

SINGLE APPROACH TO THE DESCRIPTION OF THE RELATION BETWEEN MICRO- AND MACROSTATES IN REVERSIBLE AND IRREVERSIBLE DEFORMATION OF POLYCRYSTALS

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The problem of the relationship between local and general mechanical parameters that describe the thermoreological properties of polycrystalline materials is considered. The change of parameters describing the relationship between stress and strain oscillations at two levels of the structure is analyzed. The assumption of the invariance of the density distribution function of the elastic boundaries of sub-elements in the process of irreversible deformation is used. This study is based on the principles of discrepancy between the macroscopic measures and the microscopic analogs and the orthogonality of stress and strain oscillations. It is shown that at small values of the curing factor of subelements typical for the stages of easy-sliding single crystals, this model describes such specific effects as plateau or yield drop and change of elastic properties under irreversible deformations.

Keywords: tensor, stress, strain, structure, anisotropy, single crystal, polycrystal

Introduction. Experimental studies of the laws of irreversible deformation under repeated variable nonisothermal complex loading with holding revealed a very complex behavior of structural materials. One of the most fruitful concepts used to create modern theories that define the equation of state is the concept according to which the representative volume of a macroscopically homogeneous body is represented as a finite or infinite number of interconnected subelements that have different thermoreological properties. Each subelement is identified with a set of material particles within the representative volume that has the same irreversible strain tensor. It is assumed that the condition of continuity of the medium is provided by five independent slip systems. Experimentally established nonbasic slip allows us to describe the scalar properties of materials in the region of irreversible deformation in terms of the modules of the stress and strain deviators. In [5–7], a closed system of equations is derived which can be used to derive a system of macroscopic constitutive equations if the microscopic constitutive equations are known. It was assumed that the material particles are elastically isotropic. In this paper, the behavior of polycrystalline materials is analyzed considering the elastic anisotropy of material particles. In the region of irreversible deformation, the sub-elements serve as an intermediate structural level. The equation relating the fluctuations of stresses and strains is stated at the level of material particles related to this sub-element and at the level of the system of sub-elements. In this approach, the complex unrelated features of irreversible deformation of materials that are manifested during different program changes in the load and temperature become comprehensive and interdependent.

1. Basic Equations of Multi-Element Models. To describe the thermoreological behavior of materials in models that describe inhomogeneous processes of deformation and loading, we will use Hill's equations [3]:

$$t_{ij} = \langle \tilde{t}_{ij} \rangle = \frac{1}{\Delta V_0} \int_{\Delta V_0} \tilde{t}_{ij} dV, \quad d_{ij} = \langle \tilde{d}_{ij} \rangle, \quad \langle \tilde{t}_{ij} \tilde{d}_{ij} \rangle = t_{pq} d_{lq}, \quad (1.1)$$

where $\tilde{t}_{ij}, \tilde{d}_{ij}$ are the stress and strain tensors at each point of the domain ΔV_0 , respectively; $\langle \cdot \rangle$ is the sign of averaging over the volume ΔV_0 . Expressions (1.1) satisfy the equilibrium equations of the continuous medium and the geometric Cauchy equations, and the following boundary conditions are satisfied on the surface S_0 :

$$\tilde{u}_{i/S_0} = u_i = d_{ij}x_j, \quad d_{ij} = \text{const}, \quad p_{i/S_0}^{(n)} = t_{ij}n_j, \quad t_{ij} = \text{const}.$$

Equations (1.1) are necessary but insufficient to derive the system of macroscopic constitutive equations from the microscopic constitutive equations. To obtain a closed system of equations, it is necessary to state additional assumptions.

At the first stage of development of the theory, the simplest variants of interaction were used: $\tilde{t}_{ij} = t_{ij}$ is the homogeneous stress state or $\tilde{d}_{ij} = d_{ij}$ is the homogeneous strain state. Such assumptions do not allow us to describe the variety of effects observed during the deformation of materials. A more realistic scheme of interaction of material particles was proposed by Krener [4]. He discovered a new way of stating the so-called “self-consistent” scheme related to the problem of an inclusion in an infinite matrix. According to the scheme, each grain of the polycrystal is consistently considered as an inclusion in the “matrix” of all other grains; the behavior of the polycrystal is analyzed using some adequate averaging over all grains. Krener’s approach leads to a very convenient a priori law of interaction, which is easily deduced from the Eschelby solution to the inclusion problem. This simplification is based on the elastic interaction between the “matrix” and the inclusion, as a result of which Krener obtained the following kinematic equations:

$$\bar{\sigma}_{ij} - \sigma_{ij} = 2b_2(\varepsilon_{ij} - \bar{\varepsilon}_{ij}), \quad 2b_2 = 2G \frac{7-5\mu}{8-10\mu}, \quad (1.2)$$

$$\bar{\sigma}_0 - \sigma_0 = (6b_1 + 2b_2)(\varepsilon_0 - \bar{\varepsilon}_0), \quad b_1 = 2G \frac{3-5\mu}{8-10\mu}, \quad (1.3)$$

where G is the shear modulus; μ is Poisson’s ratio,

$$\tilde{\sigma}_{ij} = \tilde{t}_{ij} - \tilde{\sigma}_0 \delta_{ij}, \quad \tilde{\varepsilon}_{ij} = \tilde{d}_{ij} - \tilde{\varepsilon}_0 \delta_{ij}, \quad \sigma_0 = \frac{1}{3} \tilde{t}_{ii}, \quad \varepsilon_0 = \frac{1}{3} \tilde{d}_{ii}. \quad (1.4)$$

Equations (1.2) and (1.3) do not cohere with Hill’s third equation ($\langle \tilde{t}_{ij} \tilde{d}_{ij} \rangle = \langle \tilde{t}_{ij} \rangle \langle \tilde{d}_{ij} \rangle$) and give excessive internal stresses in the region of irreversible deformation.

To allow for the natural tendency of a material to reduce stress fluctuations within the representative volume ΔV_0 , Berveie and Zaul [1] introduced a so-called “plastic accommodation function.” This approach is possible only when the isotropic elastic-plastic interaction between the inclusion and the matrix is limited. In this model, the parameter b_2 decreases with increasing plastic strain by almost two orders of magnitude in the uniaxial tensile test of single-phase polycrystalline materials. This model and its various modifications are also inconsistent with Hill’s third equation and the first law of thermodynamics. In addition, for single-phase polycrystalline materials with cubic symmetry, they change only the deviator values during reversible and irreversible deformation. Thus, for spherical values of the stress and strain tensors, the consequences are same as in the models $\tilde{t}_{ij} = t_{ij}$ or $\tilde{d}_{ij} = d_{ij}$. Note that the concept of plastic stress relaxation is “artificial.”

A more general approach was proposed in [5–7]. In addition to Hill’s equations (1.1), the postulate of orthogonality of the stress and strain fluctuation tensors was assumed.

$$(\tilde{t}_{ij} - t_{ij})(\tilde{d}_{ij} - d_{ij}) = 0. \quad (1.5)$$

Substituting (1.4) into (1.5), we determine the first type of equations relating the microstates and macrostates:

$$(\tilde{\sigma}_{ij} - \sigma_{ij})(\varepsilon_{ij} - \tilde{\varepsilon}_{ij}) = 3(\tilde{\sigma}_0 - \sigma_0)(\tilde{\varepsilon}_0 - \varepsilon_0), \quad (1.6)$$

where the following relations are used:

$$\tilde{t}_{ij} = \tilde{\sigma}_{ij} + \tilde{\sigma}_0 \delta_{ij}, \quad \tilde{d}_{ij} = \tilde{\varepsilon}_{ij} + \tilde{\varepsilon}_0 \delta_{ij}.$$

The fluctuations of the deviatoric components are also assumed to be in linear relationship:

$$\tilde{\sigma}_{ij} - \sigma_{ij} = B(\varepsilon_{ij} - \tilde{\varepsilon}_{ij}), \quad (1.7)$$

where $B \neq 2b_2$ is the internal parameter that contains information about the microscopic properties of the sub-elements and shows the difference between the stress fluctuations and the strain fluctuations. Equations (1.5), (1.7) satisfy Hill's third equation and the first law of thermodynamics.

Equations (1.1) show that the averaging of stresses, strains, and their products over the volume only depends on the data on the surface of the representative volume. However, all microscopic variables do not have this specific property. In particular, it was shown in [5, 7] that natural macromesures of the energy of change in volume and shape differ from the average over their micromesures. To extend system (1.1), (1.6), and (1.7), the principle of the extremum of discrepancy between macroscopic measures and average microscopic analogs was proposed in [5–7]. In particular

$$\Delta = \langle \tilde{\sigma}_{ij} \tilde{\varepsilon}_{ij} \rangle - \langle \tilde{\sigma}_{ij} \rangle \langle \tilde{\varepsilon}_{ij} \rangle = Extr. \quad (1.8)$$

Expressions (1.1), (1.6)–(1.8) are considered valid for both reversible and irreversible deformation processes. Therefore, relations (1.1), (1.6)–(1.8) can be used to describe, in a unified way, the relationship between the micro- and macrostates during reversible and irreversible deformation of polycrystalline materials.

We will analyze the change of the parameter B in the region of irreversible deformation, and, on its basis, the fluctuations of stresses and strains depending on the yield of the sub-element, the hardening factor, and the elastic constants of the crystals.

2. Testing the Model in the Elastic Region. Expressions (1.1)–(1.8) include local $(\tilde{t}_{ij}, \tilde{d}_{ij})$ and macroscopic (t_{ij}, d_{ij}) stresses and strains. In the reversible region, by $\tilde{t}_{ij}, \tilde{d}_{ij}$ are meant the average values of stresses and strains in the subset of particles with the same orientation of the crystallographic axes relative to the global coordinate system. Within this formalization, we use the local physical law

$$\tilde{t}'_{ij} = c_{ijnm} \tilde{d}'_{nm}$$

and relations (1.6)–(1.8) to establish the relationship $t_{ij} \sim d_{ij}$, where c_{ijnm} is the tensor of elastic constants in the crystallographic coordinate system; $\tilde{t}'_{ij}, \tilde{d}'_{ij}$ are the components of the corresponding tensors in the crystallographic coordinate system. The most accessible results were obtained for single-phase polycrystalline materials with a cubic lattice [7]:

$$B = 2c_{44} \sqrt{\frac{2A+3}{A(3A+2)}}, \quad A = \frac{2c_{44}}{c_{11} - c_{12}}, \quad G = c_{44} \sqrt{\frac{3A+2}{A(2A+3)}} = \sqrt{G_V G_R}, \quad (2.1)$$

$$\tilde{\sigma}'_{ij}(A, \sigma_{nm}, \Omega) = \begin{cases} \frac{5(1+A)a_{in}(\Omega)a_{jn}(\Omega)\sigma_{nm}}{2+3A+\sqrt{A(2+3A)}(3+2A)}, & i=j, \\ \frac{5(1+A)\sqrt{A}a_{in}(\Omega)a_{jn}(\Omega)\sigma_{nm}}{(2+3A)\sqrt{A}+\sqrt{(2+3A)}(3+2A)}, & i \neq j, \end{cases} \quad (2.2)$$

$$|\tilde{\sigma}_0 - \sigma_0| = \sqrt{\frac{c_{11}+2c_{12}}{6c_{44}} \sqrt{\frac{A(3A+2)}{2A+3}} (\tilde{\sigma}'_{ij} - \sigma'_{ij})(\tilde{\sigma}'_{ij} - \sigma'_{ij})}, \quad (2.3)$$

where c_{11}, c_{12}, c_{44} are the elastic constants of a cubic crystal; $a_{in}(\Omega)$ is the matrix of direction cosines of this crystallographic coordinate system relative to the global system; A is the factor of anisotropy of single crystals; G_V is the shear modulus obtained by Voigt in 1928 using the approximation $\tilde{d}_{ij} = d_{ij}$; G_R is the shear modulus obtained by Reis in 1929 using the approximation $\tilde{t}_{ij} = t_{ij}$.

According to (2.3), the fluctuations of the spherical tensor are expressed in terms of the fluctuations of the stress deviator and the anisotropy factor of the crystal. Thus, as a result of the nonlinear system of equations (1.6), (1.7), an inhomogeneous field of volume strains occurs even under pure macroscopic shear. In this paper, we study the effect of the type of

load on the value of the maximum local stress $\tilde{t}_1 = \tilde{\sigma}_1 + \tilde{\sigma}_0$. The numerical calculations performed for copper show that even under pure compression, there are material particles in which $\tilde{t}_1 > 0$. If, for example, the largest linear strain is taken as a local failure criterion, then it is affected by all the three invariants of the strain tensor and, in the irreversible region, is affected by three more invariants of the stress tensor. Thus, the elementary local failure criterion, which allows us to determine unknown material functions and constants from a simple experiment, indicates a very complex effect of all problem parameters on the strength of the material at the macroscopic level.

The values of the shear modules obtained using the Krener (G_K) and Marina (G_M) models were compared in [9]. As a result, the following fundamental inequality was determined:

$$G_K \geq G_M.$$

In the case of single-phase polycrystalline materials with cubic lattices, G_M is determined by formula (2.1), and G_K by the following cubic equation [4]:

$$G_K^3 + a_1 G_K^2 + a_2 G_K + a_3 = 0,$$

where $a_1 = \frac{1}{8}(5c_{11} + 4c_{12})$, $a_2 = -\frac{1}{8}(7c_{11} - 4c_{12})c_{44}$, $a_3 = -\frac{1}{8}(c_{11} + 2c_{12})(c_{11} - c_{12})c_{44}$.

Theoretical and experimental values of G_M and G_K for many polycrystalline materials with a cubic lattice were compared in [9]. It was shown that the studied models agree well with the experimental data, with G_M closer to G_{exp} than G_K .

In this paper, a very simple formula (2.1) ($G = \sqrt{G_V G_R}$) obtained for single-phase polycrystalline materials with cubic lattices was compared with experimental results for polycrystals of hexagonal, tetragonal, and orthorhombic symmetry (Be, Cd, Co, In, S, Sn, TiO₂, U, Y, Zn) [13]. The largest difference between the calculated and experimental data was 3.51% for zinc. Based on these comparisons, we can conclude that this formula can be used to determine the elastic constants of polycrystals with lower symmetry of the crystal lattice.

The pattern of fluctuations of the spherical tensor $\tilde{\sigma}_0$, which is absent in the Krener model and other models ($\tilde{\sigma}_0 = \sigma_0$), was determined in [8]. The established relationship between the fluctuations of the deviatoric and spherical quantities was used in [8] to describe thermomechanical effects of materials such as the dissipation of mechanical energy under load in the elastic region. The discrepancy between the values of $\langle \tilde{\sigma}_{ij} \tilde{\varepsilon}_{ij} \rangle \neq \langle \tilde{\sigma}_{ij} \rangle \langle \tilde{\varepsilon}_{ij} \rangle$, $\langle \tilde{\sigma}_0 \tilde{\varepsilon}_0 \rangle \neq \langle \tilde{\sigma}_0 \rangle \langle \tilde{\varepsilon}_0 \rangle$ serves as a macroscopic measure of such effects.

For single-phase polycrystalline materials with cubic lattices the following formula was determined in [7]:

$$\langle \tilde{\sigma}_{ij} \tilde{\varepsilon}_{ij} \rangle = \left[1 - 6 \left(\frac{A-1}{5\sqrt{A} + \sqrt{(2+3A)(3+2A)}} \right)^2 \right] \langle \tilde{\sigma}_{ij} \rangle \langle \tilde{\varepsilon}_{ij} \rangle. \quad (2.4)$$

After simple transformations in (1.1) and (2.4), we obtain the expression

$$\langle \tilde{\sigma}_0 \tilde{\varepsilon}_0 \rangle = \langle \tilde{\sigma}_0 \rangle \langle \tilde{\varepsilon}_0 \rangle + 6 \left(\frac{A-1}{5\sqrt{A} + \sqrt{(2+3A)(3+2A)}} \right)^2 \langle \tilde{\sigma}_{ij} \rangle \langle \tilde{\varepsilon}_{ij} \rangle. \quad (2.5)$$

It can be seen from formula (2.5) that the discrepancies $\langle \tilde{\sigma}_0 \tilde{\varepsilon}_0 \rangle - \langle \tilde{\sigma}_0 \rangle \langle \tilde{\varepsilon}_0 \rangle$ depend on the anisotropy factor A and the macroscopic measure $\langle \tilde{\sigma}_{ij} \rangle \langle \tilde{\varepsilon}_{ij} \rangle$. For copper [13], $A = 3.21$ and the relative discrepancy of measures (2.4) is 7.8%, while for aluminum, $A = 1.21$ and the discrepancy is only 0.23%.

3. Formalization of a Crystalline Medium in the Irreversible Deformation Region. To formalize the behavior of polycrystalline materials in the irreversible deformation region, we have to use various simplifying assumptions. As in [5–9, 11, 12], we take a sub-element identified with the set of all material particles in ΔV_0 that has the same deviator of irreversible strains as a local structural unit. Particles belonging to the same sub-element may have different positions and orientations of the crystal lattice in the representative volume ΔV_0 . The number of all particles with the same deviation of irreversible deformation determines the weight of one sub-element, which does not change during loading. Since the grains in polycrystals are deformed unevenly, then, according to the definition, the mass or volume of one sub-element can be as small as possible. Within this

concept, the domain ΔV_0 , which contains enough particles to show the average thermoreological properties of the material, is represented as a finite or infinite number of interconnected sub-elements with different thermoreological properties.

When loading in the irreversible region, the components of the deviations of the strains of the sub-elements, $\bar{\varepsilon}_{ij}$, and the body element, ε_{ij} , are represented as the sum of the reversible \bar{e}_{ij}, e_{ij} and irreversible components \bar{p}_{ij}, p_{ij} :

$$\bar{\varepsilon}_{ij} = \bar{e}_{ij} + \bar{p}_{ij}, \quad \varepsilon_{ij} = e_{ij} + p_{ij}. \quad (3.1)$$

Although only the total strain can be measured in experiments, the use of two strain components does not contradict the concept of developing a theory using quantities to be observed. It was shown in [6] that only the total strain appears in the system of macroscopic equations. The local relationship between the elastic and irreversible strains rather than between elastic and irreversible stresses was established in [5, 11, 12]. According to the law of central increment proposed in [5], the ultimate elastic strains of sub-elements can be represented as the sum of two independent components:

$$\bar{e}_{ij} = \bar{\tau}_{ij} + \bar{s}_{ij}. \quad (3.2)$$

Here $\bar{\tau}_{ij}$ are the components of the deviator of ultimate elastic strains of sub-elements in a structurally stable state; \bar{s}_{ij} is the increment of the deviator components of the ultimate elastic strains of the sub-elements as a result of changes in the structure under irreversible deformation. The quantities $\bar{\tau}_{ij}$ and \bar{s}_{ij} represent the thermoviscoplastic properties of the sub-elements without and with regard to the change in the structure of the material.

The extension of this concept to anisotropic material particles radically simplifies the analysis of irreversible deformation processes on the one hand and, on the other hand, allows us to generalize a number of ideas that are successfully used to describe irreversible processes in elastically isotropic materials.

The transition of sub-elements in the annealed state of the material ($\bar{s}_{ij} = 0$) from the reversible state to the irreversible state is described by the criterion

$$\bar{e}_{ij}\bar{e}_{ij} - \tau^2 = 0, \quad \tau^2 = \tau_{ij}\tau_{ij},$$

whence it is seen that τ is the initial limit of elasticity of the sub-element, which is assumed to depend on the average irreversible strain rate $-\dot{\bar{\varepsilon}}_T$,

$$\gamma = \frac{1}{\Psi'} \int_0^{\Psi'} \sqrt{\dot{\bar{p}}_{ij}\dot{\bar{p}}_{ij}} d\Psi, \quad \nu = \int_0^1 \bar{\varepsilon}_T d\Psi, \quad (3.3)$$

where the overdot indicates the derivative of irreversible strain with respect to time; $\bar{\varepsilon}_T$ is the purely thermal strain of the sub-element; Ψ' is the weight of irreversibly deformed sub-elements. Then

$$\tau = \tau(\Psi, \gamma, \nu), \quad 0 \leq \Psi \leq 1. \quad (3.4)$$

Here, the weight of the sub-element at the moment of its transition from the reversible state to the irreversible state under the initial load is selected as a parameter that determines the affiliation of the yield point to a certain sub-element.

The tensor properties of the subelement are defined assuming that the components of the elastic strain deviator \bar{e}_{ij} can be expanded along \bar{p}_{ij} and $d\bar{p}_{ij}/d\bar{\lambda}$:

$$\bar{e}_{ij} = (\bar{\tau} + \bar{s}) \frac{d\bar{p}_{ij}}{d\bar{\lambda}} + \bar{r} \frac{\bar{p}_{ij}}{\bar{p}}, \quad p = \sqrt{p_{ij}p_{ij}}, \quad d\bar{\lambda} = \sqrt{d\bar{p}_{ij}d\bar{p}_{ij}}.$$

With these assumptions, Eq. (1.7) can be represented as

$$\bar{e}_{ij} - e_{ij} = b(\varepsilon_{ij} - \bar{\varepsilon}_{ij}) = m(p_{ij} - \bar{p}_{ij}), \quad b = \frac{B}{2G} = \frac{m}{1-m}. \quad (3.5)$$

For variables that describe the effect of hardening of the sub-elements on the ultimate elastic strains of the sub-elements, we use the simplest laws

$$\dot{\bar{s}} = \begin{cases} a_0 \dot{\lambda}, & \bar{s} < x(\psi, \gamma, \nu), \\ \dot{x}(\psi, \gamma, \nu), & \bar{s} = x(\psi, \gamma, \nu), \end{cases}$$

$$\bar{r} = \begin{cases} a_r \bar{p}, & a_r \bar{p} < x_1(\psi, \gamma, \nu), \\ x_1(\psi, \gamma, \nu), & a_r \bar{p} = x_1, \end{cases}$$

where a_0 is the factor of isotropic hardening; a_r is the kinematic hardening.

Note that in multi-element models, averaging is performed over the set of realizations rather than over the volume, i.e., the ergodic hypothesis is considered to be valid. Considering τ as a single random parameter of the problem, we get

$$\langle \bar{e}_{ij} \rangle = \int_0^1 \bar{e}_{ij}(\psi) d\psi = \int_{\tau_0}^{\tau_{\max}} \bar{e}_{ij}(\tau) d\psi(\tau),$$

$$\langle \bar{p}_{ij} \rangle = \int_0^1 \bar{p}_{ij}(\psi) d\psi = \int_{\tau_0}^{\tau_{\max}} \bar{p}_{ij}(\tau) d\psi(\tau), \quad (3.6)$$

where $\psi(\tau)$ is the integral distribution function of the initial ultimate elastic strains; τ_{\max} and τ_0 are the largest and smallest limits of elasticity of sub-elements, respectively.

The structure of the integral distribution function, along with these physical laws, affects the macroscopic system of constitutive equations. When specifying the integral distribution function in [5, 6, 12], it was assumed that the initial deformation diagrams for different constant values of the state parameters γ, ν do not depend on the parameter $m: e = \varphi(p, \gamma, \nu) + s$. Then, the relation $\psi \sim \tau$ can be found in a parametric form using (3.2), (3.5) [5]:

$$\psi(p, m, \gamma, \nu) = \frac{m+a}{m+\varphi_{,p}}, \quad \tau(p, m, \gamma, \nu) = \varphi(p, \gamma, \nu) + mp. \quad (3.7)$$

According to (3.7), there may be different functions of the integral distribution $\psi \sim \tau$ depending on the value of the parameter. Under these conditions, a simple formula for the parameter m follows from (1.8) [5]:

$$m = -a + \sqrt{a + a^2}, \quad a = a_0 + a_r. \quad (3.8)$$

According to (3.8), the relationship between the fluctuations of reversible and irreversible strains depends only on the hardening factor of the sub-element a .

Our purpose here is to show that based on principle (1.8) we can describe the pattern of change in the parameter B in the irreversible strain region in the case where the diagram $e \sim p$ depends on the parameter m , without any additional assumptions (plastic relaxation, scalar accommodation function, etc.). To make the results more accessible for review, consider the case of proportional loading at constant values of the state parameters $\gamma = \text{const}, \nu = \text{const}$ and the linear law of hardening.

From the definition of sub-element, it follows that the elastic anisotropy of material particles should be taken into account together with the fluctuations of stresses and strains within each sub-element. Due to this fact, the fundamental concepts of stress and strains are introduced at three levels of structure: material point: $\tilde{t}_{ij} = \tilde{\sigma}_{ij} + \tilde{\sigma}_0 \delta_{ij}, \tilde{d}_{ij} = \tilde{\varepsilon}_{ij} + \tilde{\varepsilon}_0 \delta_{ij}$; sub-element:

$$\bar{t}_{ij} = \bar{\sigma}_{ij} + \bar{\sigma}_0 \delta_{ij}, \bar{d}_{ij} = \bar{\varepsilon}_{ij} + \bar{\varepsilon}_0 \delta_{ij}, \text{ and body element: } t_{ij} = \sigma_{ij} + \sigma_0 \delta_{ij}, d_{ij} = \varepsilon_{ij} + \varepsilon_0 \delta_{ij}.$$

The values of $\bar{t}_{ij}, \bar{d}_{ij}$ are determined by averaging over orientation factor of the crystal lattice:

$$\bar{t}_{ij} = \langle \tilde{t}_{ij} \rangle_{\Omega}, \quad \bar{d}_{ij} = \langle \tilde{d}_{ij} \rangle_{\Omega}, \quad \bar{\sigma}_{ij} = \langle \tilde{\sigma}_{ij} \rangle_{\Omega}, \quad \dots,$$

and the values of t_{ij}, d_{ij} are determined by averaging over the scatter parameter τ or weight function ψ .

Writing relation (1.7) in the form

$$\tilde{\sigma}_{ij} - \bar{\sigma}_{ij} + \bar{\sigma}_{ij} - \sigma_{ij} = B(\varepsilon_{ij} - \bar{\varepsilon}_{ij} + \bar{\varepsilon}_{ij} - \tilde{\varepsilon}_{ij}),$$

we establish two types of relations:

$$\tilde{\sigma}_{ij} - \bar{\sigma}_{ij} = B(\bar{\varepsilon}_{ij} - \tilde{\varepsilon}_{ij}), \quad (3.9)$$

$$\bar{\sigma}_{ij} - \sigma_{ij} = B(\varepsilon_{ij} - \bar{\varepsilon}_{ij}). \quad (3.10)$$

Expanding $\tilde{\varepsilon}_{ij}, \bar{\varepsilon}_{ij}$ into reversible, $\tilde{e}_{ij}, \bar{e}_{ij}$, and irreversible components, $\tilde{p}_{ij}, \bar{p}_{ij}$,

$$\tilde{\varepsilon}_{ij} = \tilde{e}_{ij} + \tilde{p}_{ij}, \quad \bar{\varepsilon}_{ij} = \bar{e}_{ij} + \bar{p}_{ij}$$

and considering that $\tilde{p}_{ij} = \bar{p}_{ij}$ by definition, we can represent Eq. (3.9) as

$$\tilde{\sigma}_{ij} - \bar{\sigma}_{ij} = B(\bar{e}_{ij} - \tilde{e}_{ij}). \quad (3.11)$$

According to (3.11) and (3.10), the equations relating microstates and macrostates (1.7) split into two types of relations: stress fluctuations and reversible strains in the sub-element structure and stress and strains fluctuations in the sub-element system. If the elastic isotropy of material particles is assumed, then $\tilde{e}_{ij} = \bar{e}_{ij}, \tilde{\sigma}_{ij} = \bar{\sigma}_{ij}$ and the relationship between microstates and macrostates is reduced to only one type of Eqs. (3.5).

With such assumptions, the principle of discrepancies of measures (1.8) splits into discrepancies that occur in the structure of sub-elements

$$\Delta' = \langle \tilde{\sigma}_{ij} \tilde{e}_{ij} \rangle - \langle \tilde{\sigma}_{ij} \rangle \langle \tilde{e}_{ij} \rangle \quad (3.12)$$

and the system of sub-elements

$$\Delta'' = \langle \bar{\sigma}_{ij} \bar{e}_{ij} \rangle - \langle \bar{\sigma}_{ij} \rangle \langle \bar{e}_{ij} \rangle. \quad (3.13)$$

In real interactions, we have

$$\Delta = \Delta' + \Delta'' = \text{Extr}. \quad (3.14)$$

From expressions (3.12) and (3.14), it follows that the elastic anisotropy of material particles affects the discrepancies of measures in the system of sub-elements.

4. Specification of Expressions for Discrepancies of Measures. To simplify the analysis of changes in the internal parameter B , which shows the inhomogeneity of the strains and stresses in the representative volume ΔV_0 under irreversible loading, we assume that the sub-elements are elastically isotropic. Then the effect of anisotropy of material particles is described by Eq. (3.11) only. In this case, Eq. (3.10) is simplified and takes the form (3.5).

Substituting (3.5) into (3.13) and performing simple transformations, we obtain

$$\Delta'' = 2Gm(1-m)(\langle p_{ij} - \bar{p}_{ij} \rangle \langle \bar{p}_{ij} - p_{ij} \rangle), \quad m = \frac{B}{2G+B}. \quad (4.1)$$

Expression (4.1) can be represented as

$$\Delta'' = 2Gm(1-m)(\langle \bar{p} \rangle^2 - \langle \bar{p}^2 \rangle), \quad \bar{p} = \sqrt{\bar{p}_{ij} \bar{p}_{ij}}. \quad (4.2)$$

In the case of single-phase polycrystalline materials with a cubic lattice, the formula for the discrepancies of measures in the elastic region was derived in [7]:

$$\Delta = \frac{-3B(2c_{44} - c_{11} + c_{12})^2 \sigma_{ij} e_{ij}}{[5B + 4c_{44} + 3(c_{11} - c_{12})][5c_{44}(c_{11} - c_{12}) + (3c_{44} + c_{11} - c_{12})B]} = \text{Extr}. \quad (4.3)$$

Formula (4.3) can be extended to a system of elastically isotropic sub-elements:

$$\Delta' = \frac{-12(A-1)^2 B(m)c_{44} \langle \bar{\sigma}_{ij} \bar{e}_{ij} \rangle}{[5AB(m) + 2c_{44}(3+2A)][(2+3A)B(m) + 10c_{44}]}, \quad (4.4)$$

where $c_{11} - c_{12} = 2c_{44} / A$ is taken into account. During irreversible deformation, not only the parameter B changes, but also does the shear modulus G . The analysis is simplified if we use the following formula obtained in [9]:

$$B(m) = \frac{c_{44}}{5A} \left[\frac{m}{1-m} (2+3A) - 3 - 2A + \sqrt{\left[\frac{m}{1-m} (3A+2) - 2A - 3 \right]^2 + 100A \frac{m}{1-m}} \right]. \quad (4.5)$$

The clearest results on change in B are obtained for a proportional load:

$$\frac{\bar{\sigma}_{ij}}{\bar{\sigma}} = \frac{\bar{\varepsilon}_{ij}}{\bar{\varepsilon}} = \frac{\bar{e}_{ij}}{\bar{e}} = \frac{\bar{p}_{ij}}{\bar{p}} = \text{const}, \quad \bar{\sigma} = \sqrt{\bar{\sigma}_{ij} \bar{\sigma}_{ij}}, \quad \bar{\varepsilon} = \sqrt{\bar{\varepsilon}_{ij} \bar{\varepsilon}_{ij}}.$$

With this type of load, expressions (3.5) are reduced to a scalar equation:

$$\bar{e} - e = b(\varepsilon - \bar{\varepsilon}) = m(p - \bar{p}). \quad (4.6)$$

In the region of linear hardening of sub-elements we have

$$\bar{e} = \tau + \chi(\varepsilon - \tau) = \tau(1 - \chi) + \chi\bar{\varepsilon},$$

or

$$\bar{e} = \tau + a\bar{p}, \quad a = \frac{\chi}{1 - \chi}. \quad (4.7)$$

These relations are valid beyond outside elasticity $\tau \leq \bar{e}$. In the sub-elements with $\tau > \bar{e}$ we have $\bar{p} = 0$. Using (4.7), we determine the yield point τ' in the boundary sub-element:

$$\tau' = e + mp = \frac{e + b\varepsilon}{1 + b}. \quad (4.8)$$

Using (4.6)–(4.8), we derive formulas for determining the modules of reversible and irreversible strains:

$$\bar{e}(\tau, \tau', m) = \begin{cases} \frac{m\tau + a\tau'}{m + a}, & \tau \leq \tau', \\ \tau', & \tau > \tau', \end{cases} \quad (4.9)$$

$$\bar{p}(\tau, \tau', m) = \begin{cases} \frac{\tau' - \tau}{m + a}, & \tau \leq \tau', \\ 0, & \tau > \tau'. \end{cases} \quad (4.10)$$

Integrating (4.10) over the parameter τ , we find

$$p = \frac{1}{m + a} \int_{\tau_0}^{\tau'} (\tau' - \tau) y(\tau) d\tau = \frac{1}{m + a} \varphi(\tau'), \quad (4.11)$$

where $y(\tau)$ is the density distribution of the elastic limits of the sub-elements τ , τ_0 is the smallest elastic limit,

$$\varphi(\tau') = \int_{\tau_0}^{\tau'} (\tau' - \tau) y(\tau) d\tau.$$

From (4.11) and (4.8), we find

$$\tau' = \varphi^{-1}[(m + a)p] = e + mp,$$

or in the form

$$e = \varphi^{-1}[(m+a)p] - (m+a)p + ap = F[(m+a)p] + ap, \quad (4.12)$$

where $F(x) = \varphi^{-1}(x) - x$.

Formula (4.12) allows us to find diagrams $e \sim p$ from one scheme of connection of sub-elements based on diagram calculated using another scheme.

If the integral function of the distribution of elastic limits is given as the initial information about the material, then relation (4.2) with (4.10) is represented in the form

$$\Delta''(\tau', m) = \frac{2Gm(1-m)}{(m+a)^2} \left[\left(\int_{\tau_0}^{\tau'} (\tau' - \tau) y(\tau) d\tau \right)^2 - \int_{\tau_0}^{\tau'} (\tau' - \tau)^2 y(\tau) d\tau \right]. \quad (4.13)$$

We can use (3.14), (4.4), and (4.13) to study the pattern of change in the parameter m during irreversible deformation taking into account the elastic anisotropy of material particles.

5. Numerical Analysis of the Pattern of Change in the Parameter m for Polycrystalline Materials under Loading.

Consider, as an example, a hypothetical polycrystalline material with a cubic lattice for which the integral function of the distribution of elastic limits is given by

$$y(z, k) = k^2 z e^{-kz}, \quad \psi(z, k) = \int_0^z y(z, k) dz = 1 - (1 + kz) e^{-kz}, \quad (5.1)$$

$$z = \tau' - \tau_0 = e - \tau_0 + mp. \quad (5.2)$$

Substituting (5.1) into (4.11) and taking into account notation (5.2), we obtain the relationship $e \sim p$ in the following parametric form:

$$(m+a)p = \frac{1}{k} \left[kz - 2 + (kz + 2)e^{-kz} \right],$$

$$e = \tau_0 + ap + \frac{2}{k} - \left(\frac{2}{k} + z \right) e^{-kz}. \quad (5.3)$$

Expression (5.3) can be written as

$$y = 2 - (2 + x + y) e^{-(x+y)}, \quad (5.4)$$

where

$$y = k(e - \tau_0 - ap), \quad x = k(m+a)p, \quad z = x + y. \quad (5.5)$$

The implicit type of relationship $y \sim x$ given by (5.4) complicates the numerical analysis. However, with high accuracy (deviation does not exceed 1%), expression (5.4) can be approximated by the function

$$y(x) = \begin{cases} 2 \sin \sqrt[3]{x}, & x \leq \left(\frac{\pi}{2} \right)^3, \\ 2, & x > \left(\frac{\pi}{2} \right)^3. \end{cases} \quad (5.6)$$

Given notation (5.5) in (5.6), the relationship among e , p , and m takes the form

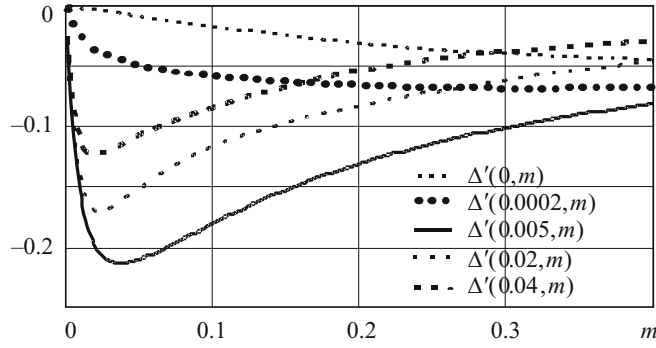


Fig. 1

$$e(p, m, a, k) = \begin{cases} \tau_0 + ap + \frac{2}{k} \sin \left[\sqrt[3]{k(m+a)p} \right], & k(m+a)p \leq \left(\frac{\pi}{2} \right)^3, \\ \tau_0 + ap + \frac{2}{k}, & k(m+a)p > \left(\frac{\pi}{2} \right)^3. \end{cases} \quad (5.7)$$

In this case, the material function F , according to (4.12) and (5.7), is defined by

$$F[(m+a)p] = \begin{cases} \tau_0 + \frac{2}{k} \sin \left[\sqrt[3]{k(m+a)p} \right], & k(m+a)p \leq \left(\frac{\pi}{2} \right)^3, \\ \tau_0 + \frac{2}{k}, & k(m+a)p > \left(\frac{\pi}{2} \right)^3. \end{cases} \quad (5.8)$$

Integrating (4.14) and taking into account (5.1) and (5.2), we obtain the following expressions for the discrepancy Δ'' :

$$\Delta''(\tau', m, a, k) = \frac{2Gm(1-m)}{k^2(m+a)^2} \left\{ \left[\left(2 + 2k\Delta\tau + (k\Delta\tau)^2 \right) e^{-k\Delta\tau} - 2 \right]^2 - \left[6 - \left(6 + 6k\Delta\tau + 3(k\Delta\tau)^2 + (k\Delta\tau)^3 \right) e^{-k\Delta\tau} \right] \right\}. \quad (5.9)$$

Expressing τ in (5.9) in terms of p and using formulas (5.2), (5.7)

$$\Delta\tau = \tau' - \tau_0 = \frac{2}{k} \sin \left(\sqrt[3]{k(m+a)p} \right) + (m+a)p, \quad (5.10)$$

then the discrepancy Δ'' can be represented as a function of the variables p , m , and k ($\Delta'' = \Delta''(p, m, a, k)$).

To identify some specific features of the change in the quantities being considered, we will use the relative discrepancy

$$\bar{\Delta}(p, m, a, k) = \frac{\Delta'(m) + \Delta''(p, m, a, k)}{2G(m, a, k)e(e+p)},$$

$$G(m, a, k) = \frac{1-m}{2m} B(m, a, k). \quad (5.11)$$

Figure 1 shows the graphs of change $\bar{\Delta}(p, m, a, k)$ for different constant values of irreversible strain p in a hypothetical material with $\tau_0 = 10^{-3}$, $k = 1000$, $c_{11} = 23.7 \times 10^4$, $c_{12} = 14.1 \times 10^4$, $c_{44} = 11.6 \times 10^4$ MPa.

The graphs show that the largest deviation of the relative discrepancy first increases, reaching 21.4% and then decreases. The value of the parameter m at which the function $\bar{\Delta} = \bar{\Delta}(p, m)$ for the given value of p takes extreme values constantly decreases.

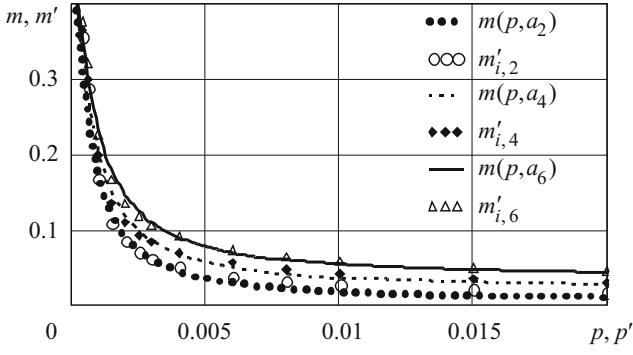


Fig. 2

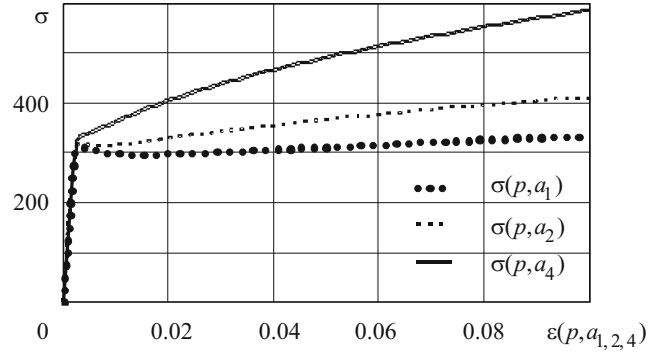


Fig. 3

Figure 2 shows the dependence of the parameter m on the irreversible strain assuming that the density of the elastic limits of the sub-elements is given by (5.1) ($k = 1000$) and the elastic constants $c_{11} = 23.7 \times 10^4$, $c_{12} = 14.1 \times 10^4$, $c_{44} = 11.6 \times 10^4$ MPa, for three values of the hardening factor a : $a_2 = 0.003$, $a_4 = 0.01$, $a_6 = 0.02$ denoting the values of $m_{i,j}$ found from (3.14) with (4.4) and (5.9) for different strains p_i and six constant hardening factors a_j .

The symbols in Fig. 2 represent the calculated results, while the solid lines, the approximating function

$$m(p, a, k) = \frac{m_0 + 0.29\sqrt{a}(kp)^{1.3}}{1 + (1.9 - 5.8\sqrt{a})(kp)^{1.3}}, \quad (5.12)$$

where m_0 is the value of the parameter m in the elastic deformation region. Functions (5.12) are specified on the basis of a detailed numerical analysis of system (3.14), (4.4), (5.7)–(5.10). We can use (5.7) and (5.12) to describe the relationship between stresses and strains at the macroscopic level if we know the elastic constants of the crystals, the hardening factor of the sub-element, and the value of the parameter appearing in the distribution law. To simplify the figures, the parameter k , which is assumed to be 1000, is not indicated. The functions of three variables p , a , k are everywhere represented as functions of two variables p and a . Figure 2 demonstrates that the parameter m decreases sharply at the first stage of irreversible deformation and then tends to some constant value. In this case, the parameters m and $b = \frac{m}{1-m}$ in the irreversible region decrease by more than

one order of magnitude. Numerically, this result differs by 40–50% from the predicted Berweier–Saul model, which uses the idea of “plastic relaxation.”

Figure 3 shows the deformation diagrams calculated by formula (5.7) ($\sigma = 2Ge(p, m(p, a, k), a, k) = 2Ge(p, a, k)$) for three values of the hardening factor a : $a_1 = 0.0002$, $a_2 = 0.0015$, $a_4 = 0.01$. The effect of reduction in the parameter m with irreversible strain can be interpreted as weakening of the kinematic coupling between sub-elements, which leads to the natural tendency of the material to reduce stress fluctuations and the shear modulus. Figure 3 demonstrates that for small values of a (typical for the first phase of hardening of single crystals) the load diagram $\sigma \sim \epsilon$ displays a plateau or a yield drop. It is possible to numerically determine the length of the yield plateau. If at the end of this section, the process of single slip stops and the further process occurs with multiple slip, then the deformation diagram has the same form as the corresponding experimental load diagram. In the section of multiple slip, the hardening factor a is usually greater than 0.01. Note that such deformation effects are described using the principle of extremum of discrepancy of measures.

The physical explanation of such effects follows from the pattern of changes in the weight of irreversibly deformed sub-elements with increasing p . Figure 4 demonstrates that for the values of a that correspond to the second stage of hardening $a_4 = 0.01$ (multiple slip), the volume of irreversibly deformed sub-elements increases with increasing p . However, for values of a that are typical for easy slip, a sharp decrease in the parameter m leads to the stop of this process and, in some cases, to a decrease in the number of irreversibly deformed sub-elements. In the latter case, unloading occurs in a part of the sub-elements. Thus, for small values of the hardening parameter, irreversible strains are concentrated in small volumes of the body element. This conclusion is in good agreement with the results of numerous experiments. The numerical analysis was conducted using formulas (5.1) with (5.2), (5.7), (5.12).

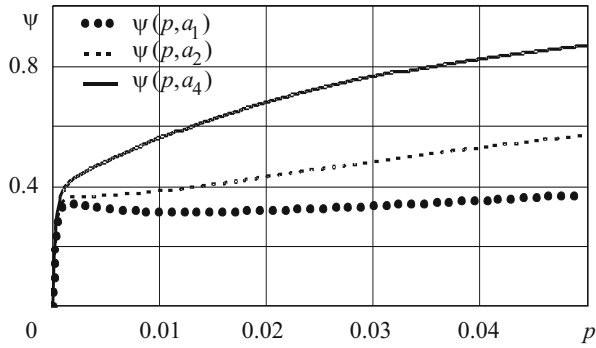


Fig. 4

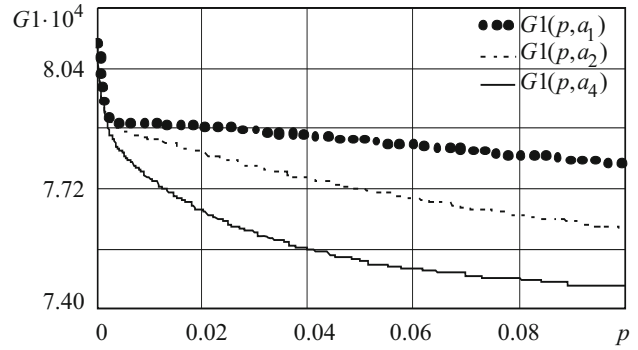


Fig. 5

The effect of stress drop at the initial moment of macroyielding strengthens if the material properties are sensitive to the strain rate. According to (3.3), (3.4), the yield points of sub-elements depend on the rate parameter γ . In [6], it was shown that at the initial moment of yielding

$$\gamma = \lim_{\psi' \rightarrow 0} \frac{\int_0^{\psi'} \sqrt{\dot{p}_{ij} \dot{p}_{ij}} d\psi}{\psi'} = \frac{\sqrt{\dot{\epsilon}_{ij} \dot{\epsilon}_{ij}}}{m+a} = \frac{\dot{\epsilon}}{m+a},$$

where $\dot{\epsilon}$ is the rate of change in the deviatoric total macroscopic strain tensor. If the experiment is performed with $\dot{\epsilon} = \text{const}$, the parameter γ decreases sharply at the initial stage of irreversible deformation, as a result of which the yield points of the sub-element are reduced, resulting in a yield drop.

The pattern of change in the shear modulus during irreversible deformation for polycrystalline materials with a cubic lattice can be established using formulas (4.5) and (5.12). Considering that

$$\frac{B}{2G} = b = \frac{m}{1-m}, \quad m = m(p, a, k), \quad b = b(p, a, k),$$

we find

$$G'(p, a, k) = \frac{c_{44}}{10Ab(p, a, k)} \left[(2+3A)b(p, a, k) - 3 - 2A + \sqrt{[(2+3A)b(p, a, k) - 3 - 2A]^2 + 100A - b(p, a, k)} \right]. \quad (5.13)$$

Formula (5.13) shows that the change in the shear modulus during irreversible deformation depends on the elastic constants of the crystals and the parameter k , which affects the shape of the load diagram on the nonlinear hardening section. If the anisotropy factor $A = 1$, then $G'(p, a, k) = c_{44}$ follows from (5.13). Therefore, in the case of elastically isotropic materials, the shear modulus does not change during irreversible deformation.

To describe the patterns of changes in the elastic properties of a body element during irreversible deformation, it is necessary to make assumptions on the interaction of material particles in the sub-elements. Two simple assumptions are noteworthy: the current values of the parameter m (or b) affect the interaction of material particles equally in reversibly and irreversibly deformed sub-elements or only in irreversibly loaded sub-elements. In the former case,

$$G(p, a, k) = G'(p, a, k),$$

in the latter case,

$$G(p, a, k) = G'(p, a, k)\psi'(p, a, k) + (1 - \psi'(p, a, k))G^*, \quad (5.14)$$

where G^* is the initial elastic modulus of the material, calculated by formula (2.1); ψ' is the weight of irreversibly deformed sub-elements. Based on assumption (5.14), Fig. 5 shows graphs of changes in the relative shear modulus $G1(p, a, k) = G(p, a, k) / G(0, a, k)$ for three values of the hardening factor a : $a_1 = 0.001$, $a_2 = 0.01$, $a_4 = 0.02$.

Many publications [2, 10, etc.] address experimental study of the effect of change in G with p . However, the published results can be used only for qualitative testing of formulas (5.13) and (5.14), as they do not provide the values of the elastic constants of the crystals and the load diagram $\sigma \sim \varepsilon$, on the basis of which we can calculate the factor k . We can conclude that the shear modulus changes a little for materials in which A is close to one, and can decrease by 8–10% in the case of iron and copper. This interval is consistent with the experimental results [2, 10, etc.]. Figure 5 shows that the shear modulus decreases rapidly at the first stage of irreversible deformation, and then asymptotically tends to a constant value.

Conclusions. The equation relating the fluctuations of the stress and strain tensors occurring at the levels of material anisotropic particles that are part of the structure of sub-elements and at the level of the system of sub-elements is derived. The pattern of the change in the relationship between the fluctuations of stresses and strains has been studied using the principle of extremum of discrepancies between the macroscopic measures and the corresponding average microscopic analogues. It has been shown that the discrepancy of measures is influenced by the elastic properties of crystals, hardening factors, and the type of the density function of the distribution of the elastic limits of the sub-elements.

Based on numerical analysis of the expressions for the discrepancies of measures, it has been shown that the ratio of stress fluctuations to strain fluctuations decreases sharply at the first stage of irreversible deformation, and then tends to some constant value. If the distribution function of yield points does not depend on the change in the kinematic relations between sub-elements, and the crystal anisotropy factor of the crystals coincides with the anisotropy factor of iron, this ratio at irreversible strains of about 10% is about 30 times less than in the elastic region.

It is shown that based on the principle of extremum of discrepancies of measures, even such specific effects as the plateau or yield drop, the length of these sections, and changes in the macroscopic elastic sections in the irreversible deformation region are described naturally without any additional conditions.

The proposed approach to the description of the pattern of change in stress and strain fluctuations at local levels allows us to describe, in a united way, a wide range of phenomena observed in monotonic and nonmonotonic nonisothermal loading of materials.

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