.

There are three points worth stressing in a discussion of creep. First, everything creeps. Actually, solids creep even at zero external load, due to the fact that practically no polycrystalline body is in thermodynamic equilibrium. Second, creep is an energy driven phenomenon. Materials creep in order to decrease their energy (or other thermodynamical potential, depending on the external conditions). The energy of a polycrystal, for example, can be decreased by moving grain boundaries. This occurs in reality, but very slowly, by means of thermodynamic fluctuations. The rate of change is magnified significantly by elevating the temperature and/or applying an external load. Third, the mechanisms of creep are stress and temperature dependent.

Two major creep mechanisms are movement of dislocations and diffusion of vacancies. A typical deformation mechanism map is shown in the stress–temperature plane in Fig. 1. Above the curve (high stresses) the dominating mechanism is dislocation motion. Below the curve (low stresses) deformations occur by the diffusion of vacancies. It is believed that at low temperatures, vacancies move mostly over the grain boundaries (Coble creep), while for high temperatures, motion of vacancies through the lattice dominates (Herring–Nabarro creep or bulk diffusional creep). Diffusional creep is the leading phenomenon in many technological processes at high temperatures. Superplasticity, sintering and void formation occur mostly by diffusional creep. In this paper we focus on a thermodynamically consistent theory of diffusional
creep. The foundations of this theory were laid down by Nabarro [1], Herring [2], Coble [3] and Lifshitz [4]. Extensive reviews of various aspects of creep theory can be found in [5-24].

The mechanism of plastic deformation caused by bulk diffusional creep can be viewed as follows. Let a monocrystal be loaded by an external force (Fig. 2). Consider the right-hand side of the monocrystal. A surface external force might be thought of as a set of forces applied to each atom of the very right column of atoms (Fig. 2(a)). Because of thermal fluctuations some of the atoms of this column can jump to a new equilibrium position (Fig. 2(b)). Then the next atoms may jump into the vacant places and we see that vacancies enter the crystal body. Then vacancies can migrate inside the body and leave the body at the free surface (Fig. 2(d)).

The motion of vacancies is accompanied by the corresponding motion of material in the opposite direction. The moved material is shaded in Fig. 2(e). Since the motion of vacancies is dispersed over the material, one observes an effective elongation of the specimen (Fig. 2(f)).
In the case of boundary diffusion, material flows over the boundaries from unloaded to loaded pieces of the boundary and that yields some macroscopic plastic deformation. This process is shown schematically in Fig. 3, the moving material is shadowed.

A typical strain–time dependence for constant stresses is shown in Fig. 4. There are two different regimes of the plastic flow. Initially, strains grow fast, then the strain rate decays until it approaches some limiting value. These two regimes are referred to as primary and secondary creep.

The aim of this paper is to construct the microequations of diffusional creep in the framework of continuum mechanics and develop a homogenization procedure to derive macroequations of creep. There are a number of reasons for pursuing these goals. First, a phenomenological approach to the derivation of macroequations for creep provides too many options. Realization of our program may help to choose the right one.

Second, the problem seems challenging from the perspective of continuum mechanics. Looking at the sketch of boundary diffusional creep shown in Fig. 5, one may observe that the basic notion of continuum mechanic, Lagrangian coordinates, cannot be used in this case. Really, material points which were on the grain boundary moves into the grain body, which is in clear contradiction to the main postulate of continuum mechanics [25, 26] on the existence of a diffeomorphism between the deformed and undeformed states and, as a consequence, to the existence of Lagrangian coordinates. If a continuum deformation were a diffeomorphism, the material points, which are on the boundary, stay on the boundary forever. Lagrangian coordinates are used in continuum mechanics, for example, in the definition of velocity: one has to ask “velocity of what?” We suggest a way to overcome this difficulty.
Third, a theory of diffusional creep must be a building block for the theory of dislocational climb which is, at the moment, in a primitive stage.

The contents of the paper are as follows. Section 2 describes the main feature of the model for bulk diffusional creep, which is the existence of a plastic displacement field. This is an unusual situation in plasticity. The general kinematic relations for the bulk diffusion and surface diffusion are given in Section 3. In Section 4 the closed system of equations of diffusional creep is developed from thermodynamic considerations. The linear version of the general theory is presented in Section 5. In the rest of the paper a linear theory of bulk diffusional creep is studied, which aims to derive macroscopic laws for grain structure starting from a micromodel. This is referred to as a homogenization problem. In Section 6 the formulation of the homogenization problem is given for a particular case of periodic grain structure. The theorem of uniqueness of the solution is proved, which is evidence for the correctness of the basic equations. In Section 7 the general type of macroscopic constitutive relations is established. Secondary creep is considered in Section 8. It is proved that, under constant loads, the transient solution tends to a steady-state solution and the closed system of equations is found, which allows one to find the macrocharacteristics of the secondary creep without "tracing" the transient solution. A numerical example of the solution of this system is presented in Section 9. A dimensional analysis of the equations and numerical modeling of the transient process are discussed in Section 10.

2. MICROMECHANICS OF BULK DIFFUSIONAL CREEP: A LOGICAL SKELETON OF THE THEORY

The logical structure of the theory is especially simple in the case of bulk diffusional creep and before going into detailed discussion, we outline it briefly. The key point of the bulk diffusional creep is that plastic strains $\varepsilon^{(p)}_{ij}$ are compatible. There exists plastic displacement $w^{(p)}_i$ such that (in the linear case)

$$
\varepsilon^{(p)}_{ij} = \frac{1}{2} \left( \frac{\partial w^{(p)}_i}{\partial x_j} + \frac{\partial w^{(p)}_j}{\partial x_i} \right). \tag{1}
$$

Here, and in the following, small Latin indices run through values 1, 2 and 3, and correspond to projections on the Cartesian axis of the observer frame; $x_i$ are the observer coordinates.

The compatibility of plastic deformation is a pure kinematic hypothesis. It aims to model the process of deformation shown schematically in Fig. 2(e). In contrast to a general creep theory where six additional equations are to be given for six unknown functions $\varepsilon^{(p)}_{ij}$, in bulk diffusional creep one has to give only three additional equations for $w^{(p)}_i$.

It is clear that the plastic rate $\dot{w}^{(p)}_i$ should be related to vacancy motion. Some kinematical and thermodynamical consideration shows that the corresponding relation (in its simplest version) is

$$
\dot{w}^{(p)}_i = D \frac{\partial c}{\partial x_i} \tag{2}
$$

where $c$ is vacancy concentration, dot denotes time derivative and $D$ is the diffusion coefficient. Equation (2) reduces the number of closing equations to one: an equation for vacancy concentration $c$. This last equation is the diffusion equation for $c$

$$
\frac{\partial c}{\partial t} = D \Delta c. \tag{3}
$$

Equations (1)–(3) should be complemented by the usual equations of elasticity and provided with the boundary conditions. Now we proceed to detailed considerations.
3. CONTINUUM KINEMATICS

We are going to model, in terms of continuum mechanics, the following physical phenomenon. If an external load is applied to an atomic lattice containing a cloud of vacancies, vacancies migrate in some preferred direction. The motion of vacancies causes the motion of atoms in the opposite direction. The motion of atoms is perceived by an observer as an irreversible plastic deformation of the material. Our first step is to establish a kinematical relation which relates the motion of vacancies to the motion of the material.

We model the motion of vacancies and material by two continua with velocities $u_i$ and $v_i$ correspondingly. We assume that vacancies are not created inside the material and can only come from the boundary. Then, as we shall argue:

$$v_i^{(e)} = (1 - c)u_i + cu_i$$

where $v_i^{(e)}$ is an "elastic" velocity. If the elastic velocity $v_i^{(e)}$ is zero, the relation equation (4) expresses velocity of material (atoms) $v_i$ in terms of velocity of vacancies $u_i$ and vacancy concentration $c$.

Usually, vacancy concentration is negligible in comparison to unity. Nevertheless, we keep the factor $(1 - c)$ until the final calculations in order to underline the physical origin of various terms. Equation (4) is a postulate which is motivated by the following reasons.

Consider a piece of crystal lattice, a "representative volume of material," and think of $v_i$ as the average velocity of all the atoms of this piece

$$v_i = \frac{1}{N_a} \sum_a v_i^a$$

where $N_a$ is the number of atoms, $v_i^a$ is the velocity of the $a$th atom and the sum is taken over all of atoms of the piece. Similarly, velocity of vacancies is the average value of the velocities of all vacancies:

$$u_i = \frac{1}{N_v} \sum_a u_i^a.$$  

Here $N_v$ is the number of vacancies and $u_i^a$ is the velocity of the $a$th vacancy. The volume average velocity $\bar{v}_i$ is, by definition:

$$\bar{v}_i = \frac{1}{N} \left( \sum_a v_i^a + \sum_a u_i^a \right)$$

where $N$ is the total number of lattice sites

$$N = N_a + N_v.$$  

It follows from equations (5)-(8) that

$$\bar{v}_i = (1 - c)u_i + cu_i$$

where the volume fraction of vacancies $c$ is, by definition,

$$c = \frac{N_v}{N}.$$  

Relation equation (9) holds for a mixture of any two substances. Now we must express in some way the fact that we are dealing with diffusion of vacancies. We may assume that in the process of position exchange between an atom and a vacancy the velocities of the atom and the vacancy are equal in magnitude and opposite in sign. Therefore, in accordance with equation (7), $\bar{v}_i = 0$. Then equation (9) links the velocities of atoms and vacancies. It is clear that atoms and vacancies might have another common additional velocity. Then $\bar{v}_i$ is not zero, but equal to this
additional velocity. The additional velocity is not related to the process of vacancy diffusion or irreversible deformation. We identify this velocity with "elastic" velocity and denote it by $v^{(e)}$. Then equation (9) takes the form equation (4).

Note that the term "elastic" velocity is not quite exact. If one defines elasticity as, that part of deformation which disappears after unloading, then velocity $v^{(e)}$ might have a contribution from a plastic rigid motion, a motion of the monocrystal after unloading as a rigid body. However, we take some liberties in the terminology to simplify the notations and use the term elastic velocity for the sum of the "real" elastic velocity and plastic velocity of rigid motion.

The flux of vacancies relative to material $J_i$ is given by

$$J_i = c(u_i - v^{(e)}). \tag{11}$$

In accordance with equations (4) and (11) material velocity $v_i$ can be expressed in terms of elastic velocity and vacancy flux as

$$v_i = v^{(e)} - \frac{1}{1 - c} J_i. \tag{12}$$

This is a key kinematical relation.

Since vacancies can be generated only on the boundary, vacancy concentration obeys the conservation law

$$\frac{\partial c}{\partial t} + \frac{\partial c u_i}{\partial x_i} = 0. \tag{13}$$

Equations (4), (11)–(13) form the basic kinematical relations of bulk diffusional creep. Now we are going to incorporate into this picture the surface diffusion.

Consider a grain in a polycrystal. It occupies a region $V$. Region $V$ depends on time. Imagine that at an initial instance, $t_0$, we cut the grain out of the polycrystal and unload it. The grain occupies some region, $V_0$, in an unloaded state. We refer both regions to some Cartesian coordinates, $x'$. Besides, we introduce in the region $V_0$ some coordinates curvilinear in general, $\xi^a$, which, in a "usual" situation, play the role of Lagrangian coordinates. Indices $a, b$ and $c$ run through values 1, 2 and 3, and correspond to projections on the axis $a$.

There is one-to-one correspondence between the observer's coordinates $x$, and coordinates $\xi^a$.

$$x' = \xi'(\xi^a). \tag{14}$$

Without loss of generality mapping equation (14) may be identical, however, it is convenient to leave it without specifications because coordinates $x'$ and $\xi^a$ obey to different groups of transformations [27]. This is why we use another group of Latin indices, $a, b$ and $c$, in the notation for Lagrangian coordinates.

At each moment of time, $t$, there is mapping of the region, $V_0$, to region $V$

$$x' = x'(\xi^a, t). \tag{15}$$

If this mapping is a diffeomorphism, then $\xi^a$ are Lagrangian coordinates. In this case, if a point, $\xi^a$, lies on the boundary, $\partial V$, of the region, $V$, its image is on the boundary, $\partial V$, of the region, $V$, for all instants, $t$. Velocity is defined as the velocity of the particle $\xi^a$: $v' = \partial x'(\xi^a, t)/\partial t$. This is a classical kinematical scheme of continuum mechanics (see, for example, [25–27]). As one sees from Fig. 5, this is not the case for boundary diffusion creep and we have to change the kinematical scheme. We introduce, as a "primary" kinematical object, the region $V$ which is changed in time. In this region two velocity fields, material velocity $v'$ and vacancy velocity $u'$ are defined. If mapping equation (15) were a diffeomorphism and $v' = \partial x'(\xi^a, t)/\partial t$, then the normal velocity of the boundary surface $\partial V$ is equal to $v' n_i$. In the case of boundary diffusion these velocities are different. We denote the difference by $u$:

$$u_{\text{boundary}} = v' n_i + u. \tag{16}$$

Velocity, $u$, is caused by the material flow over the boundary. It appears as an additional
independent kinematical characteristic. However, a "more fundamental" characteristic might be introduced as primary characteristics of boundary diffusion: boundary mass flux $J^\alpha$. Boundary mass flux is defined in the following way. The mass of the material is conserved in the boundary flow, therefore, a law of conservation of mass should exist. Denote by $J^\alpha$ the vector of mass flow on the surface. Greek indices run through values 1 and 2, and correspond to projections on the boundary surface. If $\gamma$ is a curve on the boundary and $\nu_\alpha$ is the unit normal vector to $\gamma$ at a point $P$, then the scalar $J^\alpha \nu_\alpha \Delta s$ means the mass flow through the arc of $\gamma$ of the length $\Delta s$ at the point $P$. Let $\rho$ be the mass density of material. Then the law of conservation of mass has the form

$$\rho u = \nabla_\alpha J^\alpha$$

where $\nabla_\alpha$ is the covariant derivative on the surface $\partial V$.

Mass density obeys also the law of conservation of mass inside the region $V$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$  

Equations (16)–(18) provide the conservation of mass in volume $V$

$$\frac{\partial}{\partial t} \int_{V(t)} \rho d^3x = \int_V \frac{\partial \rho}{\partial t} d^3x + \int_{\partial V} \rho \mathbf{v} \cdot \mathbf{n} d^2s = - \int_V \frac{\partial \rho \mathbf{v}}{\partial x^1} d^3x + \int_{\partial V} \rho \mathbf{v} \cdot \mathbf{n} d^2s = 0.$$

It is natural to consider $J^\alpha$ as the primary characteristics of boundary diffusion, then velocity $u$ is determined by equation (17).

Now we come to the point where we have to introduce displacements. It is natural to define a field of elastic displacements $w^{(e)}(t,x)$ which has the domain $V(t)$. Vector $w^{(e)}(t,x)$ means the displacement of a crystal from the imaginary unloaded state to the actual state $V(t)$. If there are no plastic strains, the displacement $w^{(e)}(t,x)$ relates to velocity by the formula

$$\frac{\partial w^{(e)}_i}{\partial t} + v^{(e)}_k \frac{\partial w^{(e)}_i}{\partial x_k} = v^{(e)}_i.$$

Equation (19) can be rewritten as

$$\left( \delta_i^k - v^{(e)}_k \frac{\partial w^{(e)}_i}{\partial x_k} \right) v^{(e)}_i = \frac{\partial w^{(e)}_i}{\partial t}.$$

The latter relation can be considered as a system of linear equations with respect to velocity $v^{(e)}_i$, if the displacement field is known. We keep formulas equations (19) and (20) as the definition of the vector of elastic displacements if velocity $v^{(e)}_i$ is considered as a primary quantity. Remember that, by our convention, plastic (and, hence, elastic) deformations are consistent for diffusional creep and a vector of elastic displacements exists.

4. THERMODYNAMICS OF DIFFUSIONAL CREEP

We derive the basic equations of diffusional creep following the usual thermodynamical approach: we assume an expression for free energy of the material and construct the equations in a way to warrant the negativity of the time derivatives of free energy.

The free energy $F$ of a polycrystal has, by our assumption, an energy density per unit volume $F$:

$$\mathcal{F} = \int_{V(t)} F d^3x.$$
We accept that energy density $F$ is a function of the gradient of elastic displacement $w_i^{(e)}(= \partial w_i^{(e)}/\partial x^j)$, vacancy concentration $c$ and temperature $T$:

$$F = F(w_i^{(e)}, c, T). \quad (22)$$

Temperature $T$ is maintained constant.

Note that the assumption equation (22) taken together with the definition of elastic displacements equation (19) extracts a special class of models. For example, if elastic displacement is defined, instead of equation (19), by the formula

$$\frac{\partial w_i^{(e)}}{\partial t} + u_k \frac{\partial w_i^{(e)}}{\partial x_k} = v_i^{(e)}, \quad (23)$$

which may have some virtue, we would arrive at a class of models which differs from the one under consideration in the nonlinear case.

Let us find the time derivative of free energy. We assume first that region $V(t)$ is occupied by a crystal and all fields are smooth inside $V$. We have

$$\frac{d\tilde{\mathcal{\Gamma}}}{dt} = \int_V \left( \frac{\partial F}{\partial w_i^{(e)}} \frac{\partial}{\partial x^j} w_i^{(e)} + \frac{\partial F}{\partial c} \frac{\partial c}{\partial t} \right) d^3x + \int_{\partial V} \left( v'n_i + u \right) d^2x. \quad (24)$$

After substituting in equation (24) the expression for $(\partial w_i^{(e)}/\partial t)$ from equation (13) and integration by parts we obtain

$$\frac{d\tilde{\mathcal{\Gamma}}}{dt} = \int_V \left[ -\left( \frac{\partial}{\partial x_k} \frac{\partial F}{\partial w_i^{(e)}} \right) (\delta_{im} - w_i^{(e)} v_j^{(e)} k + w_i^{(e)} + J^t) \frac{\partial}{\partial x^j} \frac{\partial F}{\partial c} \right] d^3x + \int_{\partial V} \left[ \frac{\partial F}{\partial w_i^{(e)}} n_i (\delta_{ik} - w_i^{(e)} v_j^{(e)} k - \frac{\partial F}{\partial c} (c v_j^{(e)} + J^t) n_i + F(v'n_i + u) \right] d^2x. \quad (25)$$

Here we expressed also $\frac{\partial w_i^{(e)}}{\partial t}$ in terms of elastic velocity from equation (20).

For further transformations we need an identity [27]

$$\left( \frac{\partial}{\partial x_k} \frac{\partial F}{\partial w_i^{(e)}} \right) (\delta_{im} - w_i^{(e)} v_j^{(e)} k + w_i^{(e)} + J^t) \frac{\partial}{\partial x^j} \frac{\partial F}{\partial c} = \frac{\partial}{\partial x_k} \frac{\partial F}{\partial w_i^{(e)}} (\delta_{im} - w_i^{(e)} v_j^{(e)} k + w_i^{(e)} + J^t) - \frac{\partial F}{\partial c} \frac{\partial c}{\partial x^m}. \quad (26)$$

This identity can be checked by direct inspection. Using equations (26) and (12) we can rewrite equation (25) in the form

$$\frac{d\tilde{\mathcal{\Gamma}}}{dt} = \int_V \left( -\frac{\partial \sigma_{km}^{(e)}}{\partial x^k} v_m^{(e)} + J^i \frac{\partial}{\partial x^j} \frac{\partial F}{\partial c} \right) d^3x + \int_{\partial V} \left( \sigma_i^{(e)} n_i^{(e)} - \left( \frac{\partial F}{\partial c} + \frac{F}{1-c} \right) J' n_i + Fu \right) d^2x. \quad (27)$$

Here we introduced a notation

$$\sigma_i^{(e)} = \frac{\partial F}{\partial w_i^{(e)}} (\delta_{mi} - w_i^{(e)}/m_i) + \left( F - c \frac{\partial F}{\partial c} \right) \delta_i^{(e)}. \quad (28)$$

It is seen from this expression that $\sigma_i^{(e)}$ have the sense of components of a stress tensor.
Assume that \( J^i \) do not depend on \( v^{(e)}_m \). Since \( \sigma^i_\alpha \) do not depend on \( v^{(e)}_m \) as well and \( v^{(e)}_m \) can be chosen arbitrarily, equation (27) can comply with negativity of \( \frac{dF}{dt} \) if, and only if, the equilibrium equations hold

\[
\frac{\partial \sigma^i_\alpha}{\partial x^i} = 0. \tag{29}
\]

The simplest expression for the vacancy flux which does not contradict the negativity of \( \frac{dF}{dt} \) is

\[
J^i = - D^{ij} \frac{\partial}{\partial x^j} \frac{\partial F}{\partial c} \tag{30}
\]

where \( D^{ij} \) is a positive tensor.

Consider now the boundary terms. Let \( V \) be a polycrystal. Denote by \( \Sigma \) the grain boundary surface. Then the surface terms in \( \frac{dF}{dt} \) take the form

\[
\int_\Sigma \left( \left[ \sigma^{i\alpha}(v^{(e)}_n) - \frac{\partial F}{\partial c} \right] n_j + \left[ F \right] \right) d^2x \tag{31}
\]

where for any quantity \( A \) the symbol \( [A] \) means the difference of \( A \) at two sides of the surface \( \Sigma \).

Let us present the surface force \( \sigma_{n\alpha} n_j \) as a sum of normal force \( \sigma_{mn} n^i (\sigma_{mn} = \sigma_{ij} n_j) \) and tangent traction. Similarly, \( v^{(e)}_n \) is the sum of the normal velocity \( v^{(e)}_n (v^{(e)}_n = v^{(e)}_n n^i) \) and the tangent velocity. Then

\[
\sigma^i_\alpha v^{(e)}_n n_j = \sigma^i_\alpha v^{(e)}_n n_j + \sigma_{mn} v^{(e)}_n.
\]

Greek indices \( \alpha, \beta, \gamma \) run through values 1 and 2, and correspond to projection on the tangent plane to \( \Sigma \). Using also equation (12) we rewrite equation (31) in the form

\[
\int_\Sigma \left( \left[ \sigma^{i\alpha}(v^{(e)}_n) n_j + \sigma_{mn} (v_n + u) \right] + \left[ \left( \frac{\sigma_{mn} - F}{1 - c} - \frac{\partial F}{\partial c} \right) J^i \right] n_j + \left[ (\sigma_{mn} - F) u \right] \right) d^2x. \tag{32}
\]

It is natural to require continuity of the total normal velocity of the adjacent grains

\[
[v_n + u] = 0. \tag{33}
\]

Since \( \sigma_{mn} \) (as well as other “generalized forces” in equation (32)) does not depend on velocity, it is necessary that \( \sigma_{nn} \) be continuous:

\[
[\sigma_{nn}] = 0. \tag{34}
\]

The normal vacancy flux \( J^i n_j \) can be arbitrary and vacancies on two sides of the grain boundary seem to be produced at independent rates. Therefore, it is natural to accept that the corresponding coefficient at \( J^i n_j \) in equation (32) are zeros: at both sides of the boundary surface

\[
\frac{\sigma_{mn} - F}{1 - c} - \frac{\partial F}{\partial c} = 0. \tag{35}
\]

In accordance with equation (17), the last term in equation (32) can be written as

\[
\int_\Sigma \left[ (\sigma_{mn} - F) u \right] d^2x = \int_\Sigma \left[ \frac{\sigma_{mn} - F}{\rho} \nabla_u J^\alpha \right] d^2x = - \int_\Sigma \left[ J^\alpha \nabla_u \frac{\sigma_{mn} - F}{\rho} \right] d^2x. \tag{36}
\]
Here we integrated by part and dropped the term on the polycrystal boundary. Finally,

$$\frac{dF}{dt} = \int_V J^\alpha \frac{\partial}{\partial x^i} \frac{\partial F}{\partial c} \, d^3x + \int_{\partial V} \left( [\sigma^{\alpha\beta}[v^{(c)}])n_j - \left[ J^\alpha \nabla_\alpha \frac{\sigma_{\alpha\alpha} - F}{\rho} \right] \right) \, d^2x. \quad (37)$$

There are different models which obey the negativity of equation (37). The most plausible version is based on the assumptions that $\sigma^{\alpha\beta}n_j$ are continuous and surface fluxes of material $J^\alpha$ are independent on both sides of $\Sigma$. Then, neglecting reciprocal effects, one can put

$$\sigma^{\alpha\beta}n_j = -\mu^{\alpha\beta}[v^{(c)}] \text{ on } \Sigma \quad (38)$$

$$J^\alpha = d^{\alpha\beta} \nabla_\beta \left( \frac{\sigma_{\alpha\alpha} - F}{\rho} \right) \text{ on each side of } \Sigma. \quad (39)$$

Note that, in contrast to $\sigma_{\alpha\alpha}$, the energy density is not continuous on $\Sigma$, therefore, material fluxes $J^\alpha$ are different on the two sides of $\Sigma$. However, this is a nonlinear effect. The equations derived in this section close the system of equations of diffusional creep.

5. LINEARIZED THEORY

In the linear case the system of equations is simplified greatly. First, in this case one can neglect the changes of region $V$ in the process of deformation. Second, kinematical relations take a simple form

$$v^{(e)} = \frac{\partial w^{(e)}_i}{\partial t} = v_i + cu_i \quad (40)$$

$$v_i = v^{(e)}_i - J_i \quad (41)$$

$$\frac{\partial c}{\partial t} + \frac{\partial J_i}{\partial x_i} = 0 \quad (42)$$

$$\rho u = \nabla_\alpha J^\alpha. \quad (43)$$

Third, energy density is a quadratic function of elastic strains

$$e^{(e)}_{ij} = \frac{1}{2} \left( \frac{\partial w^{(e)}_i}{\partial x^j} + \frac{\partial w^{(e)}_j}{\partial x^i} \right) \quad (44)$$

and the deviation $s = c - c_0$, of vacancy concentration from its equilibrium value $c_0$, (for brevity from now on the function $s$ will be referred to as vacancy concentration)

$$F = \frac{1}{2} A^{\text{ik}} e^{(e)}_{ij} e^{(e)}_{jk} + \frac{1}{2} As^2 + \text{function of } T. \quad (45)$$

Here $A^{\text{ik}}$ are Young moduli, while $A$ is an additional material constant. From some statistical reasoning [5]

$$A = \frac{\rho_0 T}{mc_0} \quad (46)$$

where $m$ is the mass of one atom, $\rho_0$ is the mass density of an ideal lattice. In equation (45) we neglect an interaction term $A^{\text{ik}} e^{(e)}_{ij}(c - c_0)$. 


In accordance with equation (28), the stress tensor \( \sigma^{ij} \) in the linear theory has the form
\[
\sigma^{ij} = A^{ijk} e_k^{(r)}.
\] (47)

It obeys the equilibrium equations
\[
\frac{\partial \sigma^{ij}}{\partial x^j} = 0.
\] (48)

Vacancy flux \( J^i \) is given by equation (30)
\[
J^i = -AD^{ij} \frac{\partial s}{\partial x^j}.
\] (49)

Therefore, equation (42) transforms to the usual diffusion equation
\[
\frac{\partial s}{\partial t} = \frac{\partial}{\partial x^i} \left( AD^{ij} \frac{\partial s}{\partial x^j} \right).
\] (50)

We assume that diffusion constants obey the positive definiteness condition
\[
D^{ij} \xi_i \xi_j \geq D \xi_i \xi_i > 0.
\] (51)

On the grain boundary we have from equations (33)–(35), (38) and (39)
\[
[u_n] = 0
\] (52)
\[
[\sigma_{nn}] = 0
\] (53)
\[
\sigma_{nn} = A s \text{ at each side of grain boundary}
\] (54)
\[
\sigma^{ij} n_j = -\mu^{\alpha \beta} \left[ \frac{\partial w^{(r)}}{\partial t} \right]
\] (55)
\[
J^\alpha = d^{\alpha \beta} \nabla_\beta \sigma_{nn} \text{ at each side of the grain boundary.}
\] (56)

It follows from equations (43) and (56) that the law of growth of grain boundaries due to boundary diffusion
\[
\rho u = \nabla_\mu \frac{d^{\alpha \beta}}{\rho} \nabla_\alpha \sigma_{nn}.
\] (57)

Equations (40)–(57) form a closed system of equations of diffusional creep.

6. HOMOGENIZATION PROBLEM

From now on we shall consider a special case of the linearized theory, formulated in Section 5, when there is no boundary diffusion and, hence, the only irreversible deformation is due to the bulk vacancy diffusion. Formally this means that coefficients \( d^{\alpha \beta} \) in equation (39) are supposed to be zero, which eliminates equations (56), (43) and (57) from the system equations (40)–(57).

Further we assume that constants \( \mu^{\alpha \beta} \) in boundary conditions equation (55) are zero, which neglects the tangent stresses at the grain boundary:
\[
\sigma^{ij} n_j = 0 \text{ at each side of grain boundary.}
\] (58)

This is equivalent to an additional assumption that the process of shear stress relaxation at the grain boundaries is much faster than the bulk diffusion process and is completed immediately.
after the load is applied, so that the adjacent grains can slide without resistance along their common boundary.

In the absence of the boundary diffusion the deformation of the region $V$ is described by the displacement field $w_i(x,t)$, defined in $V$ and related to the velocity $v_i$ by the formula

$$v_i(x,t) = w_i(x,t) x \in V.$$  

We introduce also the plastic displacements, which are determined by the flux $J_i$ by means of the relation

$$\dot{w}_i^{(p)}(x,t) = - J_i(x,t) x \in V.$$  

Then the displacements $w_i$ are the sum of the elastic and plastic displacements

$$w_i = w_i^{(e)} + w_i^{(p)}.$$  

Similarly for the strains:

$$\varepsilon_{ij} = 1/2 \left( \frac{\partial w_i^{(e)}}{\partial x^j} + \frac{\partial w_j^{(e)}}{\partial x^i} \right), \quad \varepsilon_{ij}^{(p)} = 1/2 \left( \frac{\partial w_i^{(p)}}{\partial x^j} + \frac{\partial w_j^{(p)}}{\partial x^i} \right) \varepsilon_{ij} = \varepsilon_{ij}^{(e)} + \varepsilon_{ij}^{(p)}.$$  

Instead of equation (52), the continuity condition of normal displacement will be employed:

$$[w_n] = 0.$$  

Condition equation (52) follows from equation (63), but not vice versa. The difference is that equation (63) excludes the possibility that the normal displacements are discontinuous at the moment $t = 0$ when the load is applied.

It is also necessary to complement the equations above with initial conditions for vacancy concentration and plastic displacements:

$$s(x,t) = 0, x \in V, t = 0$$

$$w_i^{(p)}(x,t) = 0, x \in V, t = 0.$$  

The closed system of equations in the case considered in the absence of boundary diffusion and with zero boundary shear stresses, consists of the equations (44), (47)-(50), (53), (54), (58) and (60)-(65).

Consider a polycrystalline body containing a huge number of grains. We are going to derive a theory for predicting the mechanical behavior of the body. The experience gained in the averaging of random structures shows that most results for bodies with random and periodic structures are qualitatively similar. (See, for example, [27].) Therefore, we consider a body with a periodic microstructure (Fig. 6) loaded with some constant or variable traction. The problem is to find microfields of elastic and plastic deformations and macroscopic constitutive equations.

For simplicity and consistency with the performed numerical modeling, only the 2-D plane strain case of regular hexagonal periodical microstructure (Fig. 6(b)) will be considered. The reason is that with boundary condition equation (58) not all microstructures can withstand the
instantaneous application of the external traction. For example, the rectangular microstructure (Fig. 6(a)) cannot be loaded by shear stresses, applied parallel to the grain boundaries. In other words, any macrodeformation of the structure should be the result of the application of macrostresses. Here we decided to use one structure which possesses the necessary properties rather than to formulate general restrictions on the grain geometry, which can be solved in 2-D, as well as in the 3-D case. An accurate formulation of that property will be done at the end of this section after the formulation of the homogenization problem.

We consider the asymptotical statement of the homogenization problem when the period of the microstructure \( L \) tends to zero and averaged equations are the corresponding limit equations (see, for example, [27]). Before presenting the results, some description of the periodic structure is to be done.

We assume that the grains coincide with the cells of the periodic structure. Let \( \omega^+ \) be an arbitrary cell and \( \epsilon \) be half the distance between the opposite hexagon edges, which will be taken for the characteristic size of the grain. The boundary \( \partial \omega^+ \) of the cell \( \omega^+ \) is comprised of three pairs of lines \( S_1, S'_1, S_2, S'_2, S_3, S'_3 \) such that for every line \( S_\alpha \), there exists a translation \( l_\alpha \in G \), mapping \( S_\alpha \) onto \( S'_\alpha \). This notation is explained in Fig. 7.

The periodical regular hexagonal grain structure \( M \) is obtained by translation of that cell by all elements of translation symmetry group, generated by vectors \( \mathbf{I}^1 \) and \( \mathbf{I}^2 \):

\[
G = \{ \mathbf{l}^m \mathbf{k}^n | m^1 + k^2, m, k = 0, \pm 1, \pm 2, \ldots \}.
\]

For \( \mathbf{l} \in G \) we denote by \( \omega(\mathbf{l}) \) the image of the cell \( \omega^+ \) under the translation \( \mathbf{l} \). Different cells \( \omega(\mathbf{l}) \) may have in common the boundary points only, and the union of the cells covers the whole plane. Obviously, the translation \( -l_\alpha \) maps \( S'_\alpha \) onto \( S_\alpha \). Thus, the periodic structure induces the certain mapping of the cell boundary \( \partial \omega^\prime \leftrightarrow \partial \omega^+ \), which will be used for the formulation of the boundary conditions. For every point \( x \in \partial \omega^+ \) we denote by \( \mathbf{l}(x) \) the corresponding translation vector. The points \( x \) and \( x' = x + \mathbf{l}(x) \) will be referred to as the corresponding points. Note that \( \mathbf{l}(x) \) is constant within each line \( S_\alpha, S'_\alpha \).

The unit normal \( \mathbf{n} \) to the cell boundary is assumed to be directed outward from the cell, therefore at the corresponding points \( x \) and \( x' \) we have

\[
\mathbf{n}(x) + \mathbf{n}(x') = 0, \mathbf{l}(x) = -2 \epsilon \mathbf{n}(x).
\]
Let \( f(x) \) be an arbitrary function, which is continuous within each grain, but may be discontinuous at the grain boundaries. Function \( f(x) \) is called periodic if

\[
f(x + \mathbf{l}) = f(x) \quad \text{for any } x \in \omega^+ \text{ and for any } \mathbf{l} \in G.
\]

(68)

Here \( \omega^+ \) is the interior of a cell \( \omega^+ \).

If function \( f(x) \) is known within any cell, it can be extended to the whole space by the formula equation (68). From now on the term “periodic function” will be used in the sense of the above definition, unless otherwise is explicitly indicated.

Denote by \( \omega^- \) the cell, such that \( S_i = \omega^+ \cap \omega^- \). It follows from equation (68) and the definition of the corresponding points that

\[
[f] = f^+ - f^- = f(x^+, t) - f(x^-, t) = f(x, t) - f(x', t) \quad \text{for } x \in S_i.
\]

(69)

Thus, for periodic functions the discontinuity conditions can be expressed in terms of function values within one cell, which allows us to formulate the cell problem. Instead of applying the formal procedure of homogenization (see, for example, [27]) we use here an “intuitive” approach, which is easier to implement. Of course, it gives the same results as the general approach.

Averaged constitutive equations by their physical sense relate a macroscopically homogeneous deformation of a “large” (compared with grain size \( \varepsilon \)) specimen to averaged stresses. Instead of “large” specimen we consider the whole plane loaded by stress \( \delta\gamma(t) \) at infinity. One has to find microstresses in periodic structure and macrostrains \( \delta\gamma(t) \). One may prescribe at infinity macrostrains \( \delta\gamma(t) \) as functions of time; then macrostresses \( \delta\gamma(t) \) and microdeformations in periodic structure should be found. For definiteness, we consider the case of given macrostresses.

If there were no grain boundaries, the homogeneous plane deformation history would be generated by the displacement field

\[
\tilde{\omega}(x, t) = \tilde{\varepsilon}_{ij}(t)x^j.
\]

(70)

The grain structure results in additional periodic displacements \( W_j(x, t) \), so that total displacements are given by the sum

\[
w_j(x, t) = \tilde{\varepsilon}_{ij}(t)x^j + W_j(x, t).
\]

(71)

Since the first term in equation (71) is obviously continuous over space coordinates, it follows from equations (63) and (69) that the field \( W_j(x, t) \) satisfies the condition

\[
W_n(x, t) + W_n(x', t) = 0 \quad \text{for } x \in \partial\omega^+ \Rightarrow \tilde{W}_n(x, t) + \tilde{W}_n(x', t) = 0.
\]

(72)

The vacancy concentration \( s \) is a periodic function. With equation (69) taken into account, equations (53) and (54) link the normal stress values and vacancy concentration at the corresponding points of the boundary:

\[
\sigma_{mn}(x, t) = \sigma_{mn}(x', t) \quad \text{for } x \in \partial\omega^+ (73)
\]

\[
s(x, t) = s(x', t) \quad \text{for } x \in \partial\omega^+.
\]

(74)

The macrostresses, or averaged stresses, are defined by formula

\[
\tilde{\sigma}^{\gamma}(t) = \frac{1}{|\omega^+|} \int_{\omega^+} \sigma^{\gamma}(x, t) \, d^2x.
\]

(75)

The full set of equations is as follows: equations (44), (47)–(50), (53), (54), (58), (60)–(62), (71)–(75). For further references that system of equations is referred to system \( P \). Initial conditions for the system \( P \) are equation (64) and (65). It is implied that all equations included in system \( P \) and initial conditions should be satisfied in the cell \( \omega^+ \).

Now we are going to show, that the chosen microstructure cannot be subjected to instantaneous macrodeformation, if stresses are zero. With zero stresses and zero vacancy
concentration $s$, the elastic strain coincides with the total strain and is equal to zero, hence the displacement field $w_i$ within cell $\omega^+$ is rigid body motion:

$$w_i = \mathbf{e}_{ii}x^i + W_i = \lambda e_{ii}x^i + a_i, x \in \omega^+, \lambda, a_i = \text{const}, e_{11} = e_{22} = 0, e_{12} = -e_{21} = 1. \quad (76)$$

Relation equation (76) allows us to express the displacement $W_i$ in terms of macrostrains and rigid body motion:

$$W_i = \mathbf{e}_{ii}x^i + \lambda e_{ii}x^i + a_i. \quad (77)$$

Inserting equation (77) into the continuity condition equation (72) yields

$$0 = W_n(x) + W_n(x') = (\mathbf{e}_{ii}x^i + \lambda e_{ii}x^i + a_i)n^i(x) + (\mathbf{e}_{ii}x'^i + \lambda e_{ii}x'^i + a_i)n^i(x')$$

$$= (\mathbf{e}_{ii}x^i + \lambda e_{ii}x^i + a_i)n^i(x) - (\mathbf{e}_{ii}x'^i + \lambda e_{ii}x'^i + a_i)n^i(x)$$

$$= (\mathbf{e}_{ii}x^i + \lambda e_{ii})n^i(x) = (\mathbf{e}_{ii}x'^i + \lambda e_{ii})n^i(x')$$

$$= (\mathbf{e}_{ii}x^i + \lambda e_{ii})n^i(x) - \lambda n^i(x) \otimes \mathbf{l}(x) = \mathbf{e}_{ii}n^i(x), x \in \partial \omega^+. \quad (78)$$

The vector product $\mathbf{n} \otimes \mathbf{l}$ in equation (78) vanishes because these vectors are collinear at each boundary point (see equation (67)). Since normal is constant along each edge of the hexagon, equation (78) provides three homogeneous linear equations with respect to three macrostrain components $\mathbf{e}_{ii}$. A direct check shows that its determinant is not zero, which implies that all macrostrains have to be zero.

Let $R$ be the set of periodic displacement fields $V_i$, defined at the cell $\omega^+$ by formula for rigid body motion

$$V_i = \lambda e_{ii}x^i + a_i, \lambda, a_i = \text{const} \quad (79)$$

and extended to the whole plane by the periodicity condition equation (68). Under the displacement $V_i$ each cell shifts by the constant vector $a_i$ and rotates around its center by the angle $\lambda$. It follows from equations (76)–(78) that any such a field satisfies the continuity condition equation (72) and does not produce macroadef ormation. Figure 9 illustrates the movement of the cells. The holes that one can see at the corners of the hexagons, are a second-order effect and are ignored by the small deflection theory used here.

**Theorem 1.** Consider the solution of the system $P$ with initial conditions equations (64) and (65). Macrostresses $\sigma^{ij}(t)$ are given functions of time. The total and elastic displacements of this solution are defined with the accuracy of the arbitrary displacement field from set $R$. All the other components of the solution, such as vacancy concentration, plastic displacements and strains, elastic strains, macrostrains and stresses are uniquely defined.

**Proof.** Introduce the notations

$$I(t) = \frac{1}{2} \int_{\omega^+} A \varepsilon^2 d^2x + \frac{1}{2} \left[ \varepsilon^{(e)}, \varepsilon^{(e)} \right] \left[ \varepsilon^{(e)}, \varepsilon^{(e)} \right] = \int_{\omega^+} A^{ijkl} \varepsilon^{(e)}_{ij} \varepsilon^{(e)}_{kl} d^2x,$$

$$\left[ \nabla s, \nabla s \right] = \int_{\omega^+} AD^j \frac{\partial s}{\partial x^j} \frac{\partial s}{\partial x^j} d^2x. \quad (80)$$

Since the system $P$ is linear, it is sufficient to prove, that if macrostresses are zero, then the system $P$ with initial conditions equation (64) and (65) has only zero solution for all components with the exception of displacements, which belong to the set $R$. At the initial moment $t = 0$ the plastic displacement is zero because of equation (65), the displacements coincide with the elastic displacements and since the macrostresses are zero, the macrostrains are also zero at the moment $t = 0$. Hence

$$I(0) = 0. \quad (81)$$
Using inequality equation (C.6) for \( t^* = 0 \) from Appendix C, we know that functional \( I(t) \) is zero for \( t \geq 0 \). Hence

\[
\begin{align*}
    s(t) = 0, & \quad e_{ij}^{(pt)} = 0, \\
    \sigma_{ij} = 0, & \quad e_{ij}^{(p)} = 0.
\end{align*}
\] (82)

Hence, the displacement of the cell is rigid body motion, given by the formula equation (76). It was proved above, that in order to satisfy the continuity condition equation (72), the macrostrains have to be zero. The uniqueness theorem is proved.

**Remark 1.** Let us consider the loading case when the non-zero macrostresses are applied only at some time interval \([0,t^*]\), and were removed afterwards. Then from inequality equation (C.6) we conclude that vacancy concentration \( s \) and elastic strains \( e_{ij}^{(p)} \) exponentially tend to zero, hence the stresses also tend to zero. In other words, after unloading the residual stresses are relaxing to zero exponentially with respect to time.

We conclude this section with the presentation of averaged stresses in terms of values of normal microstresses at the grain boundary (see Appendix B):

\[
\bar{\sigma}_{ij} = \frac{\epsilon}{|\omega^\perp|} \int_{\partial \omega} \sigma_{n'n'} dx.
\] (83)

Relation equation (83) is valid for an arbitrary stress field satisfying equilibrium equation (48) and boundary conditions equations (58) and (73). With equation (54) taken into account, the averaged stresses can be expressed in terms of the values of vacancy concentration at the grain boundary:

\[
\bar{\sigma}_{ij} = \frac{A \epsilon}{|\omega^\perp|} \int_{\partial \omega} s n'n'dx.
\] (84)

It can be checked (see Appendix B) that for arbitrary constant \( C \), the following identity holds:

\[
C \delta_{ij} = \frac{\epsilon}{|\omega^\perp|} \int_{\partial \omega} Cn'n'dx.
\] (85)

It follows from equations (84) and (85), that if vacancy concentration is constant over the grain boundary then the corresponding macrostress tensor is spherical and the plane is under hydrostatic compression or tension.

### 7. BOLTZMAN SUPERPOSITION PRINCIPLE AND MACROEQUATIONS.

As has already been stated above, the macromodel should provide the relations between macrostresses and macrostrains \( \bar{\sigma}_{ij}(t) \) and \( \bar{e}_{ij}(t) \). It seems almost obvious, that any parabolic type linear system such as \( P \) satisfies the Boltzman superposition principle and, hence, the stress–strain relation would involve an integral operator.

Let us first assume that at \( t = 0 \) the unit tension along axis \( x^1 \) is instantaneously applied to the polycrystal and remains unchanged for \( t > 0 \). Then the only non-zero stress component is \( \bar{\sigma}_{11}(t) = 1 \). Denote by \( N(t) \), the solution of system \( P \) with initial conditions equations (64) and (65), corresponding to load case under consideration:

\[
N(t) = [\bar{e}_{ij}(t), \sigma_{ij}(\cdot,t), e_{ij}(\cdot,t), e_{ij}^{(p)}(\cdot,t), e_{ij}^{(pt)}(\cdot,t), s(\cdot,t), W(\cdot,t), w(\cdot,t), w^{(p)}(\cdot,t)].
\] (86)

Solution \( N(t) \) is defined only for \( t \geq 0 \). Let us formally define it for \( t < 0 \):

\[
N(t) = 0 \text{ for } t < 0.
\] (87)
If the same tension \( \sigma_{11}(t) = 1 \) is applied at some time \( t_1 > 0 \), then the solution is obviously equal to \( N(t - t_1) \) for \( t > 0 \). Let us stress that \( N(t - t_1) = 0 \) for \( t < t_1 \) because of the definition equation (87).

The next step is to consider the load history, when at discrete moments \( t_i = i \Delta, i = 1,2, \ldots, k \) tension increments \( d\sigma_{11}(t_1), d\sigma_{11}(t_2) \ldots, d\sigma_{11}(t_k) \) are applied. Then at any particular time \( t \), \( t_m < t < t_{m+1} \), the total tension \( \sigma_{11}(t) \) is given by the formula

\[
\sigma_{11}(t) = \sum_{i=1}^{m} d\sigma_{11}(t_i) \tag{88}
\]

and the solution is given by the sum

\[
\sum_{i=1}^{m} d\sigma_{11}(t_i)N(t - t_i). \tag{89}
\]

Extension of the formula equation (89) to a continuous loading process provides the following formula for the solution:

\[
\int_{0}^{t} \sigma_{11}(\xi)N(t - \xi)\,d\xi. \tag{90}
\]

Let us denote by \( R_{ijk}(t) \) the macrostrain \( \varepsilon_{ijk}(t) \) corresponding to the application of the macrostress \( \sigma_{kk}(t) = 1, t > 0 \). The values \( R_{ijk}(t) \) at \( t = 0 \) are components of the tensor of elastic compliances of a polycrystal. Because of that it is convenient to decompose \( R_{ijk}(t) \) into the sum

\[
R_{ijk}(t) = R_{ijk}(0) + K_{ijk}(t), \quad K_{ijk}(0) = 0. \tag{91}
\]

By its mechanical sense the function \( K_{ijk}(t) \) is the \( \varepsilon_{ij} \) creep strain component caused by constant load \( \sigma_{kk}(t) = 1 \), while the other macrostress components are equal to zero. Then for an arbitrary loading process the following holds:

\[
\varepsilon_{ij}(t) = \int_{0}^{t} R_{ijk}(t - \xi)\sigma_{kk}(\xi)\,d\xi = R_{ijk}(0)\sigma_{kk}(t) + \int_{0}^{t} \frac{\partial K_{ijk}(t - \xi)}{\partial t} \sigma_{kk}(\xi)\,d\xi. \tag{92}
\]

Equations of the type equation (92) are widely used for creep modeling of polymers and concrete.

So we arrive at the conclusion. In order to find macrostrains, caused by an arbitrary loading process, it is necessary and sufficient to know instantaneous elastic moduli tensor \( R_{ijk}(0) \) and creep tensor \( K_{ijk}(t) \), which components are creep strains caused by the corresponding constant macrostresses. Thus, in numerical modeling or experiment one may consider only loading cases when constant load is instantaneously applied to the body and remains unchanged. This is nothing else, but the classical experiment to find the creep property of a material.

Inversion of equation (92) renders

\[
\sigma_{ij}(t) = \int_{0}^{t} Q_{ij,kt}(t - \xi)\varepsilon_{kk}(\xi)\,d\xi = Q_{ij,kt}(0)\varepsilon_{kk}(t) + \int_{0}^{t} \frac{\partial Z_{ij,kt}(t - \xi)}{\partial t} \varepsilon_{kk}(\xi)\,d\xi \tag{93}
\]

\[
Q_{ij,kt}(t) = Q_{ij,kt}(0) + Z_{ij,kt}(t), \quad Z_{ij,kt}(0) = 0. \tag{94}
\]

Here \( Q_{ij,kt}(t) \) is the macrostress component \( \sigma_{ij}(t) \) caused by the instantaneous application of a macrostrain \( \varepsilon_{kk}(t) = 1 \), while all the other macrostrain components are equal to zero. The tensor \( Q_{ij,kt}(0) \) is the elastic moduli tensor of the polycrystal.
It is worth mentioning that creep curves \( K_{ij,k}(t) \) for small values of \( t \) have an asymptotic behavior

\[
K_{ij,k}(t) \sim t^{1/2}, \quad \frac{\partial K_{ij,k}(t)}{\partial t} \sim t^{-1/2}
\]

and, hence, the creep rate tends to infinity as \( t^{-1/2} \) when \( t \) tends to zero:

\[
\dot{e}_{ij}(t) \sim t^{-1/2}, \quad t \to 0.
\]

An important feature of the constitutive equations (92) and (93) is that these relations are not local: there is a memory of the history of the process. This means that local theories of primary creep are not adequate at least in the case of bulk diffusional creep.

8. SECONDARY CREEP

Generally speaking, the macroscopic constitutive equations are given by the integral operators equations (92) and (93). However, for "slow" loading processes and a developed creep it is possible to use as an approximation the creep law

\[
\dot{e}_{ij} = E_{ijkl} \ddot{\sigma}^{kl}, \quad \ddot{\sigma}^{kl} = \ddot{\sigma}^{kl} - \delta^{kl} \ddot{\sigma}_{xx}/2
\]

or

\[
\ddot{\sigma}^{ij} = \epsilon^{ijkl} \dot{e}_{kl}.
\]

Also the incompressibility condition is imposed:

\[
\dot{e}_{kk} = 0
\]

which reflects the physically obvious fact that there is no volume change from bulk vacancy diffusion. A tensor \( \epsilon^{ijkl} \) is the inverse tensor to \( E_{ijkl} \).

The macrocharacteristics of the secondary creep \( E_{ijkl} \) are the limits of the creep rates \( \dot{K}_{ijkl}(t) \) when \( t \to \infty \). The fact that under constant applied macrostresses the creep rates tend to some constants when \( t \to \infty \) will be formulated and justified below and constitutes the basis of the approximation equations (98) and (99).

We start from formal description of how to compute the constants involved in the secondary creep law equation (98). It turns out that they may be found from the following variational principle. Let \( k_{ij} \) be an arbitrary constant macroscopic creep rates, satisfying the incompressibility condition equation (99). Denote by \( J(s) \) the following functional of function \( s(x) \):

\[
J(s) = \int \left[ \frac{1}{2} \left( \nabla s, \nabla s \right) - \epsilon \right] \int e_{ij} n_i n_j s \, dx.
\]

Here the notation equation (80) is used. Consider the minimization problem

\[
J(s) \to \min_s.
\]

Minimum is sought on the set of all functions \( s \) obeying the constraints equation (74). It follows from equations (85) and (99) that the term linear with respect to \( s \) in equation (100) is zero for \( s = \text{const} \), hence the solution \( s^* \) of the problem is determined up to an arbitrary constant. We fix this constant by the condition

\[
\int s^*(x)n_i n_j s \, dx = 0.
\]
The necessary and sufficient condition of the minimum is the following identity, which should hold for every function satisfying the condition equation (74)

\[ [\nabla s^*, \nabla s] = \epsilon \int_{\partial \omega^*} \epsilon_{ij} n^i s^j d x \text{ for } \nabla s s(x) = s(x'), \quad x \in \partial \omega^* . \]  

(103)

The differential form of the problem equation (101) is derived from equation (103):

\[ \frac{\partial}{\partial x^i} AD^j \frac{\partial s}{\partial x^j} = 0, \quad x \in \omega^* \]  

(104)

\[ [J_n](x) = - 2 \epsilon \epsilon_{ij} n^i(x), \quad x \in \omega^* , \]  

\[ [J_n](x) = J_n(x) + J_n(x'), \quad x \in \omega^* , \]  

\[ J_n(x) = - AD^j \frac{\partial s(x)}{\partial x^j} n_j(x), \quad x \in \omega^* . \]  

(105)

After the solution \( s^* \) of the variational problem equations (100), (74), (101) and (102) are found, the deviator of macrostresses is defined by the formula equation (84) which takes the form

\[ \tilde{e}^{ij} = \frac{A \epsilon}{|\omega^*|} \int_{\partial \omega^*} s^* n^i n^j d x . \]  

(106)

Macrostresses \( \tilde{e}^{ij} \) are deviatoric because of condition equation (102) since

\[ \tilde{e}^{ij} \]  

are deviatoric because of condition equation (102) since

\[ \sum_{kl} M^{kl} \frac{\partial s}{\partial x^k} n^l(x) = 0. \]  

(107)

The solution \( s^* \) depends linearly on the parameters \( \tilde{e}^{ij} \). Hence, by putting this solution into equation (106) one obtains macrostresses in terms of creep velocities \( \tilde{e}^{ij} \), i.e. the relation equation (98). In more detail, consider two solutions, corresponding to two linear independent loading cases:

\[ s^{12} = s^{21} \]  

corresponds to \( \tilde{e}_{12} = \tilde{e}_{21} = 1/2, \tilde{e}_{11} = 0, \tilde{e}_{22} = 0 \),

\[ s^{11} = - s^{22} \]  

corresponds to \( \tilde{e}_{12} = \tilde{e}_{21} = 0, \tilde{e}_{11} = - \tilde{e}_{22} = 1/2 \).  

(108)

Then the solution \( s^* \) is the linear combination

\[ s^* = \tilde{e}^{ij} s^{ij} . \]  

(109)

Substitution of equation (109) into equation (106) provides the formulas for the macrocharacteristics \( e^{ijkl} \):

\[ e^{ijkl} = \frac{A \epsilon}{|\omega^*|} \int_{\partial \omega^*} (s^{kl}) n^i n^j d x . \]  

(110)

It is obvious that only two constants among \( e^{ijkl} \) are independent.

So far it was shown how to find the deviator of macrostresses if macroscopic constant incompressible creep rates are given. Let us prove that the secondary creep law is reversible. Multiplying equation (106) by \( \delta^{ij} \) we obtain after summation over repeated indices and using equation (103):

\[ \tilde{e}^{ij} \delta^{ij} = \frac{A \epsilon}{|\omega^*|} \int_{\partial \omega^*} s^* \delta^{ij} n^i n^j d x = \frac{A \epsilon}{|\omega^*|} [\nabla s^*, \nabla s^*] . \]  

(111)

The left-hand side of the relation equation (111) is zero if and only if all creep rates \( \tilde{e}^{ij} = 0 \),
which means that the matrix of the quadric form \( \tilde{e}_{ij} = e^{\beta \gamma \lambda} \tilde{e}_{ij} \tilde{e}_{\lambda} \) is positive definite, hence the law equation (98) may be inverted.

Now we can describe how to find creep rates and vacancy concentration for secondary creep. Let macrostresses \( \tilde{\sigma}^{0ij} \) be given constants. First, the deviator of tensor \( \tilde{\sigma}^{0ij} \) should be calculated

\[
\tilde{\sigma}^{0ij} = \tilde{\sigma}^{0ij} - \delta^{ij} p, \quad p = \sigma^{0kk}/2. \tag{112}
\]

Then the creep rates \( \tilde{\varepsilon}_{0ij} \) are found satisfying the creep law equations (97)-(99). The vacancy concentration \( s^0 \) is the sum of the constant \( A^{-p} \) and the solution of the variational problem equation (101), corresponding to creep rates \( \tilde{\varepsilon}^{0ij} \).

\[
s^0(x) = A^{-1} p + \tilde{\varepsilon}^{0ij}(x). \tag{113}
\]

The last step to define the microcharacteristics of the secondary creep is to determine the elastic strains and stresses within the cell \( \omega^+ \). The normal stresses at the cell boundary are determined from equation (51), since the vacancy concentration \( s^0 \) is found:

\[
\sigma_{nn}(x) = A s^0(x), \quad x \in \partial \omega^+. \tag{114}
\]

Formulas equations (58) and (114) define surface tractions at the grain boundary. Thus, the elastic displacements, elastic strains and stresses inside the cell may be found from the solution of the elasticity problem equations (44), (47), (48), (58) and (114), if the principal vector and moment produced by surface tractions are zero, which they are as is shown in Appendix B. Denote this solution as \( w_i^{(e)}(x), e_i^{(e)}(x), \sigma^{0ij} \). At this point all the characteristics of secondary creep are determined.

**Theorem 2.** Under constant applied macrostresses \( \tilde{\sigma}^{0ij} \) the solution of the system \( P \) with initial conditions equations (64) and (65) reveals the following asymptotic behavior:

\[
s(x,t) \to s^0(x), \tilde{\varepsilon}^{0ij}(x,t) \to \tilde{\varepsilon}^{0ij}(x,t), e_i^{(e)}(x,t) \to e_i^{(e)}(x,t), \sigma^{0ij}(x,t) \to \sigma^{0ij}(x). \tag{115}
\]

**Proof.** It is shown in Lemma 2, Appendix C, that the difference between two arbitrary solutions of the system \( P \), corresponding to the same loading process \( \tilde{\sigma}^{0ij}(t) \), tends to zero in the following sense:

\[
s^1(x,t) - s^2(x,t) \to 0, \tilde{\varepsilon}^{0ij}(t) - \tilde{\varepsilon}^{0ij}(t) \to 0, e_i^{(e)}(x,t) - e_i^{(e)}(x,t) \to 0, \sigma^{0ij}(x,t) - \sigma^{0ij}(x,t) \to 0. \tag{116}
\]

Let us stress that solutions need not satisfy initial conditions equations (64) and (65) and need not have the same initial conditions. This means that if some particular solution of the system \( P \) is found, then any other solution tends to it, regardless of the initial conditions. Thus, to find the asymptotics of the solution of the problem it is sufficient to find some particular solution of the system \( P \). We shall use upper case index "0" for all quantities related to this solution. This implies that the functions introduced above with the same index are part of this particular solution.

Let us first define macrostresses as a constant strain rate process:

\[
\tilde{\varepsilon}^{0ij}(t) = \tilde{\varepsilon}^{0ij}. \tag{117}
\]

Second, define the plastic displacement. Since the plastic displacement velocity is expressed in terms of the vacancy concentration from equations (60) and (49), the only freedom left is to define the plastic displacements at \( t = 0 \). We pose

\[
w_i^{0(x)}(x,0) = - w_i^{0(x)}(x) \in \omega^+. \tag{118}
\]

Then

\[
w_i^{(e)}(x,t) = - w_i^{0(e)}(x) - \mathcal{J}_i^0(x), \quad \mathcal{J}_i^0 = - A D^{0ij} \frac{\partial s^0}{\partial x^j}, \quad x \in \omega^+. \tag{119}
\]

Third, since the elastic and plastic displacements are defined over the cell, the additional displacement in the equation (71) ought to be as follows:

\[
\mathcal{W}_i^0(x,t) = - t \tilde{e}^{0ij} - \mathcal{J}_i^0(x), \quad x \in \omega^+. \tag{120}
\]
To conclude the construction of the particular solution, it is necessary to check the continuity condition equation (72). It obviously holds at $t=0$ and, hence, it is enough to check a second condition in equation (72) for $t>0$. It follows from equations (105) and (119) that

$$[\dot{W}_n^0] = -\epsilon^0 n' n - [J_n^*] = 0. \quad (121)$$

The theorem is proved.

Remark 2. Let us normalize the diffusivity tensor:

$$D^{ij} = D\tilde{D}^{ij} \quad (122)$$

where $D$ is some characteristic value of tensor $D^{ij}$ and introduce dimensionless coordinates

$$y' = \frac{x}{\epsilon} \quad (123)$$

which maps the cell $\omega^*$ onto unit cell $\Omega$. The functional equation (100) is transformed to

$$J(s) = \frac{1}{2} \int_{\omega} \tilde{D}^{ij} \frac{\partial s}{\partial y'} \frac{\partial s}{\partial y} d^2 y - \frac{\epsilon^2}{AD} \int_{\omega} \tilde{e}_{ij} n's d^2 y. \quad (124)$$

Then secondary creep macrocharacteristics can be represented as follows:

$$e^{ijkl} = \tilde{e}^{ijkl} \frac{\epsilon^2}{D}, E_{ijkl} = \tilde{E}_{ijkl} \frac{D}{\epsilon^2} \quad (125)$$

where dimensionless constants $\tilde{e}^{ijkl}$ and $\tilde{E}_{ijkl}$ depend on the constants $\tilde{D}^{ij}$ and the unit cell shape only. An important consequence is that secondary creep rates do not depend on the elastic properties and even on the value of the constant $A$. Elastic properties influence only stress microfields.

14. NUMERICAL RESULTS FOR SECONDARY CREEP

For definiteness, it was assumed that grains are isotropic, and hence only four physical constants are needed: Young modulus $E$, Poison ratio $\nu$, the constant $A$ in equation (54), diffusivity constant $D$ in equation (122) (with $\tilde{D}^{ij} = \delta^{ij}$) and the grain size $\epsilon$.

14.1 Secondary creep rates.

In creep, the periodic hexagonal structure behaves isotropically. Thus, the creep law equation (97) contains just one macrocharacteristic—the viscosity $\mu$:

$$\tilde{\sigma}^{ijkl} = \mu \tilde{e}^{ijkl} \quad (126)$$

The dimensional analysis of the cell problem shows that $\mu$ depends on the grain size $\epsilon$ and the diffusivity coefficient $D$ only

$$\mu = a \frac{\epsilon^2}{D} \quad (127)$$

where $a$ is some constant. Numerical simulations give the following value of the constant $a$ for the hexagonal structure

$$a = 0.26. \quad (128)$$

Formulas equations (127) and (128) inspire an assumption that a similar relation between macro- and micro-characteristics exists for the random structure as well, where $\epsilon$ is the averaged.
grain size and $D$ is the characteristic diffusion coefficient of monocrystals, while the coefficient $a$ is of the order of unity.

14.2 Microdeformation.

The distribution of creep velocity over the cell in the regime of secondary creep is shown in Fig. 8. The orientation of shear stress applied is given at the right top of Fig. 8. It is seen that there are three pairs of opposite cell sides with different properties. Material departs from one pair of sides and arrives at the other pair of sides. The remaining two sides consist of two pieces: material leaves one piece and arrives at the other one.

15. DIMENSIONAL ANALYSIS AND TRANSITION TIME TO SECONDARY CREEP

Let $E$ be some characteristic value of tensor $A_{ijkl}$. Similar to equation (122), normalize the tensor $A_{ijkl}$ using the value $E$:

$$\tilde{A}_{ijkl} = \frac{A_{ijkl}}{E}.$$ (129)

Let us assume that dimensionless parameters $\tilde{A}_{ijkl}$ and $\tilde{D}_{ijkl}$ remain unchanged in our analysis. Then a solution of the system $P$ depends on four constants: $E, D, A$ (see equation (54)) and $\epsilon$-characteristic grain size.

Fig. 8. Creep velocity distribution during the secondary creep.
Our intent is to transform the system $P$ to dimensionless form. In addition to dimensionless space coordinates $y'$ (see equation (122)) introduce intrinsic time $\tau$ and normalized displacements and flux:

$$
\tau = t \frac{AD}{\epsilon^2} : \dot{f} = \frac{\partial f}{\partial \tau}, \dot{w} = \frac{1}{\epsilon} W, \dot{w} = \frac{1}{\epsilon} W,
$$

$$
\dot{w}^{(r)} = \frac{1}{\epsilon} W^{(r)}, \dot{w}^{(p)} = \frac{1}{\epsilon} W^{(p)}, \dot{j} = \frac{1}{\epsilon} \frac{e^2}{AD} J, \dot{\sigma}^{ij} = \frac{1}{A} \sigma^{ij}.
$$

(Vacancy concentration and strains need not to be normalized. Then system $P$ is reduced to the system $\tilde{P}$:

$$
e^{(r)} = 1/2 \left( \frac{\partial \tilde{w}^{(r)}}{\partial y'} + \frac{\partial \tilde{w}^{(r)}}{\partial y} \right),
$$

$$
\tilde{\sigma}^{ij} = e A^{q \varepsilon} \epsilon^{(r)}
$$

$$
\frac{\partial \tilde{\sigma}^{ij}}{\partial y'} = 0
$$

$$
\dot{j} = -\tilde{B}^{ij} \frac{\partial s}{\partial y'}
$$

$$
\frac{\partial s}{\partial \tau} = \frac{\partial}{\partial y'} \left( \tilde{B}^{ij} \frac{\partial s}{\partial y'} \right)
$$

$$
\tilde{\sigma}_{nn} = s, y \in \partial \Omega
$$

$$
\tilde{\sigma}^{ij} n_j = 0, y \in \partial \Omega
$$

$$\tilde{w}^{(p)}(y, \tau) = -\tilde{j}(y, \tau), y \in \Omega
$$

$$\tilde{w}_i = \tilde{w}_i^{(r)} + \tilde{w}_i^{(p)}
$$

$$
e_{ij} = 1/2 \left( \frac{\partial \tilde{w}_i}{\partial y'} + \frac{\partial \tilde{w}_j}{\partial y} \right), e_{ij}^{(p)} = 1/2 \left( \frac{\partial \tilde{w}_i}{\partial y'} + \frac{\partial \tilde{w}_j}{\partial y} \right) e_{ij}^{(r)} + e_{ij}^{(p)}
$$

$$\tilde{w}_i(y, \tau) = \tilde{e}_{ij}(\tau) y_j + \tilde{W}_i(y, \tau)
$$

$$\tilde{W}_n(y, \tau) + \tilde{W}_n(y', \tau) = 0 \text{ for } y \in \partial \Omega \to \tilde{W}_n(y, \tau) + \tilde{W}_n(y', \tau) = 0
$$

$$\tilde{\sigma}_{nn}(y, \tau) = \tilde{\sigma}_{nn}(y', \tau) \text{ for } y \in \partial \Omega
$$

$$s(y, \tau) = s(y', \tau) \text{ for } y \in \partial \Omega
$$

$$\tilde{\sigma}^{ij}(\tau) = \frac{1}{[\Omega]} \int_\Omega \tilde{\sigma}^{ij}(y, \tau) d^2 y.
$$

(Initial conditions:

$$s(y, \tau) = 0, \tilde{w}^{(p)}(y, \tau) = 0, y \in \Omega, \tau = 0.
$$

We see that the only dimensionless parameter, $e = E/A$, remains in the equations. To get a feeling what may be the actual value of parameter $e$, let us consider copper at 1000 K temperature. It is known that equilibrium value of vacancy concentration varies in broad range is $C_0 \sim 10^{-8} - 10^{-4}$. Then it follows from equation (46) that $e \sim 0.01 - 100$.

Let us study numerically how the solution depends on parameter $e$. For simplicity computations were done for the problem of compression of a single crystal by absolutely rigid
frictionless pistons (see [4]). Region $\Omega$ is a square, the characteristic size is the distance from its center to the edges (see Fig. 10). Vertical crystal edges are free. For simplicity let us assume that the crystal is isotropic. Under this assumption the compression of the crystal will not result in piston rotation and from symmetry considerations we may assume that the displacement of the cell center is zero. Let $\tilde{\epsilon}(\tau)$ be the vertical displacement of the upper piston, which is the unknown function and which is analogous to the macrostrain in system $P$. The normal average stress $\overline{\sigma}$ at the contact between the pistons and the crystal surfaces serve as an analog to the macrostresses. The piston is loaded by a constant force, such that the average stress is equal to $-1$.

$$\overline{\sigma} = \frac{1}{2} \int_{-1}^{1} \sigma_{nn}(y_1, 1, \tau) dy_1 = \frac{1}{2} \int_{-1}^{1} \sigma_{nn}(y_1, -1, \tau) dy_1 = -1. \quad (147)$$

The system of equations of the problem of compression of a single crystal is the set equations (131)–(139) and (147), initial conditions equation (146) plus boundary conditions:

$$\sigma_{nn}(\pm 1, y_2, \tau) = 0, \quad -1 \leq y_2 \leq 1 \quad (148)$$

$$\hat{\omega}_n(y_1, \pm 1, \tau) = \pm \tilde{\epsilon}(\tau), \quad -1 \leq y_1 \leq 1. \quad (149)$$

The Theorems 1 and 2 can be proven for this problem as well.

The steady-state solution for secondary creep can be obtained in closed form and the value of the steady-state creep rate is $\dot{\epsilon} = 1.7$. Hence, the analog of the formulas equations (126) and (127) in this case is

$$\dot{\sigma} = 0.588 \dot{\epsilon} \frac{\varepsilon^2}{D}. \quad (150)$$

One may notice that the numerical coefficients in equations (126) and (128) and in equation (150) are of the same order of magnitude.
Let us discuss numerical results for the transient solution. Parameter $e$ values were chosen to be 0.1, 1, 10, which is in the middle of the expected range.

1. As was expected, for small values of dimensionless time $\tau$ creep rates fit very well the asymptotic $\sim \tau^{-1/2}$ (See Fig. 11–13).

2. When $\tau$ is large, a steady-state creep rate of 1.7 is achieved (see Table 1). A practically steady-state is reached at $\tau \sim 1$ (see Table 1).

3. Parameter $e$ somewhat affects the transition time necessary to reach the steady-state creep rate. The smaller the $e$ the larger the transition time. However, the modeling results do not allow us to conclude what kind of dependency is it. As one can see from Table 1, the transition time for $e=0.1$ is much larger, than for $e=1$, but there is no noticeable difference between cases with $e=1$ and 10.

4. At the first moment of load application, the only non-zero stress component is $\sigma^{22}$ and it is equal to $-1$ over $\Omega$. With creep developed, stresses tend to limit, which do not depend on the parameter $e$, which is as it should be because of Theorem 2. Figure 14
Fig. 13. shows the stress distribution at the piston–crystal contact for \( e = 10, \tau = 0.5 \). Stars mark asymptotical the steady-state stress distribution. The transition time to steady-state stresses is of the same magnitude, as the transition time needed for the creep rate to become constant.

Table 1. Stabilization of the creep rate for various values of parameter \( e \)

<table>
<thead>
<tr>
<th>( e )</th>
<th>0.1</th>
<th>1</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau )</td>
<td>2.5</td>
<td>0.8</td>
<td>0.65</td>
</tr>
<tr>
<td>( \dot{\varepsilon} )</td>
<td>1.74</td>
<td>2</td>
<td>1.72</td>
</tr>
</tbody>
</table>

Asymptotic value of \( \dot{\varepsilon} = 1.7 \)
16. CONCLUSIONS.

Three interesting results of this study seem worth noting. First, the constitutive macroequations of diffusional creep turn out to be nonlocal. It is not obvious how to eliminate the nonlocality by introducing additional internal variables. Probably, the elimination of the nonlocality on the macroscale is impossible in principle. Since this seems to be the case, a search for adequate local constitutive equations for creep is doomed to failure. Second, there is an intrinsic material time $\tau = tDA/\varepsilon^2$. Strain–time dependence (for constant stresses) is universal for intrinsic time in the sense that it does not depend on the material and on the temperature (the temperature dependence comes from the material constants $D$ and $A$). Third, as the variational principle shows, creep rates do not depend on the elastic properties in secondary creep: only diffusion constants, the grain size and the grain geometry are important. Formula equation (87) is an example of such a dependency.

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APPENDIX

A. THE EFFECT OF GRAIN BOUNDARY STRESS RELAXATION ON APPARENT ELASTIC MODULUS

The assumption equation (58) that shear stresses at the grain boundaries can be neglected in creep problem is believed to be correct by many authors. It would be interesting to find an experimental evidence that such an effect is real. It may not be an easy task, because the numerical modeling revealed surprisingly low influence of grain shear stress relaxation on apparent elastic modulus. In more detail, the averaged elastic properties were computed for the periodic structure described in Section 6. Boundary conditions equation (58), (72) and (73) were applied and averaged elastic moduli were calculated from the solution of the periodic elasticity problem. For definiteness it was assumed that grains are isotropic and, hence, only two elastic constants need to be calculated. In addition, it is obvious that if the hydrostatic pressure tensor is applied to the plane, the structure does not "feel" the cuts made and, hence, the bulk modulus of the polycrystal is the same as the bulk modulus of the grain itself:

$$\frac{E^*}{2(1 - v^*)} = \frac{E}{2(1 - v)}$$

where $E$, $v$ and $E^*$, $v^*$ are Young's modulus and Poisson's ratio of the grain and the polycrystal correspondingly. Because of that the ratios $E^*/E$ and $G^*/G$ depend only on Poisson's ratio. Results are listed in Table 2 and as one can conclude the Young and shear moduli drop no more than 20% as a result of shear stress relaxation.

B. PROPERTIES OF PERIODIC STRESS FIELDS, SATISFYING THE EQUILIBRIUM CONDITIONS

Let us prove formulas equations (83) and (85), which hold for an arbitrary stress field satisfying equilibrium equation (48) and boundary conditions equations (73) and (58). Multiplying equation (48) by $x^k$ and integrating over cell $\omega$ we
Formula equation (83) follows from equation (B.1) and definition equation (75). In order to prove equation (85) let us note that spherical tensor \( \sigma^{ij} = C_{s}^{ij} \) may be substituted in equation (83), which is reduced in this case to equation (85). Let \( s \) be an arbitrary function, satisfying periodicity condition equation (74). Let us define surface tractions on the cell boundary \( \partial \Omega \) by formulas equations (58) and (54). Then the principal vector \( F \) and principal moment \( M \) applied to the grain from these tractions, are zeros.

\[
F = \int_{\Omega} \sigma_{mn}(x)n(x)dx = 0 \quad \text{(B.2)}
\]

\[
M = \int_{\Omega} \sigma_{mn}(x)n \otimes dx = \sum_{r=1}^{3} \left( \int_{S_{r}} \sigma_{mn}(x)n(x) \otimes (x - x')dx \right) - \sum_{r=1}^{3} \left( \int_{S_{r}} \sigma_{mn}(x)n(x) \otimes (x + n(x'))dx' \right) = 0 \quad \text{(B.3)}
\]

The last term in equation (B.3) is zero because of equation (67).

**C. ASYMPTOTIC BEHAVIOR OF THE SOLUTION AT LARGE TIME.**

**Lemma 1.** For every solution of the system \( P \) the following identity holds:

\[
\frac{d}{dt} + A[\nabla s, \nabla s] = |\omega|^{2} \sigma_{ij} \psi_{ij}. \quad \text{(C.1)}
\]

**Proof.** It follows from equations (50) and (54) that

\[
Q = \frac{d}{dt} + A[\nabla s, \nabla s] = A[\nabla s, \nabla s] + \int_{\Omega} A_{s} \frac{\partial s}{\partial t} d^{2}x + \int_{\Omega} A_{ij} \epsilon_{ij}^{st} \epsilon_{ij}^{st} d^{2}x
\]

\[
= A[\nabla s, \nabla s] - \int_{\Omega} A_{s} \frac{\partial s}{\partial t} d^{2}x + \int_{\Omega} A_{ij} \epsilon_{ij}^{st} \epsilon_{ij}^{st} d^{2}x = A[\nabla s, \nabla s] + \int_{\Omega} \sigma_{mn} \phi_{mn} d^{2}x + \int_{\Omega} \sigma_{mn} \phi_{mn} d^{2}x. \quad \text{(C.2)}
\]

With equations (62) and (71) the elastic strains are expressed in terms of averaged strains, plastic strains and strains \( \epsilon_{ij}^{st}(W) \) generated by field \( W \):

\[
\epsilon_{ij}^{st} = \epsilon_{ij}^{s} + \epsilon_{ij}^{p}(W) - \epsilon_{ij}^{st}(W) = \frac{1}{2} \left( \frac{\partial w_{ij}}{\partial x^{i}} + \frac{\partial w_{ij}}{\partial x^{j}} \right) \epsilon_{ij}^{st} = \epsilon_{ij}^{s} + \epsilon_{ij}^{p}(W) - \epsilon_{ij}^{st}(W). \quad \text{(C.3)}
\]

Substitution of equation (C.3) into equation (C.2) yields

\[
Q = \int_{\Omega} \sigma_{mn} \phi_{mn} d^{2}x + \int_{\Omega} A_{ij} \epsilon_{ij}^{st} \epsilon_{ij}^{st} d^{2}x
\]

\[
= \int_{\Omega} \sigma_{mn} \phi_{mn} d^{2}x + \int_{\Omega} A_{ij} \epsilon_{ij}^{st} \epsilon_{ij}^{st} d^{2}x + \int_{\Omega} \sigma_{mn} (W_{mn} - \phi_{mn}) d^{2}x = |\omega|^{2} \sigma_{ij} \psi_{ij}. \quad \text{(C.4)}
\]

Boundary conditions equations (73) and (72) were used in the derivation equation (C.4). Lemma 1 is proved.
LEMMA 2. Let us assume that for \( t \geq t^* \) macrostresses are equal to zero:
\[
\sigma^{\text{m}}(t) = 0, \quad t \geq t^*.
\] (C.5)

Then for an arbitrary solution of the system \( P \) the following estimations hold:
\[
I(t) \approx e^{-\beta t}, \quad t \geq t^*, \beta = \text{const} > 0
\] (C.6)
and the following components of the solution tend to zero:
\[
s \to 0, \quad e_{ij}^{(p)} \to 0, \quad \sigma^{ij} \to 0, \quad \dot{e}_{ij} \to 0, \quad t \to 0.
\] (C.7)

PROOF. For \( t \geq t^* \) the identity equation (C.1) is reduced to the following:
\[
\frac{dl(t)}{dt} + A[\nabla s, \nabla s] = 0.
\] (C.8)

It follows from equations (C.5) and (84) that
\[
\int_{\Omega_0} s_n n^2 d\Omega = \int_{\Omega_0} s d\Omega = 0, \quad t \geq t^*.
\] (C.9)

Then the following inequalities hold [28]:
\[
\int_{\Omega_0} A \frac{\partial s^{(r)}}{\partial x^2} d\Omega \leq C_4[\nabla s, \nabla s], \quad (C.10)
\]
\[
\int_{\Omega_0} A \frac{\partial s^{(r)}}{\partial x^2} d\Omega \leq C_4[\nabla s, \nabla s]. \quad (C.11)
\]

Adding, if necessary, to the solution some field \( V e^R \) we may modify the elastic solution so that at each moment \( t \) averaged over the cell \( \omega^* \) elastic displacements and rotation are zero:
\[
\int_{\omega^*} \omega^{(r)} d\Omega = 0 \quad (C.12)
\]
\[
\int_{\omega^*} \left( \frac{\partial w^{(r)}}{\partial x^1} - \frac{\partial w^{(r)}}{\partial x^2} \right) d\Omega = 0. \quad (C.13)
\]

Then [29]
\[
\int_{\Omega_0} \left( w^{(r)} \right)^2 d\Omega \leq C_4[\nabla e^{(r)}, \nabla e^{(r)}], \quad C_4 = \text{const}. \quad (C.14)
\]

Let us prove that
\[
[\nabla e^{(r)}, \nabla e^{(r)}] \leq C_4[\nabla s, \nabla s]. \quad (C.15)
\]

With equations (48), (58) and (54) taken into account, the left-hand side of equation (C.15) is reduced to
\[
\left[ e^{(r)}, e^{(r)} \right] = \int_{\Omega_0} \sigma^{(r)} e_{ij}^{(r)} d\Omega = \int_{\Omega_0} \sigma^{(r)} e_{ij}^{(r)} d\Omega = \int_{\Omega_0} \sigma^{(r)} e_{ij}^{(r)} d\Omega
\]
\[
= \int_{\Omega_0} A \frac{\partial w^{(r)}}{\partial x^1} d\Omega \leq \sqrt{\int_{\Omega_0} A \frac{\partial w^{(r)}}{\partial x^1} d\Omega^2} \leq \sqrt{\int_{\Omega_0} \left( w^{(r)} \right)^2 d\Omega} \leq C_4 \sqrt{\left[ \nabla e^{(r)}, \nabla e^{(r)} \right] \left[ \nabla s, \nabla s \right]}. \quad (C.16)
\]

The inequalities in equation (C.16) follow from equations (C.14) and (C.11). Estimation equation (C.15) follows from equation (C.16).

Combining equations (C.15) and (C.10) we obtain
\[
A[\nabla s, \nabla s] \geq \beta I(t), \quad \beta = \text{const}. \quad (C.17)
\]

It follows from equations (C.8) and (C.17) that
\[
0 = \frac{dl(t)}{dt} + A[\nabla s, \nabla s] \geq \frac{dl(t)}{dt} + \beta I(t)
\] (C.18)

which results in the basic relation
\[
I(t) \leq e^{-\beta t} - e^{-\beta t^*} I(t^*) \Rightarrow I(t) \to 0, \quad t \to \infty. \quad (C.19)
\]

The first three statements in equation (C.7) follow immediately from equation (C.18). Since elastic strains and vacancy concentration tend to zero, the same is true for elastic and plastic strain rates, if the solution of the system \( P \) is sufficiently smooth. Hence
\[
\Delta_n = \dot{e}_{ij} + e_{ij}^{(p)} \to 0, \quad t \to \infty. \quad (C.20)
\]

Using Levi-Civita formulas, we obtain the following equalities:
\[
\dot{W}_i = - \dot{e}_{ij}^x + \lambda e_{ij} x^i + a_i + T(\Delta_n) \lambda, \quad a_i = \text{const}, \quad T(\Delta_n) \to 0. \quad (C.21)
\]

The second and third terms in equation (C.21) represent the rigid body displacement, the last term stands for Levi-
Cvita integrals. Substitution of equation (C.21) into continuity condition equation (72) is made similarly to evaluation equation (78) and yields
\[ \tilde{\varepsilon}_i \tilde{p}(x) n_i(x) + T_{x,1}(\Delta \tilde{\varepsilon}_1), T_{x,2}(\Delta \tilde{\varepsilon}_2), \to 0, t \to \infty. \] (C.22)

Since the normal vector is constant over \( S_r, r = 1,2,3 \), the relation equation (C.22) provides three different conditions, which may be considered as a system of linear equations with respect to three components \( \tilde{\varepsilon}_r \). The determinant of this system is not zero, and then it follows from equation (C.22) that \( \tilde{\varepsilon}_r \to 0, t \to \infty \). Lemma 2 is proved.

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