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A THREE-LEVEL CONSTITUTIVE MODEL DESCRIBING THE BEHAVIOR OF POLYCRYSTALS WITH MONOTONIC AND NON-MONOTONIC STRAIN DIAGRAMS

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Abstract. A three-level constitutive model is considered that describes from a concurrent positions the behavior of materials with monotonic and non-monotonic strain diagrams. An effect of the anisotropy and strengthening coefficients of the crystal, the average value of the grain diameter and distribution density of structural defects on the macroscopic behavior of the polycrystal is established. Thereto, three postulates are used: averaged connections, the extremum of discrepancy between the macroscopic measures and their microscopic analogues, and orthogonality of stress and strain fluctuations. Based on the constructed system of governing equations, the specific effects of the structural characteristics of a polycrystal on macroscopic strain diagrams and elasticity constants are studied.

Key words*:* constitutive model, structure, crystal, polycrystal, subelement, stress, strain, anisotropy, strengthening, discordance of measures.

Introduction.

The most effective models that describe a wide range of properties of polycrystalline materials include structural models of the medium [2, 6, 10, 19] and approaches in which each grain of the polycrystal is consistently considered as an inclusion in the "matrix" of all other grains [9, 11, 12, 15]. The striking contrast between the underlying elementary properties of structural elements/subelements, which can be established in the simplest experiments, and a wide range of reflected effects indicates the decisive role of microplastic deformations and associated microstresses on the behavior of materials. It is important to note that the indicated deformations and stresses play the role of material memory carriers for the prehistory of loading and heating.

The disadvantages of the model [2, 6, 10, 19] include the assumption of equality of strains $\tilde{d}_{ij} = d_{ij}$ or stresses $\tilde{t}_{ij} = t_{ij}$ of subelements, which narrows the possibility of describing processes under complex non-isothermal loading. In the approach based on the problem of inclusion in an infinite matrix [15], linear relationships were established between stress and strain fluctuations $\tilde{t}_{ij} - t_{ij} = B_{ijnm}(d_{nm} - \tilde{d}_{nm})$. A weak point of research in this area is the inconsistency of the linear equations of the connection of macro and microstates with the first law of thermodynamics. In [3] shown:

$$\left\langle \int_0^t \tilde{t}_{ij} \dot{\tilde{d}}_{ij} dt \right\rangle < \int_0^t \langle \tilde{t}_{nm} \rangle \left\langle \dot{\tilde{d}}_{nm} \right\rangle dt$$

for any options for changing B_{ijnm} tensor, except for the limit: $B_{ijnm} = 0$ or $B_{ijnm} = \infty$, where $\langle . \rangle -$ sign of averaging over representative volume.

In the conditions of impossibility of detailed accounting of interactions of material particles in a representative volume, it is advisable to construct the equations of connection of macro and microstates that would be consistent with the laws of thermodynamics, take into account the phenomenon of coherence of local deformation processes and meet the condition of uniqueness of the solution of the problem of representing a real material in a model [3 – 5, 17]. The theory of constitutive equations developed in [3 – 5, 17] is based on three principles: of averaged connections, of the extremum of discrepancy between the macroscopic measures and the microscopic analogs and orthogonality of stress and strain fluctuations. In works [3 – 5, 17], a closed system of equations is established on the basis of which it is possible to construct constitutive equations at the macroscopic level, if the physical equations at the microscopic level are known. Although the possibilities of the theory have been significantly expanded, nevertheless, it turned out that within the framework of the two levels of the model it is impossible to describe from a unified position the behavior of materials with monotonic and no monotonic deformation diagrams (with a platform or a yield tooth), changes in elastic constants in the process of irreversible deformation, and a number of other observed phenomena in the destruction of materials. It is also important to note the difference between the accepted concepts of primary structural elements in the description of reversible and irreversible deformation processes. If in the study of reversible processes an anisotropic grain is chosen as the primary element of the structure, then an elastically isotropic subelement is used to describe irreversible processes. Due to this difference, it is not possible to obtain a coherent theory for reversible and irreversible deformation processes, which from a general point of view describes many diverse and externally unrelated effects of fast and long-term deformation, single, cyclic non-isothermal deformation, and failure along straight or curvilinear loading trajectories. The capabilities of the model can be extended by leading the analysis to the intermediate level of the structure [7, 8, 16].

In this paper, we analyze the behavior of the model in the coupled and uncoupled substitution of the extremum of the mismatch of measures at the levels of material particles and the system of subelements. Let us construct a constitutive equation for the relationship between macro and microstates, containing both characteristics of properties at the level of crystals and at the level of systems of subelements, and on its basis, we will analyze the specific effects of individual parameters of the material structure on the macroscopic deformation diagram.

§1. Formalization of a continuous medium taking into account the elastic anisotropy of crystals.

In the reversible region of deformation, the representative volume of a polycrystal can be represented as an infinite number of differently oriented crystals. Within the framework of such a schematization, the fundamental concepts of stress and strain, in the elastic region, are introduced only at two levels of structure: material particles $\tilde{t}_{ij}$, $\tilde{d}_{ij}$, and body element t_{ij}, d_{ij}. By $\tilde{t}_{ij}, \tilde{d}_{ij}$ we mean the average value of stresses and strains in crystals with the same orientation of the crystal lattice.

In the irreversible region of deformation, as a local structural unit, we take a subelement, which is identified with the set of all material particles inside the representative volume ΔV_0, having the same deviator of irreversible deformations. Particles belonging to the same subelement may have different positions and orientations of the crystal lattice in a representative volume ΔV_0. The number of all particles with the same irreversible deformation deviator determines the weight of one subelement, which does not change during loading. Within the framework of this concept, the area ΔV_0 is represented as an infinite number of interconnected subelements with different thermorheological properties.

Based on the above definition of the concept of a subelement, it follows that when taking into account the elastic anisotropy of material particles, it is necessary to take into account stress and strain fluctuations within each subelement. Because of this, stresses and strains are introduced at three levels of the structure: material point – $\tilde{t}_{ij} = \tilde{\sigma}_{ij} + \tilde{\sigma}_0\delta_{ij}$, $\tilde{d}_{ij} = \tilde{\varepsilon}_{ij} + \tilde{\varepsilon}_0\delta_{ij}$, subelement – $\overline{t}_{ij} = \overline{\sigma}_{ij} + \overline{\sigma}_0\delta_{ij}$, $\overline{d}_{ij} = \overline{\varepsilon}_{ij} + \overline{\varepsilon}_0\delta_{ij}$ and body element $-t_{ij} =$ $= \sigma_{ij} + \sigma_0\delta_{ij}$, $d_{ij} = \varepsilon_{ij} + \varepsilon_0\delta_{ij}$.

When constructing the equations of connection between macro and microstates, we will use Hill's equations [13]

$$t_{ij} = \langle \tilde{t}_{ij} \rangle = \frac{1}{\Delta V_0} \int\limits_{\Delta V_0} \tilde{t}_{ij} dV; \quad d_{ij} = \langle \tilde{d}_{ij} \rangle; \quad \langle \tilde{t}_{ij} \tilde{d}_{ij} \rangle = t_{pq} d_{lq}, \tag{1.1}$$

where $\tilde{t}_{ij}$, $\tilde{d}_{ij}$ – stress and strain tensors at each point of the area ΔV_0 respectively, $\langle . \rangle$ – volume averaging sign ΔV_0.

Equations (1.1) are obtained under the constraint that the displacements and trains are small. In this study, we will assume that relations (1.1) can also be extended to the case of finite strain, if by the symmetric tensor d_{ij} we mean the tensor

$$d_{ij} = \sum_{n=1}^{3} r_{ni} r_{nj} \ln \lambda_n; \quad \lambda_n = \sqrt{C_n}; \quad C_{ij} = F_{ni} F_{nj}, \tag{1.2}$$

where $\lambda_1, \lambda_2, \lambda_3$ – principal elongations referred to some state of reference for a material element; C_n – eigenvalues of the Cauchy-Green tensor C_{ij}; r_{ij} – direction cosines of the principal tensor system C_{ij} (principal coordinate systems of tensors C_{ij} and d_{ij} – coaxial); F_{ni} – strain gradient. According to [13] a measure of strain on a logarithmic scale is the norm; with its help, any other function $f(\lambda)$ can be expanded into a power series.

Accordingly, for each strain tensor d_{ij}, a symmetric stress tensor t_{ij}, is introduced, using the strain work differential $d\omega$, which coincides with the Cauchy stress tensor.

When defining the strain tensor d_{ij} in the form (1.2), the first invariant d_{ii} is calculated by the formula

$$d_{ii} = 3\varepsilon_0 = \ln(\lambda_1 \lambda_2 \lambda_3) = \ln(\rho_0/\rho), \tag{1.3}$$

where ρ_0 and ρ – density in the initial and deformed states. From (1.3), the physical meaning of the first invariant d_{ij} and the spherical strain tensor $\varepsilon_0\delta_{ij}$ are revealed: monotonic functions of changing the volume of a body element. This is especially important because the mechanical properties of the material under all-round tension (compression) differ significantly from the properties under other types of stress states. Selecting from d_{ij} the part that characterizes the volume changes, we obtain the expression for the deviator of the strain tensor

$$\varepsilon_{ij} = d_{ij} - \varepsilon_0\delta_{ij} = \sum_{n=1}^{3} r_{ni} r_{nj} \ln \frac{\lambda_n}{\sqrt[3]{\lambda_1 \lambda_2 \lambda_3}}; \quad \tilde{\varepsilon}_{ij} = \tilde{d}_{ij} - \tilde{\varepsilon}_0\delta_{ij}. \tag{1.4}$$

By analogy with the strain tensor, we decompose the stress tensor into the components of the spherical tensor $\sigma_0\delta_{ij}$ and the deviator σ_{ij}

$$t_{ij} = \sigma_{ij} + \sigma_0\delta_{ij}; \quad \tilde{t}_{ij} = \tilde{\sigma}_{ij} + \tilde{\sigma}_0\delta_{ij}. \tag{1.5}$$

Equations (1.1) are necessary but not sufficient for constructing a system of defining equations at the macroscopic level based on physical relationships at the microscopic level. To obtain a closed system of equations, the following principles were formulated in [3 – 5, 17]: established on the basis of three postulates: averaged connections, of the extremum of discrepancy between the macroscopic measures and the microscopic analogs and orthogonality of stress and strain fluctuations. Based on the principle of averaged bonds, the phenomenon of coherence of local deformation processes is taken into account. It is assumed that interactions between material particles in a representative volume are formed under the influence of only averaged bonds. Then consistency with the first law of thermodynamics can be ensured on the basis of the postulate of the orthogonality of stress and strain oscillations

$$(\tilde{t}_{ij} - t_{ij})(\tilde{d}_{ij} - d_{ij}) = 0. \tag{1.6}$$

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 [3 – 5, 17] that the natural macro measures of the energy of change in volume and shape differ from the average over their micro measures. To extend system (1.1), (1.6) in [3 – 5, 17], the principle of the extremum of discrepancy between macroscopic measures and average microscopic analogs was proposed in [3 – 5, 17]. In particular

$$\Delta = \left\langle \tilde{\sigma}_{ij}\tilde{\varepsilon}_{ij} \right\rangle - \left\langle \tilde{\sigma}_{ij} \right\rangle \left\langle \tilde{\varepsilon}_{ij} \right\rangle = Extr\ , \tag{1.7}$$

where through $\tilde{\sigma}_{ij}$ и $\tilde{\varepsilon}_{ij}$ local deviators of stresses and strains are indicated. Having decomposed in (1.6) the stress and strain tensors into deviatory and spherical components, we establish the first type of equations for the connection of macro and microstates

$$\left(\tilde{\sigma}_{ij} - \sigma_{ij}\right)\left(\varepsilon_{ij} - \tilde{\varepsilon}_{ij}\right) = 3\left(\tilde{\sigma}_0 - \sigma_0\right)\left(\tilde{\varepsilon}_0 - \varepsilon_0\right). \tag{1.8}$$

For fluctuations of the deviatory components, we take the linear dependences

$$\tilde{\sigma}_{ij} - \overline{\sigma}_{ij} = B\left(\overline{\varepsilon}_{ij} - \tilde{\varepsilon}_{ij}\right); \tag{1.9}$$

$$\overline{\sigma}_{ij} - \sigma_{ij} = B'\left(\varepsilon_{ij} - \overline{\varepsilon}_{ij}\right), \tag{1.10}$$

where B, B' – internal parameters containing information about the microscopic characteristics of subelements, which reflect the difference between stress fluctuations and strain fluctuations at the investigated structural levels.

Expressions (1.1), (1.7) – (1.10) are assumed to be valid for both reversible and irreversible deformation processes. Because of this, on the basis of relations (1.1), (1.7) – (1.10) it is possible to describe from a unified standpoint the relationship between micro and macro states during reversible and irreversible deformation of polycrystalline materials. Having decomposed the strains $\tilde{\varepsilon}_{ij}, \overline{\varepsilon}_{ij}$ into reversible $\tilde{e}_{ij}, \overline{e}_{ij}$ and irreversible $\tilde{p}_{ij}, \overline{p}_{ij}$ components – taking into account the accepted definition of a subelement ($\tilde{p}_{ij} = \overline{p}_{ij}$),

$$\tilde{\varepsilon}_{ij} = \tilde{e}_{ij} + \tilde{p}_{ij} = \tilde{e}_{ij} + \overline{p}_{ij}; \quad \overline{\varepsilon}_{ij} = \overline{e}_{ij} + \overline{p}_{ij}; \quad \varepsilon_{ij} = e_{ij} + p_{ij}, \tag{1.11}$$

relation (1.9), represent in the form

$$\tilde{\sigma}_{ij} - \overline{\sigma}_{ij} = B(\overline{e}_{ij} - \tilde{e}_{ij}). \tag{1.12}$$

Note that in multi-element models, averaging is performed not over the volume, but over the set of realizations, i.e. the use of the ergodic hypothesis is considered legitimate. The values $\overline{t}_{ij}, \overline{d}_{ij}$ are determined by averaging over the orientation factor of the crystal Ω

$$\overline{t}_{ij} = \left\langle \tilde{t}_{ij} \right\rangle_{\Omega}; \quad \overline{d}_{ij} = \left\langle \tilde{d}_{ij} \right\rangle_{\Omega}; \quad \overline{\sigma}_{ij} = \left\langle \tilde{\sigma}_{ij} \right\rangle_{\Omega}; \ \dots\ . \tag{1.13}$$

For macroscopic quantities t_{ij}, d_{ij} we accept the ratios

$$t_{ij} = \int_0^1 \overline{t}_{ij}(\tau) d\psi(\tau) = \int_{\tau_0}^{\tau_{\max}} \overline{t}_{ij}(\tau) y(\tau) d\tau; \quad d_{ij} = \int_0^1 \overline{d}_{ij}(\tau) d\psi(\tau) = \int_{\tau_0}^{\tau_{\max}} \overline{d}_{ij}(\tau) y(\tau) d\tau, \tag{1.14}$$

where $\psi(\tau)$ – integral distribution function of initial ultimate elastic strains, $y(\tau)$ – distribution density of ultimate elastic strains τ, $\tau_{\max}$, τ_0 – the largest and smallest elastic limits of the subelements, respectively.

Taking into account the equality $\tilde{p}_{ij} = \overline{p}_{ij}$ and (1.13), (1.14), we take the expression for the extremum of the discrepancy between the macroscopic measure and the appropriate average value of the microscopic analogue (1.7) in the form

$$\Delta = \Delta' + \Delta'' = Extr; \tag{1.15}$$

$$\Delta' = \left\langle \left\langle \tilde{\sigma}_{ij} \tilde{e}_{ij} \right\rangle_{\Omega} - \overline{\sigma}_{ij} \overline{e}_{ij} \right\rangle_{\Psi}; \quad \Delta'' = \left\langle \overline{\sigma}_{ij} \overline{\varepsilon}_{ij} \right\rangle_{\psi} - \sigma_{ij} \varepsilon_{ij}. \tag{1.16}$$

In formulas (1.16) $\langle . \rangle_{\Omega}$ – sign of averaging over the orientation factor of the crystal lattice Ω, a $\langle . \rangle_{\Psi}$ – by scatter parameter τ.

§2. Analyzing model behavior in disconnected substitution.

Based on the general expression for the discrepancy (1.15), taking into account equations (1.10), (1.12) and the thermorheological characteristics of the elements of the structure, it is possible to take into account the influence of the interaction of properties at different scales of the material. To assess this influence, consider the behavior of the model in an uncoupled substitution. In this approximation, it is assumed that

$$\Delta' = \left\langle \left\langle \tilde{\sigma}_{ij} \tilde{e}_{ij} \right\rangle_{\Omega} - \overline{\sigma}_{ij} \overline{e}_{ij} \right\rangle_{\psi} = Extr; \quad \Delta'' = \left\langle \overline{\sigma}_{ij} \overline{\varepsilon}_{ij} \right\rangle_{\psi} - \sigma_{ij} \varepsilon_{ij} = Extr. \tag{2.1}$$

Expressions for the macroscopic shear modulus and discordance Δ' in the reversible deformation region, for single-phase polycrystals with a cubic lattice, were obtained in [4].

$$G = C_{44} \frac{5 + (2 + 3A)b}{3 + 2A + 5Ab}; \quad A = \frac{2C_{44}}{C_{11} - C_{12}}; \quad b = \frac{B}{2C_{44}}; \tag{2.2}$$

$$\Delta' = \frac{-6(A-1)^2 b \sigma_{ij} e_{ij}}{(3 + 2A + 5Ab)\left[5 + (2 + 3A)b\right]} = Extr. \tag{2.3}$$

Here C_{11}, C_{12}, C_{44} – crystal elasticity constants; A – crystal anisotropy factor. Based on (2.2) and (2.3), under the condition $\sigma_{ij} e_{ij} = \text{const}$, the calculation formulas were obtained for G and b [4]

$$b = \sqrt{\frac{2A + 3}{A(3A + 2)}}; \quad G_M = \sqrt{G_V G_R}; \quad G_V = C_{44} \frac{3A + 2}{5A}; \quad G_R = C_{44} \frac{5}{2A + 3}, \tag{2.4}$$

where G_V – shear modulus obtained by Voigt [20] in 1928 as part of the approximation $\tilde{d}_{ij} = d_{ij}$; G_R – shear modulus obtained by Reuss [18] in 1929 as part of the approximation $\tilde{t}_{ij} = t_{ij}$. According to (2.4), it follows that the macroscopic shear modulus found on the basis of the principle of extremum discrepancy of measures (2.1) is equal to the geometric mean value of the shear modulus obtained in two limiting cases: a homogeneous stressed and a homogeneous strain state. The numerical studies carried out in [5] show that a simple formula for calculating the macroscopic shear modulus (2.4), presented in the form $G = G_M = \sqrt{G_V G_R}$, is in good agreement with the experimental data in the case of polycrystalline materials with a lower symmetry of the crystal lattice. Note that in general

$$G_V = (3C_{ijij} - C_{iijj})/30; \ K_V = C_{iijj}/3; \ C_{ijij} = C_{11} + C_{22} + C_{33} + 2(C_{44} + C_{55} + C_{66}); \ldots$$

$$G_R = 7{,}5\big/(3S_{ijij} - S_{iijj}); \quad K_R = 3/S_{iijj}; \quad S_{iijj} = S_{11} + S_{22} + S_{33} + 2(S_{23} + S_{31} + S_{12}); \ldots$$

$$C_{ijpq} S_{pqnm} = I_{ijnm}; \quad G_M = \sqrt{G_V G_R}; \quad K_M = \sqrt{K_V K_R}. \tag{2.5}$$

To construct an expression for the extremum of the discrepancy between measures (2.1) in the irreversible region, it is first necessary to formulate the physical relations for the subelements. As in [3 – 5, 17], we will formulate a local relationship not between stresses and irreversible strains, but between reversible and irreversible strains. According to the law of the central increment proposed in [4], the limiting elastic deformations of subelements can be represented as the sum of two independent parts

$$e_{ij} = \tau_{ij} + s_{ij}, \tag{2.6}$$

where $\overline{\tau}_{ij}$ – components of the deviator of ultimate elastic deformations of subelements in a structurally stable state; $\overline{s}_{ij}$ – increment of the components of the deviator of ultimate elastic deformations of subelements as a result of a change in the structure during irreversible deformation. The transition of subelements in the annealed state $(\overline{s}_{ij} = 0)$ of the material from a reversible state to an irreversible one is determined by the criterion: $\overline{e}_{ij}\overline{e}_{ij} - \tau^2 = 0$, $\tau^2 = \tau_{ij}\tau_{ij}$, from which it can be seen that τ is the initial elastic limit of the subelement, which is assumed to depend on temperature T and the average rate of irreversible deformations $-\gamma$

$$\gamma = \frac{1}{\psi'} \int_0^{\psi'} \sqrt{\dot{\overline{p}}_{ij} \dot{\overline{p}}_{ij}}\, d\psi, \tag{2.7}$$

where the top dot denotes the time derivative of irreversible deformation, ψ' – is the current weight of irreversibly deformable subelements. Then

$$\tau = \tau(\psi, \Theta); \ \Theta = \Theta(\gamma, \dot{T}) \quad 0 \le \psi \le 1. \tag{2.8}$$

When writing (2.8), the relationship between the influence of the change in speed and the temperature established in [21] was taken into account, with the difference that not the rate of general strain $\dot{\varepsilon}$, but the average rate of irreversible strain over a subset of subelements loaded beyond the yield point γ (2.7) is chosen as the speed parameter. The component $\overline{s}_{ij}$ associated with the change in the structure of the material characterizes the hardening of the subelement, which consists of the isotropic part, and the kinematic hardening – r_{ij} :

$$\dot{\overline{s}} = \begin{cases} a_0 \dot{\overline{\lambda}}, \overline{s} < x(\psi, \Theta), \\ \dot{x}(\psi, \Theta), \overline{s} = x(\psi, \Theta), \end{cases} \qquad r_{ij} = a_r p_{ij}\,. \tag{2.9}$$

Here a_0 – the strengthening isotropic coefficient; a_r – kinematic strengthening. Under the assumption of elastic isotropy of subelements, relation (1.9) under proportional loading

$$\frac{\sigma_{ij}}{\sigma} = \frac{\varepsilon_{ij}}{\varepsilon} = \frac{p_{ij}}{p}; \quad \sigma = \sqrt{\sigma_{ij}\sigma_{ij}}; \ \varepsilon = \sqrt{\varepsilon_{ij}\varepsilon_{ij}}; \ p = \sqrt{p_{ij} p_{ij}}, \tag{2.10}$$

can be represented as

$$\overline{e}-e=b'\left(\varepsilon-\overline{\varepsilon}\right)=m(p-\overline{p});\quad b'=\frac{B'}{2G};\quad m=\frac{b'}{b'+1}. \tag{2.11}$$

Here through $\overline{e}=\sqrt{\overline{\sigma}_{ij}\overline{\sigma}_{ij}}\Big/2G$ and $e=\sqrt{\sigma_{ij}\sigma_{ij}}\Big/2G$ the reversible/elastic deformations of the subelements and the body element, respectively, are indicated. If, along with the individual strengthening of the subelements, hidden strengthening is also taken into account, then the ultimate elastic deformations of the subelements, on the linear section of the strengthening, can be represented as

$$\overline{e}=\overline{\sigma}/2G=\tau+a\overline{p}+a_0p;\ a=\chi/(1-\chi);\ a_0=\chi_0/(1-\chi_0). \tag{2.12}$$

According to (2.12) hidden strengthening – a_0p it is the same for all multiple subelements, regardless of which area of deformation (reversible or irreversible) the separate subelement is loaded.

On the basis of (2.11) and (2.12), we establish formulas for the moduli of deviators of reversible and irreversible deformations in subelements

$$\overline{e}(z,z',m)=\begin{cases}\dfrac{mz+az'}{m+a}+\tau_0+a_0p,\ z<z',\\ z'+\tau_0+a_0p,\ z\ge z';\end{cases}\qquad \overline{p}(z,z',m)=\begin{cases}\dfrac{z'-z}{m+a},\ z<z',\\ 0,\ z\ge z';\end{cases} \tag{2.13}$$

$$z=\tau-\tau_0;\quad z'=\tau'-\tau_0;\quad \tau_0=R(\tau_0'+k_sd^{-1/2});\quad \tau'=e+(m-a_0)p. \tag{2.14}$$

Here τ' – yield strength in the bordering subelement (separates the zone of irreversibly deformed subelements from the reversible one); τ_0 – the lowest yield strength in the system of subelements, which is assumed to depend on the grain size d and the average orientation factor R – for the face-centered cubic lattice $R=3{,}1$, volumetrically centered cubic lattice $R=2{,}9$, for hexagonal densely packed lattice $R=6{,}5$ [14].

Considering (2.14) in (1.14), (1.15) and integrating over the spread parameter z, we find

$$p=\frac{\Phi(z',\gamma,T)}{m+a};\quad \Phi(z',\gamma,T)=\int_0^{z'}(z'-z)y(z,\gamma,T)dz; \tag{2.15}$$

$$e=\tau_0+z'-\frac{m-a_0}{m+a}\Phi(z',\gamma,T);\qquad \sigma=2Gf(\varepsilon,\gamma,T). \tag{2.16}$$

There is also a way to build a function $e=f(\varepsilon,\gamma,T)$ based on deformation diagrams obtained at various constant values of state parameters $T=\text{const},\ \gamma=\text{const}$. In [17] it was established that in experiments on the proportional loading of tubular samples by tensile force and internal pressure at different fixed values of temperature and speed of longitudinal deformation (movement of grip) $\dot{d}_{zz}=\text{const},$ the average speed of irreversible deformation (2.7) does not change during loading $\gamma=\text{const}.$ The orientation of the linear trajectory of the load in the coordinates of the axial t_{zz} and circumferential $t_{\varphi\varphi}$ stresses and the value of the average rate of irreversible strain γ are determined by the expressions

$$t_{\varphi\varphi}=\frac{2K-B'}{K+B'}t_{zz};\quad \gamma=\frac{1-\chi}{B'+2G\chi}\sqrt{2(K^2+B'^2-KB')}\left|\dot{d}_{zz}\right|.$$

Thus, to determine the orientation of the loading trajectory in the space of axial and circumferential stresses and the value of the speed parameter $\gamma,$ it is necessary to know the values of the bulk modulus of elasticity – $K,$ the shear modulus – G the coefficient of individual strengthening of the subelements χ and the parameter of the kinematic interaction scheme between the subelements B' – ratio (1.10).

If on the basis of the deformation diagrams obtained in the specified experiments it is required to be determined $\sigma = \sigma(t)$ according to the data $\varepsilon = \varepsilon(t),$ $T = T(t),$ then the equation of state is represented as [17]

$$\sigma = 2Gf(\varepsilon, \gamma, T); \quad \gamma_0 = \gamma_{/t=0} = \left(\dot{\varepsilon}(0) - \tau_{0,T}\dot{T}\right)\Big/(m+a); \tag{2.17}$$

$$\dot{\gamma} = \left[\dot{\varepsilon} - \frac{(m+a)\gamma}{m - a_0 + (1 - m + a_0)f_{,\varepsilon}}\right]\frac{1 - f_{,\varepsilon}}{f_{,\gamma}} - \frac{f_{,T}}{f_{,\gamma}}\dot{T}. \tag{2.18}$$

Integrating (2.18) under the specified initial condition, we establish the law of the speed parameter change $\gamma = \gamma(t),$ and then on the basis of (2.17) we determine the deviator modulus of the stress tensor $\sigma = \sigma(t),$ and from (2.10) its components. It should be noted that the defining equations (2.17), (2.18) describe monotonous processes of irreversible deformation of the body element when the external influence leads to active loading in the entire subset of irreversibly deformed subelements. Conditions of monotonic loading are shown in [17].

Equations (2.17), (2.18) allow to reveal important consequences of the behavior of the material in experiments with constant speed of the deviator modulus of the deformation tensor. In these experiments according to (2.18) (with isothermal loading) the speed parameter decreases during exposure within the limits: $\gamma = \dot{\varepsilon}/(m+a) \div \dot{p}.$ With small values of the parameter m, at some point in time, the rate of hardening of the body element as a result of the increase in irreversible deformation and loosening thanks to the reduction of the yield points of the subelements are balanced, then

$$\dot{\sigma}/2G = f_{,\varepsilon}\dot{\varepsilon} + f_{,\gamma}\dot{\gamma} = 0. \tag{2.19}$$

Considering expressions (2.17), (2.18) and equality $\dot{\varepsilon} = (m+a)\gamma_0$ in (2.19), we find

$$f_{,\varepsilon}\gamma_0 + \left(\gamma_0 - \frac{\gamma}{m - a_0 + (1 - m + a_0)f_{,\varepsilon}}\right)(1 - f_{,\varepsilon}) = 0. \tag{2.20}$$

Since the inequality follows from (2.20) on the whole area of irreversible deformation with $\dot{\varepsilon} = \text{const},$ $\gamma \le \gamma_0,$ from (2.20) follows the inequality

$$f_{,\varepsilon} < \frac{1 - m + a_0}{2 - m + a_0} \approx \frac{1}{2 + b'}; \quad m = \frac{b'}{1 + b'} \quad b' > 0, a_0 << m. \tag{2.21}$$

Consequently, the appearance of a yield tooth in materials sensitive to the rate of deformation is impossible without a preliminary increase in stress at the initial stage of yielding in experiments with $\dot{\varepsilon} = \text{const}.$ According to (2.21), the tangential shear modulus before the appearance of the yield tooth is at least twice less than in the elastic region. If the reverse task is set: the determination of the strain $\varepsilon = \varepsilon(t)$ process according to the given parameters $\sigma = \sigma(t),$ $T = T(t),$ then the data obtained in the specified experiments can be conveniently presented in the form $\varepsilon = e + F(e, \gamma, T),$ $e = \sigma/2G.$ In this case, the differential equation for the speed parameter γ has the form [17]:

$$\dot{\gamma} = \left[\frac{(m+a)\gamma}{1 + (m - a_0)F_{,e}} - \frac{\dot{\sigma}}{2G}\right]\frac{F_{,e}}{F_{,\gamma}} - \left(F_{,T} - F_{,e}\frac{\sigma G_{,T}}{2G^2}\right)\frac{\dot{T}}{F_{,\gamma}}. \tag{2.22}$$

The unknown parameter $m = B'/(B'+2G)$ appearing in the system of defining equations (2.17) – (2.21) is determined, in an unrelated substitution, on the basis of (2.1), which, taking into account (2.11), can be represented as

$$\Delta'' = 2G\frac{b'}{(1+b')^2}\left[\langle \overline{p}\rangle^2 - \langle \overline{p}^2\rangle\right]; \quad b' = \frac{B'}{2G}. \tag{2.23}$$

Expression (2.23) with regard to (2.11), (2.13) can also be written in two interesting forms

$$\Delta'' = 2Gb'\left(\frac{1-\chi}{b'+\chi}\right)^2\left[\langle \tau'-\tau\rangle_{\psi'}^2 - \left\langle(\tau'-\tau)^2\right\rangle_{\psi'}\right]; \tag{2.24}$$

$$\Delta'' = 2G\frac{(1-\chi)b'}{(\chi+b')(1+b')}\left[\langle \tau'-\tau\rangle_{\psi'}\langle \overline{p}\rangle_{\psi'} - \langle(\tau'-\tau)\overline{p}\rangle_{\psi'}\right], \tag{2.25}$$

where $\langle . \rangle_{\psi'}$ – sign of averaging over a subset of irreversibly deformed subelements. Quantities

$$\langle \overline{p}\rangle^2 - \langle \overline{p}^2\rangle; \quad \langle \tau\rangle_{\psi'}^2 - \langle \tau^2\rangle_{\psi'}; \quad \langle \tau\rangle_{\psi'}\langle \overline{p}\rangle_{\psi'} - \langle \tau\overline{p}\rangle_{\psi'},$$

in formulas (2.23) – (2.25) have different physical meanings. The extremum of the inconsistency of measures should be established under certain physical conditions. If we assume that the current extreme inconsistency of measures is achieved under the condition that one of the listed values is independent of the parameter b', we obtain the following values:

$$b' = 1; \quad \langle \overline{p}\rangle^2 - \langle \overline{p}^2\rangle = \varphi(p) \le 0; \tag{2.26}$$

$$b' = \chi; \quad \langle \tau'\text{-}\tau\rangle_{\psi'}^2 - \left\langle(\tau'\text{-}\tau)^2\right\rangle_{\psi'} = h(\tau') \le 0; \tag{2.27}$$

$$b' = \sqrt{\chi}; \quad \langle \tau'-\tau\rangle_{\psi'}\langle \overline{p}\rangle_{\psi'} - \langle(\tau'-\tau)\overline{p}\rangle_{\psi'} = r(p,\tau') \le 0\,. \tag{2.28}$$

The case $b' = 1$ is close to the value obtained in the elastic region, however, it leads to overestimated internal stresses during irreversible strain. The variant $b' = \chi \sim 10^{-4} \div 10^{-2}$ leads to results close to a homogeneous stress state. The case $b' = \sqrt{\chi}$ corresponds to the geometric mean of the variants: $b' = 1$, $b' = \chi$. In this case, as shown in [17], the component $\langle \tau'-\tau\rangle_{\psi'}\langle \overline{p}\rangle_{\psi'} - \langle(\tau'-\tau)\overline{p}\rangle_{\psi'}$ for the mismatch of measures Δ'' can be expressed in terms of the macroscopic quantities observed in the experiments,

$$\langle \tau'-\tau\rangle_{\psi'}\langle \overline{p}\rangle_{\psi'} - \langle(\tau'-\tau)\overline{p}\rangle_{\psi'} = 2\int_0^{\sigma} p(\sigma,\gamma,T)d\sigma - 2G(a+a_0)p^2, \tag{2.29}$$

which are not subject to change. Taking into account (2.29), the discrepancy can be represented as

$$\Delta'' = \frac{-2(1-\chi)b'}{(\chi+b')(1+b')}\left(\int_0^{\sigma} p(\sigma,\gamma,T)d\sigma - G(a+a_0)p^2\right) = Extr. \tag{2.30}$$

Note that the integral $\int p\,d\sigma$ is calculated for the current values of the state parameters. Attention should also be paid to the clear physical meaning of the components appearing in (2.29). The value $\langle \tau\overline{p}\rangle_{\psi'}$ represents that part of the work of deformation that is dissipated in the form of heat, and $\langle\tau\rangle_{\psi'}\langle\bar{p}\rangle_{\psi'}$ – the macroscopic measure of uncompensated heat. A more detailed analysis of the physical meaning $\langle\tau'-\tau\rangle_{\psi'}\langle\bar{p}\rangle_{\psi'}-\langle(\tau'-\tau)\bar{p}\rangle_{\psi'}$ of the quantity shows that the difference between the average measure of uncompensated heat and the corresponding macroscopic measure is part of the latent elastic energy of deformation of the body element. Thus, the difference between the two measures of uncompensated heat represents the latent elastic strain energy.

Taking into account (2.29), inequality (2.21) can be concluded: based on the given macroscopic constitutive equations obtained by analyzing the model in an uncoupled substitution of the discrepancy extremum Δ', Δ'', it is possible to describe a wide range of phenomena observed in experiments under nonisothermal loading of materials with monotonic strain diagrams. Problems arise when describing from a unified standpoint the behavior of materials with monotonic and nonmonotone deformation diagrams, as well as when describing complex processes occurring at the initial stage of irreversible deformation and destruction.

§3. Analyzing the behavior of a model in a coupled measure mismatch substitution.

Relationship equations (1.12) establish the relationship between fluctuations of stresses and reversible strains in the structure of a subelement, and equations (1.10) – fluctuations of stresses and strains in a system of subelements. In an uncoupled substitution, the internal parameters B and B', are determined on the basis of (2.1) as independent quantities. Because of this, the mutual influence of stress fluctuations and strain fluctuations at the considered structural levels is not taken into account. In the coupled substitution, it is necessary to set the relation $B\sim B'$. In [16], the simplest relation was considered. Then expressions (1.9), (1.10) can be represented as a single constraint equation

$$\tilde{\sigma}_{ij}-\sigma_{ij}=B(\varepsilon_{ij}-\tilde{\varepsilon}_{ij}). \tag{3.1}$$

In case (3.1), the relation for the extremum of the mismatch of measures (1.16) follows directly from expression (1.7)

$$\left\langle\left\langle\tilde{\sigma}_{ij}\tilde{\varepsilon}_{ij}\right\rangle_{\Omega}\right\rangle_{\psi}-\sigma_{ij}\varepsilon_{ij}=Extr. \tag{3.2}$$

Note that in (2.4) the parameter B is expressed in terms of the dimensionless parameter $b=B/2C_{44}$, and in (2.11), in terms of the dimensionless parameter $b'=B'/2G$. If $B=B'$, then $b'=bC_{44}/G$. In this paper, we consider the variant of the equality of dimensionless parameters

$$b'=b;\quad B'=BG/C_{44}. \tag{3.3}$$

It should be noted that the formulas for the discrepancy between measures (2.3) and (2.30) include macroscopic quantities observed in experiments

$$u_e=\sigma_{ij}e_{ij}=2Ge^2;\quad u_p=2\int_0^{\sigma}p(\sigma,\gamma,T)d\sigma-2G(a+a_0)p^2=2G\left(\langle\tau\bar{p}\rangle_{\psi'}-\langle\tau\rangle_{\psi'}\langle\bar{p}\rangle_{\psi'}\right), \tag{3.4}$$

which, when determining the extremum of the discrepancy between measures (1.15), are assumed to be independent of the parameter b. Then, taking into account the assumptions made, the expression for the discrepancy between measures (1.15) can be represented as

$$\Delta_{e,b}+\Delta_{p,b}=0; \tag{3.5}$$

$$\Delta_{e,b}=\frac{\partial\Delta_e}{\partial b}=\frac{-30(A-1)^2\left[3+2A-A(2+3A)b^2\right]u_e}{(3+2A+5Ab)^2\left[5+(2+3A)b\right]^2}; \tag{3.6}$$

$$\Delta_{p,b}=\frac{\partial\Delta_p}{\partial b}=\frac{-(1-\chi)(\chi-b^2)u_p}{(b+1)^2(b+\chi}. \tag{3.7}$$

When writing (3.6), (3.7), expressions (2.4), (2.34) and (2.12), (3.3), (3.4) were taken into account.

In the case of analyzing the behavior of a model with a variable parameter b, it is convenient to use formulas (1.14), (1.15), (2.14), (2.15), (3.4). To calculate the quantities u_e, u_p relations (3.4), taking into account (1.14), (1.15) and (2.14), (2.15), we represent in the form

$$u_p = 2G\frac{\chi+b}{(1-\chi)(1+b)}\left[\left(\int_0^{z'}(z'-z)y(z,\Theta)dz\right)^2 - \int_0^{z'}(z'-z)^2 y(z,\Theta)dz\right]; \tag{3.8}$$

$$u_e \approx 2G\left[\tau_0 + \int_0^{z'} zy(z,\Theta)dz + z'\left(1-\int_{z'}^{\infty} y(z,\Theta)dz\right)\right]^2. \tag{3.9}$$

To simplify the analysis of the interactions occurring at the levels of material particles that are part of the subelements and in the system of subelements, when writing (3.9), we neglected the influence of the hardening effect on the value u_e. In this approximation, equation (3.5) is composed of two terms. In one, only quantities A, b, χ characterizing the properties of material particles (A, χ) and the state of kinematic relations appear – b (both at the level of the system of subelements and at the level of material particles)

$$M(A,\chi,b) = \frac{(\chi+b)^{1,5}(1+b)^{0,5}}{(5Ab+3+2A)[5+(2+3A)b]}\sqrt{\frac{30(A-1)^2(3+2A-A(2+3A)b^2)}{(1-\chi)(b^2-\chi)}}, \tag{3.10}$$

and in another $y(z,\Theta)$ – distribution density of ultimate elastic strains $\tau = \tau_0 + z$ depending on state parameters and grain diameter $\Theta = \Theta(d,\gamma,T)$

$$V(z',\Theta) = \frac{\sqrt{\left(\int_0^{z'}(z'-z)y(z,\Theta)dz\right)^2 - \int_0^{z'}(z'-z)^2 y(z,\Theta)dz}}{\tau_0 + \int_0^{z'} zy(z,\Theta)dz + z'\int_{z'}^{\infty} y(z,\Theta)dz}. \tag{3.11}$$

Then the equation connecting the inhomogeneity of deformation and loading in a representative volume (3.5) with the physical characteristics of material particles can be represented as

$$M(A,\chi,b) = V(z',\Theta). \tag{3.12}$$

In what follows, expression (3.12) will be called the constitutive equation of the relationship between properties and inhomogeneity of stresses and strains in a representative volume. According to (3.10), the admissible limits of b parameter change were set from

$$(3+2A-A(2+3A)b^2 \geq 0; \quad b^2-\chi \geq 0; \quad \sqrt{\chi} \leq b \leq \sqrt{\frac{3+2A}{A(2+3A)}}. \tag{3.13}$$

For given A, χ for each parameter b value in (3.10), based on (3.12), taking into account (3.11), we determine z', and on its basis from (2.15), (2.16) we determine the relationship between macroscopic stresses and strains. At the same time, attention should be paid to the complex nature of the change in the function $M(A,\chi,b)$, which reflects the most important qualities of the behavior of the material. Fig. 1 shows diagrams $M(A,\chi,b) = M(\chi,b)$ for one value of the anisotropy coefficient A and three values of the hardening coefficient χ. From the diagrams shown in Fig. 1, one can notice not only the quantitative but also the qualitative influence of the values of the parameters of the material structure A, χ on the behavior of the model. The function $M(A,\chi,b)$ in the interval (3.13) has one (curve $M(\chi_0,b)=M(2{,}4,\chi,b)$) or two inflection points (curve $M(\chi_2,b)=M(2{,}4,\chi,b)$). At two inflection points, two extrema are found on the graph (Fig. 1). In addition, there is a critical state in which (curve $M(2{,}4,\chi,b)=M(\chi_1,b)$)

$$\frac{\partial M(A,\chi,b)}{\partial b}=0;\quad \frac{\partial^2 M(A,\chi,b)}{\partial b^2}=0. \tag{3.14}$$

As a result of a detailed numerical study of conditions (3.14), for the variant $b'=b$, $B'=BG/C_{44}$, the following relationship was established between the parameters and in the state separating the qualitative behavior of the material

$$\chi_*(A)\approx 4\cdot 10^{-3}(2-A^{0{,}47})\quad 1\le A\le 3. \tag{3.15}$$

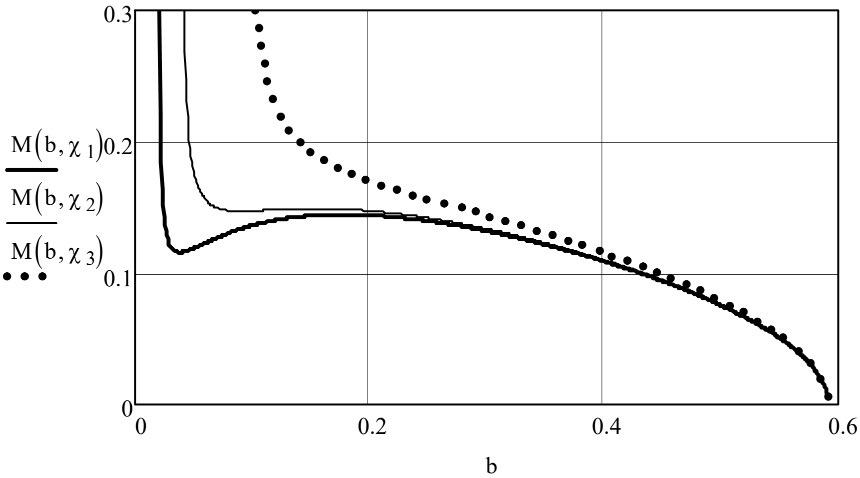

Fig. 1

Thus, if the hardening coefficient of subelements $\chi>\chi_*(A)$ from (3.10) – (3.12), (2.15), (2.16) it follows that the material deformation diagram is monotonic. If $\chi<\chi_*(A)$ then the relaxation of the kinematic bonds between the subelements, at the initial stage of the irreversible flow proceeds with such intensity that unloading occurs in a part of the irreversibly deformed subelements. Because of this, a yield tooth appears on the loading diagram. If $\chi=\chi_*(A)$, then a yield plateau is observed on the strain diagram.

§4. Numerical study of model behavior.

An analysis of experimental diagrams of deformation of polycrystalline materials shows that the following expression can be taken as a function of the distribution density $y(z)$ of a random variable z :

$$y(z,\Theta)=\Theta^2 z e^{-\Theta z}\ ;\ \psi(z',\Theta)=\int_0^{z'} y(z,\Theta)dz=1-(1+\Theta z')e^{\Theta z'};\quad \Theta=\Theta(\gamma,T). \tag{4.1}$$

In this case, expression (3.11) can be represented as $(V(z',\Theta)\Rightarrow V(x,x_0))$

$$V(\xi,\xi_0)=\frac{\sqrt{6-4\xi+\xi^2-(6+2\xi)e^{-\xi}-\left[\xi-2+(2+\xi)e^{-\xi}\right]^2}}{\xi_0+2-(2+\xi)e^{-\xi}}\ ; \tag{4.2}$$

$$\psi(\xi)=1-(1+\xi)e^{-\xi},\ \xi=\Theta z'=\Theta(\tau'-\tau_0),\ \xi_0=\Theta\tau_0. \tag{4.3}$$

Based on (2.14), (2.15), (2.16), (4.1), taking into account the notation (4.3), we represent the relationship between reversible e and irreversible deformations p in the form

$$p(b,\chi,\xi,\Theta)=\frac{(1-\chi)(b+1)}{b+\chi}\frac{\xi-2+(2+\xi)e^{-\xi}}{\Theta}; \tag{4.4}$$

$$e(b,\chi,\xi,\Theta,\tau_0)=\frac{(1-\chi)b\left[2-(2+\xi)e^{-\xi}\right]+\chi(b+1)\xi}{(b+1)\Theta}+\tau_0. \tag{4.5}$$

Note that in (2.15), (2.16) and (4.4), (4.5) the relationship is established not between stresses and strains, but between reversible and irreversible strains. The relationship among $e\sim p$ or $e\sim\varepsilon$ makes it possible to notice important regularities in the influence of structural parameters on the behavior of materials that cannot be detected when studying deformation diagrams in coordinates $\sigma\sim\varepsilon.$ In particular, if we compare the deformation curves for various pure metals with a face-centered cubic lattice and a body-centered cubic lattice, taking into account corrections for the shear modulus and melting point, it turns out that the curves for metals with a body-centered cubic lattice lie lower than the curves for metals with face-centered cubic lattice, and the degree of hardening is also significantly lower [16]. The curves $e\sim\varepsilon$ for body-centered cubic metals, as well as for FCC metals, are very sensitive to grain size: in both cases, the finer-grained material has a higher yield strength and is more intensively hardened during deformation.

If the characteristics of crystals $(A,\chi),$ grain sizes and structural defects are known, which are reflected by the parameters – $(\tau_0,\Theta),$ on the basis of (3.12), (3.10), (4.2) we establish the relationship $\xi\sim b$, which expresses the evolution of the relaxation of kinematic bonds both at the level of material particles and at the level of the system of subelements. If the dependences $\xi\sim b,$ for the data of the characteristics of the structure are established, then on the basis of (4.4) and (4.5) we determine the dependence $e\sim p$ or $e\sim\varepsilon,$ then, using the relation $\sigma=2G(b,A)e,$ we find the dependence $\sigma\sim\varepsilon=e+p.$

The procedure for establishing a connection $\xi\sim b$ can be greatly simplified if, within the change of the variable $0\le\xi\le 8$ (according to (4.3) at $\xi>8,$ $\psi(\xi)\approx 1),$ it is taken into account that expression (4.2), with sufficient accuracy for practical calculations, can be approximated by a simple function

$$V(\xi,\xi_0)\approx V'(\xi,\xi_0)=\frac{c(\xi_0)\xi^{1,5}}{1+d(\xi_0)\xi^{1,5}}; \tag{4.6}$$

$$c(\xi_0)=\frac{V(\xi_1,\xi_0)V(\xi_2,\xi_0)(\xi_1^{1,5}-\xi_2^{1,5})}{\left[V(\xi_1,\xi_0)-V(\xi_2,\xi_0)\right](\xi_1\xi_2)^{1,5}};\ d(\xi_0)=\frac{V(\xi_2,\xi_0)\xi_1^{1,5}-V(\xi_1,\xi_0)\xi_2^{1,5})}{\left[V(\xi_1,\xi_0)-V(\xi_2,\xi_0)\right](\xi_1\xi_2)^{1,5}}. \tag{4.7}$$

Comparison of functions $V(\xi,\xi_0)$ and $V'(\xi,\xi_0)$ is shown in Fig. 2. The calculations were carried out at $\xi_1=2{,}5;\xi_2=6{,}5;\xi_0=0{,}3;\ 0{,}8.$ From Fig. 2 shows good agreement between the considered functions $V(\xi,\xi_0)$ and $V'(\xi,\xi_0).$

Substituting (4.6) into (3.12) we find the following dependence for the variable ξ

$$\xi(b,\chi,A,\xi_0)=\left[\frac{M(b,\chi,A)}{c(\xi_0)-d(\xi_0)M(b,\chi,A)}\right]^{2/3}. \tag{4.8}$$

Taking into account (4.8) in (4.4), (4.5), we represent the relationship between reversible and irreversible deformations in the following parametric form

$$p(b,\chi,A,\xi_0,\tau_0)=$$
$$=\frac{(1-\chi)(b+1)}{(b+\chi)}\frac{\xi(b,\chi,A,\xi_0)-2+(2+\xi(b,\chi,A,\xi_0))e^{-\xi(b,\chi,A,\xi_0)}}{\xi_0}\tau_0; \tag{4.9}$$

$$e(b,\chi,A,\xi_0,\tau_0)=$$
$$=\left[\frac{(1-\chi)b\left[2-(2+\xi(b,\chi,A,\xi_0))e^{-\xi(b,\chi,A,\xi_0)}\right]+\chi(b+1)x(b,\chi,A,\xi_0)}{(b+1)\xi_0}+1\right]\tau_0. \tag{4.10}$$

When proceeding to the calculation of the macroscopic modulus of the stress deviator, one should also take into account changes in the shear modulus with an increase in the number of subelements involved in the irreversible flow. According to formula (2.3), the shear modulus $G=G(b,A)$ depends on the anisotropy coefficient A and the parameter reflecting the inhomogeneity of the development of stresses and strains in the elements of the material structure b. From a physical point of view, it can be assumed that the relaxation of kinematic bonds (decrease in the parameter b) occurs only between the material particles included in the subelements involved in the irreversible flow. Then we can assume that on the basis of formula (2.3) the shear modulus is determined only in irreversibly deformed subelements, the weight of which is determined on the basis of formula (4.3) – $\psi(\xi)$, and in subelements with weight $1-\psi(\xi)$ we will assume that $G=G_M$ it is determined from formula (2.5). Based on these assumptions, we establish the following law of change in the shear modulus in irreversible deformation processes

$$G(b,\chi,A,\xi_0)=$$
$$=C_{44}\left[\sqrt{\frac{3A+2}{A(2A+3)}}-\left(\sqrt{\frac{3A+2}{A(2A+3)}}-\frac{5+(2+3A)b}{3+2A+5Ab}\right)\psi\left[\xi(b,\chi,A,\xi_0)\right]\right]. \tag{4.11}$$

The parametric relationship between the shear modulus and the accumulated irreversible strain is determined on the basis of (4.3), (4.8), (4.9) and (4.11). Since a cubic crystal does not change shape under the action of hydrostatic pressure, the average bulk modulus of a polycrystal K is equal to the value measured for a single crystal $K=\sigma_0/\varepsilon_0=C_{11}+2C_{12}$, which does not change in the process of irreversible flow. Therefore, based on the law of change in the shear modulus (4.11) and the expression for K, it is possible to establish, using well-known formulas, the patterns of change in technical elastic constants: the modulus of elasticity E and Poisson's ratio, depending on the accumulated irreversible deformation $p(b,\chi,A,\xi_0)$.

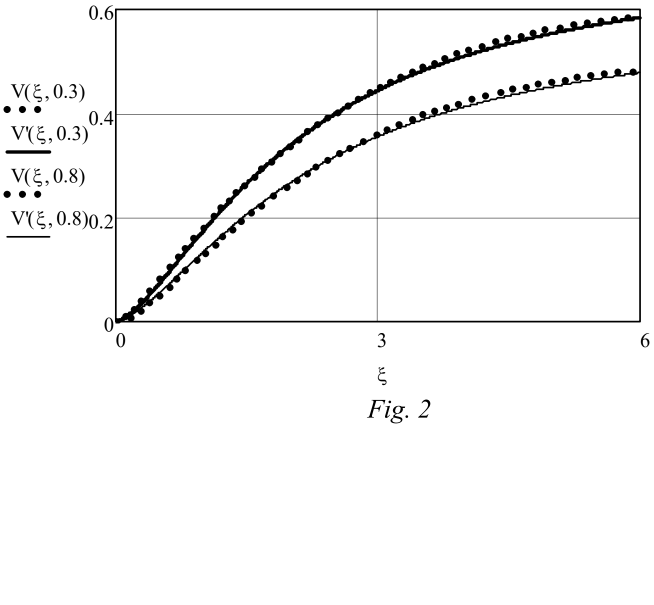

Fig. 2

In system (4.9), (4.10), the characteristics of crystals are expressed in terms of the anisotropy A and strengthening coefficients χ (in the first or second phases of deformation), and the characteristics of the granular structure of a polycrystal are expressed in terms of the average grain diameter d and density of structural defects ρ_s: $\tau_0 = \tau_0(d, \rho_s)$, $\xi_0 = \xi_0(d, \rho_s)$. The listed parameters may also depend on the state parameters γ, T. In experiments with constant state parameters $\gamma = \text{const}$, $T = \text{const}$ in the system (4.9), (4.10) there is only one variable b characterizing the inhomogeneity of deformation and loading. Therefore, for known parameters of the structure, on the basis of (4.9), (4.10) we establish the relationship between reversible and irreversible deformations $e \sim p$ or $e \sim \varepsilon$, and then, using the relation $\sigma = 2G(b, A)e$, we find the dependence $\sigma \sim \varepsilon$.

Thus, the relationship between macroscopic stresses and strains is influenced by the characteristics of crystals (A, χ) and the parameters of the function density distribution of yield strengths of subelements (ξ_0, τ_0). Based on the system of constitutive equations (3.10), (4.6) – (4.11), we consider the specific effect of each structural parameter on the polycrystal deformation diagram.

Fig. 3 shows strain diagrams $e \sim \varepsilon$:

$$e(b, \chi) \to 10^3 e(b,\ \chi,\ 2{,}6,\ 0{,}3,\ 10^{-3}) \sim \varepsilon(b, \chi) \to \varepsilon(b,\ \chi,\ 2{,}6,\ 0{,}3,\ 10^{-3})$$

obtained for three values of the hardening coefficient $\chi_1 = 10^{-4}$, $\chi_2 = 1{,}5 \cdot 10^{-3}$, $\chi_3 = 5 \cdot 10^{-3}$, at $A = 2{,}6$, $\xi_0 = 0{,}3$, $\tau_0 = 10^{-3}$. The coefficient $\chi = 10^{-4}$ corresponds to the value of the hardening coefficient at the stage of easy slip of a single crystal, and $\chi = 5 \cdot 10^{-3}$ – at the second stage of hardening (multiple slip). Note that the ratio of the hardening modulus to the shear modulus is independent of temperature, crystal orientation, and the amount of impurities. However, the experimental data presented in various works differ within the limits $\chi = 4 \cdot 10^{-3} \div 10^{-2}$. Probably, the differences are related to the peculiarities of the coordinates used in the calculations: reduced shear stress-shear strain. More convenient data are presented in [16], where the hardening parameters were obtained by stretching polycrystalline metals $t_{11} \sim d_{11}$. According to the data presented in [16], at the second stage of deformation $\chi_{11} = \dfrac{1}{E}\dfrac{dt_{11}}{dd_{11}} \approx 10^{-2}$. Based on the assumption of an elastic change in volume, the hardening modulus in coordinates $\sigma \sim \varepsilon$ is determined by the expression $\chi = 2(1+\nu)\chi_{11} / \left[3 - (1-2\nu)\chi_{11}\right]$. For Poisson's ratio $\nu = 0{,}3$, the coefficient $\chi = 0{,}0087$. It is important to note that the established theoretical value $\chi_*(A)$ (3.15), separating the zone of monotonic strain diagrams from nonmonotonic ones, lies between the experimental values of the hardening coefficients for the stages of multiple and easy slip. This fact should be considered as one of the principal methodological confirmations of the main provisions of the model under study.

From Fig. 3 shows that the numerical values of the hardening coefficient have not only a quantitative effect, but also a qualitative effect on the strain diagrams. The calculations performed show that for each value of the crystal anisotropy coefficient A there is a strengthening coefficient χ determined on the basis of formula (3.15), which separates the zone of monotonic strain diagrams from nonmonotonic ones. For, $A = 2{,}6$ the critical value is $\chi_*(2{,}6) = 1{,}5 \cdot 10^{-3}$. At $\chi > 1{,}5 \cdot 10^{-3}$, elastic strains increase monotonically with an increase in irreversible strain, and at $\chi > 1{,}5 \cdot 10^{-3}$, unloading into some subelements is observed, which leads to a decrease in macroscopic reversible strain. If $\chi > 1{,}5 \cdot 10^{-3}$, then a yield point appears on the loading diagram.

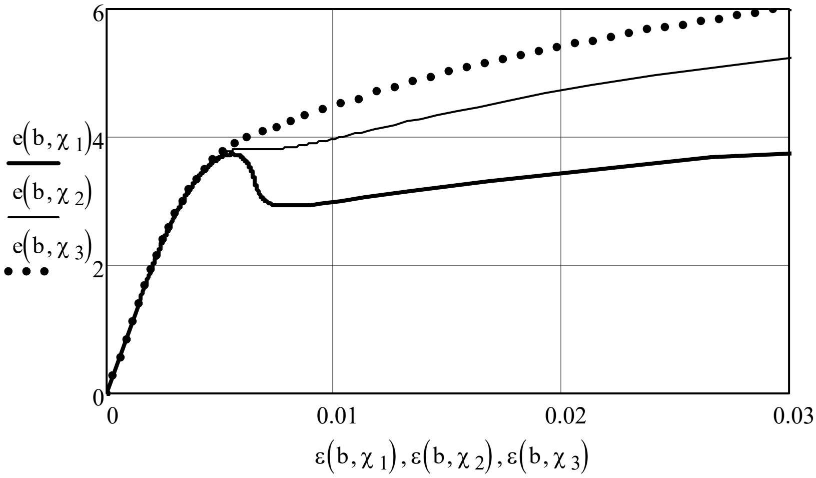

Fig. 3

Therefore, the phenomena of yield tooth, yield plateaus and monotonic diagrams are described within the framework of a single model. The transition of a new volume of material into an irreversible region of deformation is impossible without relaxation of the kinematic bonds both between material particles and between subelements. From (4.8) – (4.10) it follows that this process proceeds most intensively at the initial stage of the irreversible flow, when there is a sharp increase in deformation inhomogeneity and partial equalization of stresses. Depending on the numerical values of the structural parameters in the process of stress equalization, with a very sharp decrease in the b parameter, an active loading process continues in some subelements with an increase in irreversible macroscopic deformation, and in the other, unloading occurs. Depending on the predominance of one or another effect at the macroscopic level with the development of irreversible deformations, three options are possible: a continuous increase in stresses, a decrease or maintenance of a constant value in a certain area of deformation, after which the increase in stresses continues.

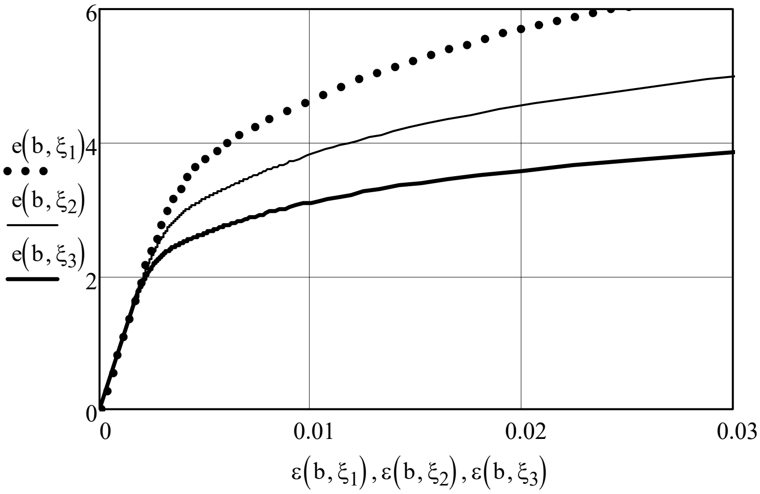

Fig.4

Influence of the function parameter of the distribution density of the initial values of the yield strengths of subelements ξ_0 on the deformation diagram, in coordinates

$$e(b,\chi) \to 10^3 e(b,\ \chi, 2{,}6, 0{,}3, 10^{-3}) \sim\ \varepsilon(b,\chi) \to \varepsilon(b,\ \chi, 2{,}6,\ 0{,}3,\ 10^{-3})$$

and three values $\xi_0 = \xi_1 = 0{,}3;\ \xi_2 = 0{,}45;\ \xi_3 = 0{,}7$ presented in Fig. 4. It can be seen from the presented diagrams that the parameter ξ_0 has a significant effect on the shape of the material deformation diagrams at all stages of the irreversible flow.

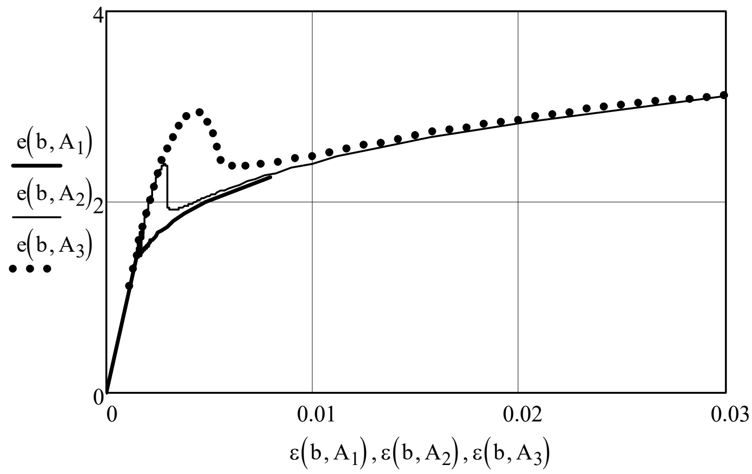

Fig.5

Fig. 5 shows the effect of the crystal anisotropy coefficient on the load diagram $e \sim \varepsilon$, in coordinates

$$e(b,\ A) \to 10^3 e(b, 10^{-4},\ A, 0{,}45, 10^{-3}) \sim \varepsilon(b,\ A) = \varepsilon(b, 10^{-4},\ A, 0{,}45, 10^{-3})$$

for a hypothetical material having the following characteristics: $\chi = 10^{-4}$, $\xi_0 = 0{,}45$, $\tau_0 = 10^{-3}$, for three values $A = A_1 = 1{,}25;\ A_2 = 1{,}8;\ A_3 = 2{,}6$. Of those presented in Fig. 5 curves, it can be seen that the crystal anisotropy coefficient has a significant effect on the deformation diagrams of the polycrystal only at the initial stage of irreversible loading. In this case, we note a strong increase in the macroscopic yield strength of the material with an increase in the anisotropy coefficient of the crystal.

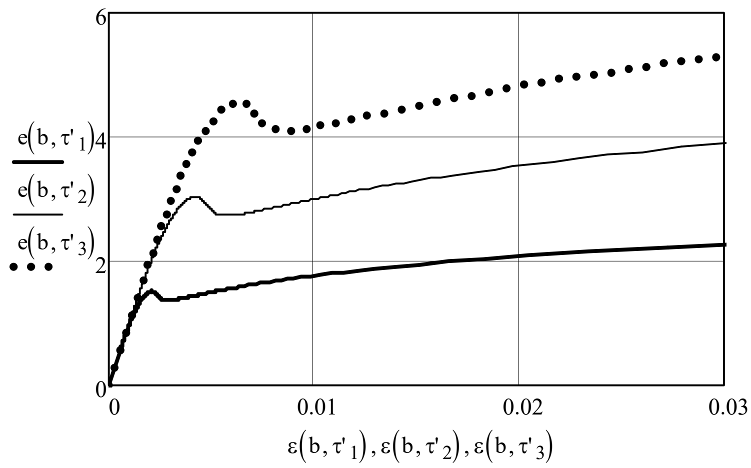

Fig. 6

Fig. 6 shows the influence of the microscopic yield stress $\tau_0 = R(\tau_0' + k_s d^{-1/2})$ on the load diagram view $e \sim \varepsilon$, in coordinates

$$e(b,\tau_0) \to 10^3 e(b, 4\cdot 10^{-4}, 2{,}4, 0{,}4, \tau_0) \sim \varepsilon(b,\tau_0) \to \varepsilon(b, 4\cdot 10^{-4}, 2{,}4, 0{,}4, \tau_0)$$

for three values $\tau_0 = \tau_1' = 0{,}5\cdot 10^{-3}, \tau_2' = 10^{-3}, \tau_3' = 1{,}5\cdot 10^{-3}$. The conducted numerical studies show the global influence of the microscopic yield strength τ_0 (depending on the grain size d) at all stages of loading the body element. At the same time, τ_0 affects the size and length of the section, which is associated with a violation of the loading monotonicity process at the initial stage of yield.

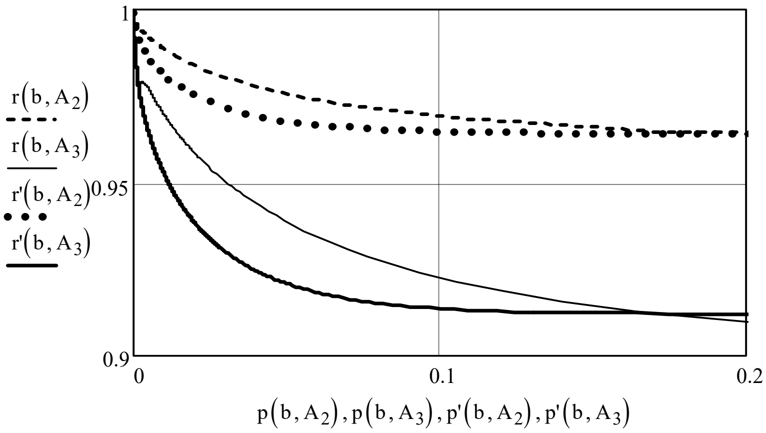

Fig. 7

Note that as the grain size decreases, the entire diagram shifts to the region of higher stresses; in this case, the values of both the upper and lower yield points also increase.

The influence of the anisotropy A and strengthening coefficients χ of the crystal on the relative change in the shear modulus $r(A,\chi) = G(b,\chi, A, 0{,}5)/G_M$ of the $p(A,\chi)$ calculated for, $A_3 = 2{,}6$, $\chi = 6\cdot 10^{-3}$, and the curves $r'(A,\chi) \sim p'(A,\chi)$ for the same values of the anisotropy coefficients A_2, A_3, but with the strengthening factor $\chi = 6\cdot 10^{-4}$. Of those presented in Fig. 7. It can be seen from curves that the anisotropy coefficient A has a significant effect on the decrease in the shear modulus of the polycrystal during irreversible flow G decreases most intensively in the initial section of irreversible deformation, and then tends to a constant value. At the same time, with a decrease χ, the tendency to a constant value of the shear modulus is achieved at higher values $p(A,\chi)$, which leads to the intersection of the curves and a qualitative change χ in the influence on the change G.

Conclusions.

The constitutive model governing equations in the coupled and uncoupled substitution of the extremum of the discrepancy of measures at the levels of material particles and systems of subelements are studied.

A constitutive equation is obtained connecting the inhomogeneities of deformation and loading in a representative volume with physical characteristics at the levels of material particles and a system of subelements. The properties of crystals are expressed in terms of the anisotropy and hardening coefficients, and the systems of subelements are expressed in terms of the parameters of the distribution density function of the initial yield strengths.

It is shown that in the reversible loading region, the relative stress fluctuations are approximately the same as the strain fluctuations. At the initial stage of the irreversible flow, there is a brusque relaxation of the kinematic bonds between material particles and between subelements, which leads to a strong increase in the inhomogeneity of strain and smoothing of stress fluctuations. With the values of the hardening coefficients characteristic of the light slip phase, in a certain area of deformation, the irreversible flow proceeds with a decrease or with a constant weight of the irreversibly deformed subelements. Then, during the loading process, the growth of the weight of irreversibly deformed particles is restored, with the same hardening coefficient.

With an increase in the anisotropy coefficient of the crystal, a strong increase in the macroscopic yield strength of the material is observed. However, outside the area of violation of the loading monotonicity, the anisotropy coefficient does not affect the shape of the deformation diagram.

In contrast to the anisotropy coefficient, the microscopic yield stress (which depends on the grain size) affects not only the magnitude of the nonmonotonic deformation region, but also beyond it. With a decrease in the grain size, the entire diagram shifts to the region of higher stresses; in this case, the values of both the upper and lower yield points also increase.

The influence of the structural parameters of a polycrystal and the magnitude of irreversible deformation on the regularity of the change in elastic constants in the process of irreversible flow is analyzed.

РЕЗЮМЕ. Розглянуто трирівневу конститутивну модель, що описує з єдиних позицій поведінку матеріалів з монотонними та немонотонними діаграмами деформування. Встановлено вплив коефіцієнтів анізотропії та зміцнення кристала, середнього значення діаметра зерен і густини розподілу дефектів структури на макроскопічну поведінку полікристалу. Для цього використано три постулати: середніх зв'язків, екстремуму невідповідності між макроскопічними мірами та їх мікроскопічними аналогами і ортогональності тензорів флуктуацій напружень та деформацій. На основі побудованої системи конститутивних рівнянь досліджено специфічний вплив структурних характеристик полікристалу на макроскопічні діаграми деформування та константи пружності матеріалу.

КЛЮЧОВІ СЛОВА: конститутивна модель, структура, кристал, полікристал, субелемент, напруження, деформація, анізотропія, зміцнення, невідповідність мір.

1. *Вильдеман В.Э., Ломакин Е.В., Третьякова Т.В.* Запаздывание текучести и пространственно-временная неоднородность пластического деформирования углеродистой стали // Известия РАН. МТТ. – 2017. – № 4. – С. 56 – 67.
2. *Гохфельд Д.Ф., Садаков О.С.* Пластичность и ползучесть элементов конструкций при повторных нагружениях. – Москва: Машиностроение, 1984. – 256 с.
3. *Марина В.Ю.* Нелокальный подход к проблеме необратимого деформирования неоднородного тела // Математические исследования. – 1987. – **94**. – С. 47 – 53.
4. *Марина В.Ю.* Принципы перехода от микро к макро напряжённо-деформированному состоянию. // Известия АН Молдовы. Серия математика. – 1998. – № 2. – С. 16 – 24.
5. *Марина В.Ю., Марина В.И.* Анализ соотношений между локальными и общими механическими параметрами, применяемыми для описания поведения поликристаллических материалов. // Металлофиз. Новейшие Технологии. – 2020. – **42**, № 3. – С. 415 – 431.
6. *Новожилов В.В., Кадашевич Ю.И.* Микронапряжения в конструкционных материалах. – Ленинград: Машиностроение, 1990. – 223 с.
7. *Трусов П.В*. Классические и многоуровневые конститутивные модели для описания поведения металлов и сплавов: проблемы и перспективы (в порядке обсуждения) // Известия РАН. МТТ. 2021. – № 1. С. 69 – 82.
8. *Трусов П.В*., *Швейкин А.И., Начаева Е.С., Волегов П.С.* Многоуровневые модели неупругого деформирования материалов и их применение для описания эволюции внутренней структуры // Физическая мезомеханика. – 2012. – **15**, № 1. – С. 33 – 56.
9. *Benedetti I., Barde F.* Modelling polycrystalline materials: an overview of three-dimensional grain-scale mechanical models // J. of Multiscale Modelling. – 2013. – **5**, N 1. – P. 1 – 51.

10. *Besseling J.F.* Theory of elastic, plastic and creep deformations of an initially isotropic material showing anisotropic strain-hardening, creep recovery and secondary creep // J. Appl. Mech. – 1958. – № 4. – P. 529 – 536.
11. *Berveiller M., Zaomi A.* An Extention of the Self-Consistent Scheme to Plastically-Flowing Polycrystals // J. Mechanics and Physics of Solids. – 1979. – **26**. – P. 325 – 344.
12. *Flipona B., Kellera C., Queyb R., Barbea F.* A Full-field Crystal – Plasticity Analysis of Bimodal Polycrystals // Int. J. Solids and Struct. – 2020. – **184**. – P. 178 – 192.
13. *Hill R*. The elastic behavior of a crystalline aggregate // Proc. Physical Soc. – 1952. – **65**, № 5. – P. 349 – 354 p.
14. *Honeycombe R.W.K.* The Plastic Deformation of Metals. – London: Edward Arnold Lid. 1968. – 408 p.
15. *Kroner E*. On the physical reality of torque stresses in continuum mechanics // Int. J. Engng. Sci. – 1963. – P. 261 – 278.
16. *Marina V.Yu., Marina V.I.* Single Approach to the Description of the Relation Between Micro-and Macrostates in Reversible and Irreversible Deformation of Polycrystals // Int. Appl. Mech. – 2021. – **57**, N 6. – P. 707 – 719.
17. *Marina V.Yu.* Equation of Elastoplastic Deformation of an Object Subject to Proportional Nonisothermic Loading // Int. Appl. Mech. – 1997. – № 2. – P. 93 – 100.
18. *Reuss A*. Berechnung der Fliesgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle // Zeitschrift fur Angewandte Mathematik und Mechanik. – 1929. – **9**, N 1. – S. 49 – 58.
19. *Shchevchenko Yu.N.* Thermoviscoelastoplastic Processes in the Deformation of Elements of a Solid (Survey) // Int. Appl. Mech. – 1994. – № 3. – P. 165 – 183.
20. *Voigt W*. Lehrbuch der Kristallphysik. – Leipzig: Teubner, 1928. – 978 s.
21. *Zener C., Hollomon J.H.* Effect of Strain Rate upon Plastic Flow of Steel // J. Appl. Phys. – 1944. – 15, N 1. – P. 22 – 32.

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