A Two-Level Elasto-Viscoplastic Model: Application to the Analysis of the Crystal Anisotropy Influence

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Abstract—Multilevel (mainly two-level) crystal plasticity models have been widely used for studying processes of inelastic deformation of polycrystalline materials over the last 15–20 years. Anisotropy of plastic strain in crystallites is usually taken into account at the mesoscale, while their elastic properties are often considered as isotropic. The purpose of this study is to assess the differences in the stress–strain characteristics (especially residual mesoscopic stress) by taking into account the anisotropy of elastic properties of materials calculated for the isothermal deformation of polycrystals with various types of crystallite lattice symmetry within a representative macroscopic volume. To this end, our results are compared with the data obtained for a material with isotropic elastic properties using the Voigt–Reuss–Hill averaging procedures. The results of the analysis for the stress–strain state of polycrystalline samples with fcc, bcc, and hcp lattices obtained in a simple shear test (up to the accumulated strain of 50%) are presented. The statistical two-level constitutive model, constructed within the geometrically nonlinear elasto-viscoplasticity theory, is used for calculations. In such constitutive models, the main fundamental relation is the law of elasticity written in the rate relaxation form in terms of the measures of the stress and strain rates, being independent of the chosen reference frame (or of the superimposed rigid motion). It is shown that the analysis of the anisotropy effect has a noticeable impact on the characteristic macroscopic volume stress–strain state only in the initial deformation stage. Subsequently, for deformations exceeding 1–1.5%, the difference becomes insignificant. At the same time, the results of calculating the residual mesoscopic stress (i.e., the stress after unloading the representative macroscopic volume), which has a significant effect on the strength characteristics of materials, with allowance for the crystal anisotropy turned out to be significantly different from those obtained under the hypothesis of isotropy.

Keywords: two-level elasto-viscoplastic model, elastic anisotropy effect, equivalent isotropic material, Voigt–Reuss–Hill averaging procedures, residual mesostress

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1. INTRODUCTION

Mathematical models with different degrees of complexity and depth are widely applied to improve existing technological processes of intense plastic deformation and develop new ones. Their most important features are constitutive models (constitutive relations) of materials, the quality of which mainly determines the adequacy of the mathematical model as a whole. It should be noted that the physical and mechanical properties of various materials are determined almost completely by their meso- and microstructure [1, 2]. In view of the aforesaid, modern models, aimed at describing and improving regimes of treatment of metals and alloys, should make it possible to trace the occurred changes in the internal structure. Multilevel (mainly two-level) models based on the introduction of internal variables and the physical theories of elasto-viscoplasticity, which have become very popular over the last decades, appear most promising for this purpose [3–9]. In such models, the mesoscopic element is a crystallite (grain or subgrain) and the macroscopic element is a representative macroscopic volume [3, 7, 8]. It should be noted that the overwhelming majority of problems arising when considering technological processes of treatment of metals and alloys are geometrically nonlinear; when constructing constitutive models, additive decomposition of the strain rate in elastic and inelastic components, obtained based on multiplicative decomposition of the gradient of site, is widely used to describe the behavior of crystallites [10–12]. Fur-
thermore, equations of a particular physical theory of elastoplasticity (elasto-viscoplasticity) are applied to determine the inelastic component of the strain rate [3, 7].

The choice of the law of elasticity plays an important role in constructing the constitutive model of a crystallite. Finite equations (i.e., in terms of the measures of the stress and strain determined in bases of the reference or unloaded configurations) can be used as such laws [13, 14]. When considering geometrically nonlinear problems, elastic relations in the rate relaxation form, stated in terms of the actual configuration, are most widely used. Note that often (especially, in the early stage of development of multilevel models) elastic deformations at the mesoscopic level were either neglected [15] or assumed to be isotropic [16], which simplifies solution of the problem, but does not have physical justification when analyzing the behavior of crystallites. This assumption is caused to some extent by the fact that there are hardly any scientific publications or handbooks containing elastic characteristics of anisotropic materials, because standard tests of structural materials (extension—compression and twisting) make it impossible to determine all the components of the their elastic constant tensor.

The rate form of the elastic defining relations is generally written as a linear or quasi-linear relationship, which does not depend on the chosen reference frame of the stress rate (as a rule, corotation derivative of the stress tensor) and the elastic component of the strain rate tensor (symmetric part of the velocity gradient). Such constitutive relations were likely introduced for the first time by Truesdell [17–19], who named them hypoelastic. However, the hypoelastic relations in the initial version could not be put into correspondence with hyperelastic physical equations; as a result, they do not satisfy additional requirements to elastic relations formulated by Xiao et al. [20–23], according to which: (i) the stress trajectory should be closed for any closed elastic strain cycle; (ii) work in any such cycle should be zero. For brevity, below we will refer to these two requirements as a condition of conservativity of elastic constitutive relations. It was also shown in the abovementioned studies that the logarithmic (Hencky) strain measure, corresponding to the actual configuration, is the only energetically conjugate (weighted Kirchhoff stress tensor) measure of deformation from the Seth–Hill strain class [24–26]; notably, the strain rate tensor is equal to the so-called logarithmic corotation derivative of the Hencky tensor [20]. Note also that the use of the constitutive hypoelastic relation with the logarithmic corotation derivative does not yield another well-known nonphysical effect: stress oscillations under monotonic simple shear strain [27, 28]. It should be noted that the proof of correctness of the hypoelastic relation reported in [20] is valid only for an isotropic material. These advantages of isotropic elastic relations likely cause their wide application (in particular, for crystallites, which appears inconsistent with the presence of anisotropy of elastic properties of real crystals (especially crystals of the middle and low symmetry classes)).

In view of the above considerations, the following question is of interest: what uncertainty to the material response is induced by replacement of the elastic-anisotropic law with the corresponding elastic isotropic law in a constitutive two-level model at the mesoscale? The purpose of this study is to analyze the influence of anisotropy of the elastic properties on the behavior of polycrystalline materials.

2. BRIEF DESCRIPTION OF THE TWO-LEVEL ELASTO-VISCOPLASTIC MODEL

The above-stated problem can be solved using the constitutive two-level statistical elasto-viscoplastic model [3]. The macroscopic element is a representative macroscopic volume of a polycrystal; the mesoscopic element is a crystallite with the isotropic or anisotropic elastic properties; it should be noted that the viscoplastic relations are formulated in terms of the shear velocities along crystallographic slip systems and, therefore, are anisotropic. The hypoelastic law was chosen to be the fundamental constitutive relation for elastic strain at the mesoscopic level. The distribution of lattice orientations of mesoscopic elements, entering the representative macroscopic volume, in the reference configuration is described by the uniform law.

When constructing constitutive models that are applicable for describing deformation processes with high gradients of displacements (geometric nonlinearity), one of the most important questions is how to decompose the motion into quasi-solid and deformation [29]; notably, the suggested decomposition should allow one to take into account the symmetry properties of crystallites. To this end, is introduced for each mesoscopic element (crystallite) an individual mobile undeformed orthogonal Cartesian coordinate system (MCS) Ox₁x₂x₃ with basis k₁, rigidly bound to one crystallographic direction and a crystallographic plane containing this direction [30]. For the coordinate system, rigidly bound with the crystallite lattice, components of the elastic constant tensor u can be assumed to be invariable. A uniform (affine) change in the configuration of each crystallite is described by the deformation gradient (transposed gradient of site) of the mesoscopic level f [26, 29]. To consider both elastic and inelastic deformations, we introduced an additional unloaded configuration, obtained from the reference configuration by transfor-
A TWO-LEVEL ELASTO-VISCOPLASTIC MODEL

formation determined by the plastic pair $P$ of the deformation gradient (or from the actual configuration using the transformation $f^{-1}$). Multiplicative decomposition of the deformation gradient $f = f^e \cdot f^p = \tilde{f}^e \cdot \mathbf{r} \cdot f^p$, proposed in [30], is used; here, $f^e$ is the elastic part of the deformation gradient, $f^p = k_k k'_0$ is the orthogonal tensor transforming the reference basis $k'_0$ of the mobile coordinate system into the current one $k$, and $\tilde{f}^e$ is the part of the deformation gradient transforming the plastically strained configuration undergone rotation into the actual configuration at the mesoscale (i.e., $\tilde{f}^e$ reflects distortion of the lattice). At this decomposition, quasi-solid motion of the crystallite is described by the rotation tensor $r$, which simultaneously determines rotation of the rigid mobile coordinate system.

Below, we present the systems of equations entering the mathematical formulation of the two-level (for macro- and mesoscopic levels) constitutive model of deformation of polycrystalline materials (from here on, macroscopic and mesoscopic parameters are denoted by corresponding capital and lowercase letters). The statistical model based on the Voigt hypothesis is used [3–6]. The complete system of equations of the mesoscopic model is as follows (number of the mesoscopic elements are omitted for brevity):

\[
\begin{align*}
\mathbf{k}^\text{cor} & \equiv \dot{\mathbf{k}} + \dot{\mathbf{k}} \cdot \mathbf{\omega} - \mathbf{\omega} \cdot \mathbf{k} = \mathbf{n} \cdot (\mathbf{l} - \mathbf{z}^\text{in} - \mathbf{\omega}), \\
\dot{\gamma}^{(k)} & = \gamma_0 (\tau^{(c)} / \tau^{(k)})^m H(\tau^{(c)} - \tau^{(k)}), \\
\tau^{(k)} & = b^{(k)} \cdot \mathbf{n}^{(k)} \cdot \mathbf{k}, \\
\tau^{(c)} & = \sum_{l=1}^{K} h^{(k,l)} \gamma^{(l)}, \\
\mathbf{z}^\text{in} & = \sum_{k=1}^{K} \gamma^{(k)} b^{(k)} \mathbf{n}^{(k)}, \\
\mathbf{l}^T & = \mathbf{l} - \mathbf{z}^\text{in}, \\
\dot{\mathbf{r}} \cdot \mathbf{r}^T & = \mathbf{\omega}.
\end{align*}
\]

Here, $\mathbf{k}$ is the weighted Kirchhoff stress tensor ($\mathbf{k} = (\det f) \sigma$, where $\sigma$ is the Cauchy stress tensor); $\mathbf{k}^\text{cor} = \dot{\mathbf{k}} + \dot{\mathbf{k}} \cdot \mathbf{\omega} - \mathbf{\omega} \cdot \mathbf{k}$ is the rate of change in the Kirchhoff stress tensor that is independent of the chosen reference frame; $\mathbf{\omega}$ is the spin tensor of the crystallite MCS, which specifies its rotation rate [30, 31]; $\mathbf{n}$ is the fourth-rank tensor of elastic properties, determined by invariable components in the basis of the rigid MCS; $\mathbf{z}^\text{in}$ is the inelastic part of the mesoscopic strain rate tensor; $\mathbf{l} = \hat{\mathbf{V}} \mathbf{V}^T$ is the transposed velocity gradient (due to the use of the Voigt hypothesis $\mathbf{l} = \hat{\mathbf{V}} \mathbf{V}^T = \mathbf{L}$, where $\mathbf{L}$ is the transposed macroscopic velocity gradient); $\dot{\gamma}^{(k)}$ is the shear rate at the $k$th slip system; $\gamma_0$ is the shear strain along the slip system when the tangential stress reaches the critical shear stress; $\tau^{(k)}$ is the working stress at the $k$th slip system; $\tau^{(c)}$ is the critical stress at the $k$th slip system; $m$ is the exponent of the strain-rate sensitivity of the material; $H(\cdot)$ is the Heaviside function; $b^{(k)}$ and $\mathbf{n}^{(k)}$ are unit vectors of, respectively, the slip direction and normal to the slip plane of the $k$th slip system (in actual configuration); and $\mathbf{r}$ is the MCS orientation tensor. Note that the tensor of elastic properties for crystallites is anisotropic in the general case, and the symmetry type is determined by the lattice; components of these tensors in the crystallographic lattice basis for various materials are known reference data.

The system of equations for the macroscopic level has the following form:

\[
\begin{align*}
\mathbf{K}^\text{cor} & \equiv \ddot{\mathbf{K}} - \mathbf{\Omega} \cdot \mathbf{K} + \mathbf{K} \cdot \mathbf{\Omega} = \mathbf{\Pi} : (\mathbf{L} - \mathbf{\Omega} - \mathbf{Z}^\text{in}), \\
\mathbf{\Pi} & = \langle \mathbf{n} \rangle, \\
\mathbf{\Omega} & = \langle \mathbf{\omega} \rangle, \\
\mathbf{Z}^\text{in} & = \langle \mathbf{Z}^\text{in} \rangle + \mathbf{\Pi}^{-1} : \langle \mathbf{n}' : \mathbf{z}^\text{in} \rangle + \mathbf{\Pi}^{-1} : \langle \mathbf{\chi}' \cdot \mathbf{\omega}' \rangle - \langle \mathbf{\omega}' \cdot \mathbf{\chi}' \rangle.
\end{align*}
\]

Here, $\mathbf{K}$ is the weighted Kirchhoff stress tensor (for the macroscopic level); $\mathbf{K}^\text{cor} = \ddot{\mathbf{K}} - \mathbf{\Omega} \cdot \mathbf{K} + \mathbf{K} \cdot \mathbf{\Omega}$ is the rate of change (corotation derivative with spin $\mathbf{\Omega}$) Kirchhoff stress tensor that is independent of the chosen reference frame; $\mathbf{\Omega}$ is the macroscopic MCS spin tensor; $\mathbf{\Pi}$ is the tensor of effective elastic properties;
$Z'$ is the inelastic component of the indifferent measure of the strain rate $Z = \hat{\nabla}\nu^T - \Omega$; $L = \hat{\nabla}\nu^T$ is the velocity gradient defined in the actual configuration; $\langle \cdot \rangle$ is the averaging operator over the representative macroscopic volume, and $a'$ denotes deviation of the tensor characteristic $a$ in the crystallite under consideration from the value averaged over the representative macroscopic volume [3, 30, 31]. The latter relation in (2) was obtained upon matching of the constitutive relations for the meso- and macroscales (i.e., establishment of the constitutive relation at the macroscopic level by averaging the corresponding relation at the mesoscopic level [3]).

As one can easily see, the two-level mathematical model described by the systems of Eqs. (1) and (2) is strongly nonlinear; hence, a corresponding procedure is required for its implementation. Let us briefly describe the algorithm of implementation of the model.

The problem of analyzing the stress–strain state of a representative macroscopic volume can be solved using a step-by-step procedure; the input parameters are specified components (in the basis of the laboratory coordinate system (LCS)) of the velocity gradient tensor at the beginning of a step. The algorithm at each step is implemented in three stages (at first, in a cycle over mesoscopic elements): finding of the solution in terms of velocities, integration of the system of equations of the model from the point of view of the MCS, and redetermination of all the model parameters because the crystallite orientation changes by the end of the time step (note that all material parameters are assumed to be “frozen” in the MCS). Afterwards, the found characteristics are averaged, and the related parameters at the macroscale are sought; then the algorithm passes to the next time step. The algorithm of implementation of the two-level elasto-viscoplastic model was described in detail in [3].

As was noted above, it was assumed in many publications on two-level models that a material is elastically isotropic and has some averaged properties. In this study, we consider polycrystalline materials consisting of homogeneous crystallites with identical elastic properties. The corresponding isotropic medium is considered to be a medium with elastic properties “spread” over the representative macroscopic volume on the assumption of uniform distribution of the orientations of crystallites entering the representative volume. Components of the tensor of elastic properties of an isotropic material, expressed in terms of the elastic moduli (Lamé coefficients $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$, modulus of elasticity $E$, and the Poisson ratio $\nu$), can be represented by the following matrix (in the Voigt notation):

$$[\bar{n}_{isotr}] = \begin{bmatrix} \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & \mu \end{bmatrix}.$$  

When accepting the hypothesis of isotropy of a polycrystalline material, one should know the best approximation of isotropic constants as functions of the anisotropic characteristics and the conditions of applicability of the found values. The detailed description of the approaches to Voigt, Reuss, Hill averaging for determining elastic moduli of corresponding isotropic elastic materials in terms of the components of the tensor of elastic properties of an anisotropic body was given in [32–34].

3. RESIDUAL MESOSCOPIC STRESS

Residual stress (RS) arises during almost all technological processes of metal treatment [35–37]; notably, first-order RS (balanced throughout a sample) are generally under consideration [37, 38]. At the same time, the operational characteristics (especially, strength ones) of various constructions depend significantly on lower-scale RS (in particular, residual mesoscopic stress, second-order RS (self-balanced RS at the polycrystal-grain scale), and third-order RS (self-balanced RS at the scale of several tens of the lattice parameter)) [36, 37]. The residual mesoscopic stress (RMS), which is the subject of this study, is considered to be a stress, which is caused by the incompatibility of mesoscopic elastic strains and balanced at the scale of the representative macroscopic volume of the material (they remain in crystallites after total unloading of the representative macroscopic volume). The RMS is used to estimate the elastic energy accumulated at the scale of the representative macroscopic volume, which may affect the occurrence and propagation of micro- and mesocracks. In this study, the influence of anisotropy of the elastic properties...
mesoscopic elements (crystallites) on the RMS is considered using the two-level elasto-viscoplastic model.

To determine RMS in numerical experiments, the stage of active elasto-viscoplastic loading should be succeeded by unloading of the representative macroscopic volume. One must take into account that the above-described two-level model based on the Voigt hypothesis is focused on kinematic setting of loading. In this context, an iterative procedure should be applied, which with kinematic loading (implemented in increments) would satisfy with a specified accuracy the condition \( \mathbf{K} = \mathbf{0} \) (the weighted Kirchhoff stress tensor, averaged over the representative macroscopic volume, equals the zero tensor).

Let us describe the procedure of unloading of the representative macroscopic volume. We assume that macroscopic stress \( \mathbf{K} \) in the representative macroscopic volume was achieved at an arbitrary previous loading stage; then, to implement the step-by-step procedure of unloading, one should know the (transposed) velocity gradient at each step. It can be found from the following condition:

\[
\mathbf{v}^T = -\chi \frac{\mathbf{K}}{\|\mathbf{K}\|}, \quad \|\mathbf{K}\| = (\mathbf{K} : \mathbf{K})^{1/2},
\]

(3)

where \( \chi \) is a parameter (in s\(^{-1}\)) related to the value of a time step, which can be obtained from numerical experiments. Note that, in view of the known problem of ambiguous determination of an unloaded configuration (which can be established only accurate to rotation of the volume under study as a rigid whole), it was assumed that the principal axes of the tensor \( \mathbf{K} \) (or the elastic strain tensor) remain invariable upon unloading. It should be noted that, despite the accepted assumption of elasticity of the unloading process for the representative macroscopic volume as a whole, its individual crystallites may undergo irreversible deformations, which results in the necessity of using a step-by-step procedure. The unloading process is considered as complete when the condition \( \|\mathbf{K}\| < \varepsilon \) is satisfied, where \( \varepsilon \) is a small positive number.

4. RESULTS OF THE NUMERICAL EXPERIMENTS

The mathematical model considered in Section 2 was applied for studying loading of representative macroscopic volumes (samples) of polycrystals with bcc, fcc, and hcp lattices. In each of the considered experiments, the representative macroscopic volumes included samples of 1000 crystallites, the initial orientations of which had a uniform distribution law. In the numerical experiments, the elastic relations with anisotropic and corresponding isotropic properties were considered for each lattice type; recall that the viscoplastic properties in all versions were assumed to be anisotropic, lattice-bound. All the other relations and material parameters were assumed to be identical for each of the considered polycrystalline types (including the laws of distribution of the lattice orientations in the reference configuration).

It is known [32] that independent components of the tensor of elastic properties (in the Voigt notation) in the MCS basis (in the reference configuration coinciding with the crystallographic coordinate system) for single crystals (mesoscopic elements) of tungsten (bcc lattice), copper (fcc lattice), and titanium (hcp lattice) are

- bcc : \( n_{11} = 512.6 \text{ GPa}, \quad n_{12} = 205.8 \text{ GPa}, \quad n_{66} = 29 \text{ GPa}, \)
- fcc : \( n_{11} = 168.4 \text{ GPa}, \quad n_{12} = 121.4 \text{ GPa}, \quad n_{44} = 75.4 \text{ GPa}, \)
- hcp : \( n_{11} = 162.4 \text{ GPa}, \quad n_{33} = 180.7 \text{ GPa}, \quad n_{12} = 92 \text{ GPa}, \quad n_{13} = 69 \text{ GPa}, \quad n_{55} = 46.7 \text{ GPa}. \)

Axes of the orthonormal Cartesian coordinate system, determined in terms of the Miller (for fcc and bcc) and Bravais (for hcp) indices, are oriented with respect to the crystallographic axes as follows:

(i) \( O_x = [100], O_x = [010], O_x = [001] \) for a cubic lattice;
(ii) \( O_x = [\overline{2} \overline{1} 0], O_x = [01 \overline{1} 0], O_x = [0001] \) for a hexagonal close-packed lattice.

Using the known approaches [32], elastic moduli of corresponding isotropic materials were calculated based on the above-presented components of the tensors of elastic properties of single crystals (see Table 1, where \( K = \frac{E}{3(1-2\nu)} \) is the bulk modulus).

As was noted above, the purposes of this study were as follows:

(i) To investigate the behavior of a material using the law of elasticity of anisotropic and corresponding isotropic bodies as constitutive relations.
(ii) To analyze the dependences of the stress intensity on the intensity of accumulated strain, triaxiality ratio, and characteristics of residual mesoscopic stress.
To this end, we performed a series of numerical simple shear tests (up to the accumulated strain of 50%) in the Ox1x3 plane of a polycrystalline sample with a rectangular cross section (in the x3 = 0 plane) in the reference configuration. To set characteristic loading axes, an immobile LCS with the basis vectors \( 1_i, \ i \in \{1, 3\} \) was introduced. When simulating simple shear, the transposed gradient of site was set in the form

\[
\lambda \in \mathbb{R}, \ 1 \leq i \leq 3, \ \lambda = \lambda_1 \mathbf{l}_1 + \lambda_2 \mathbf{l}_2 + \lambda_3 \mathbf{l}_3,
\]

where \( \lambda \) is the parameter determining the strain rate, (in s\(^{-1}\)) and \( t \) is time. All calculations were carried out at identical (except for the components of the tensor of elastic properties) values of the model parameters for each material (number of the crystallographic slip systems (SS), parameters of the hardening law, and orientations of the lattices of all crystallites in the reference configuration) and initial conditions:

\[
k_{i=a} = 0, \quad \tau^{(k)}_{i=0} = \tau^{(k)}_{e=0}, \quad \gamma^{(k)}_{i=0} = 0, \quad k = 1, ..., K, \quad r^{(k)}_{i=0} = r_0.
\]

The results of the numerical simple shear tests showed that the stress–strain curves differ significantly only in the initial stage of active deformation (in the elastic region); afterwards, they insignificantly differ for each of the materials under consideration. For the titanium sample, the dependences of the stress intensity \( K_u \) on the accumulated-strain intensity \( \varepsilon_u \), defined as a time integral of the strain rate intensity, are shown in Fig. 1. Among all the materials under consideration, the results in the elastic region for titanium differ most significantly. Figure 1b shows the initial portions of the plots on an enlarged scale. Solid curves are for the anisotropic material.

When determining the residual stress for the aforementioned set of samples, achievement of the accumulated strain intensity of 50% in them at simple shear was succeeded by unloading. Figures 2–5 show histograms of the RMS intensity distribution of crystallites (in the range of ±10 MPa with respect to the mean histogram values): (A) anisotropic properties and isotropic (V) Voigt, (R) Reuss, and (H) Hill properties.

It follows from the presented results that the difference between the RMS distributions of crystallites at high (90–110 MPa) stress intensities is largest in crystals with a cubic (fcc and bcc) lattice. Although the hcp lattice is more asymmetric, the difference between the RMS distributions of elements for titanium, obtained in calculations with anisotropic and isotropic elastic properties, were minimum among the materials under consideration (especially, for Hill determination of the averaged characteristics). This circumstance may be related to the fact that the elastic properties in the base plane for the hcp lattice are close to the isotropic ones.

It should be noted that the form of the strained state also has a great effect on the strength of products. In most works devoted to strength, the loading hardness parameter (triaxiality ratio), equal to the ratio of the average stress to the stress intensity, is used as a characteristic of the strained-state form:

\[
\Theta = \frac{K_w}{K_u}, \quad K_w = \frac{I_1(\kappa)}{3}, \quad K_u = \left( \frac{3}{2} \kappa' : \kappa' \right)^{1/2},
\]

where \( I_1(\kappa) \) is the first invariant of the second-rank tensor and \( \kappa' \) is the Kirchhoff stress deviator. The way of fracture of most materials differs for tensile and compressive average stress. As was shown experimentally, all materials (without exception) can endure fairly high stress at uniform compression, whereas at

| Averaging method | Material, lattice | \( K \), GPa | \( \mu \), GPa | \( \lambda \), GPa |
|-----------------|------------------|-------------|--------------|--------------|
| Voigt           | Tungsten, bcc    | 308.07      | 78.76        | 255.56       |
| Reuss           | 308.07           | 41.88       | 280.15       |
| Hill            | 308.07           | 60.32       | 267.85       |
| Voigt           | Copper, fcc      | 137.07      | 54.64        | 100.64       |
| Reuss           | 137.07           | 33.33       | 114.85       |
| Hill            | 137.07           | 43.98       | 107.74       |
| Voigt           | Titanium, hcp    | 107.06      | 44.00        | 78.02        |
| Reuss           | 123.54           | 38.23       | 98.31        |
| Hill            | 115.30           | 41.11       | 88.16        |

**Table 1.** Elastic moduli of corresponding isotropic materials
uniform extension they are destroyed at relatively low stress. There exist stress states, in which the destruction is brittle, without formation of plastic strain; however, in some other states, the same material can be plastically deformed. The criteria of destruction were described in more detail in numerous monographs (see, e.g., [39–41]) and reviews [42, 43].

Using the Chebyshev metric, the pairs of crystallites (of anisotropic and corresponding isotropic bodies) were found, for which the intensity of the difference between the RMS tensor components is maximum:

$$
\|\Delta \kappa_i\| = \max_{i=1,7} \left( \frac{3}{2} (\kappa_i^A - \kappa_i^N) : (\kappa_i^A - \kappa_i^N) \right)^{1/2},
$$

where $\kappa_i^A$ and $\kappa_i^N$ are the RMS deviators in the $i$th crystallite, calculated for the anisotropic (A) and corresponding isotropic elastic bodies with Voigt (N = V), Reuss (N = R), and Hill (N = H) averaging of the constants and $I$ is the number of mesoscopic elements in the representative macroscopic volume.

The following parameters were calculated after determining (using the Chebyshev metric) the pair of crystallites: (i) difference between the RMS tensors of the anisotropic and corresponding isotropic crystallites ($\Delta \kappa_N$); (ii) stress intensity $\|\Delta \kappa_N\|$; and (iii) values of the triaxiality parameters. The results obtained are listed in Table 2. It should be noted that

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**Fig. 1.** Dependence of $K_\nu$ on $\varepsilon_\nu$ with simple shear of a polycrystalline elastically isotropic titanium sample (hcp lattice) at (- -) Voigt, (· · ·) Reuss, and ( - - - ) Hill averaging of the elastic characteristics: (a) general view of the curves and (b) initial portions on an enlarged scale; the dependence for elastically anisotropic titanium (—) is presented for comparison.

**Fig. 2.** Residual mesoscopic stress intensity distribution of crystallites (tungsten).
both intensities of the RMS difference and its components differ significantly; the intensity of the RMS difference may even exceed the yield stress (in the reference configuration).

5. CONCLUSIONS

The difference between responses of materials was analyzed based on the two-level elasto-viscoplastic model using the anisotropic (with a certain symmetry class) and corresponding isotropic constitutive relations to describe elastic deformation. The calculations yielded the curves characterizing the stress—strain state, the residual mesoscopic stress (remaining in crystallites after unloading of the representative macroscopic volume of a polycrystal) was estimated, and triaxiality ratios of the pairs of crystallites (of anisotropic and corresponding isotropic bodies), for which the intensity of the difference between the residual mesoscopic stress tensor components is maximum, were found. It was shown using numerical simple shear tests that the dependences of the stress intensity on the accumulated strain intensity for a representative macroscopic volume consisting of 1000 grains differ only slightly in the developed-strain stages; some greater differences were observed for a material with a hexagonal close-packed lattice (titanium) with deformation in the elastic region.

Fig. 3. Residual mesoscopic stress intensity distribution of crystallites (copper).

Fig. 4. Residual mesoscopic stress intensity distribution of crystallites (titanium).
When analyzing residual mesoscopic stress for materials with bcc and fcc lattices, the best approximation to an anisotropic body was obtained using the elastic relations of materials, the elastic moduli in which are determined using the Reuss hypothesis. For an hcp material, the best correspondence was obtained at isotropic elastic characteristics, obtained within the Hill hypothesis. Application of different approaches to determination of elastic properties of the corresponding elastically isotropic body affects significantly the results of calculating the residual mesoscopic stress: some approaches may lead to high errors in estimating the fatigue strength of a product. Residual mesoscopic stress allows one to assess the accumulated elastic energy in crystallites as a result of the previous elastoplastic deformation and forecast crack formation and propagation at the mesoscale, which should be taken into account when predicting strength properties of products. The processes of damage accumulation and destruction are also affected significantly by the form of the strained state; the triaxiality ratio is often used as the main characteristic of the strained-state form. The calculation results based on the two-level model showed that, when applying anisotropic and corresponding isotropic laws to describe elastic deformations, the triaxiality ratios for the RMS yield differences as large as 23%, which may also affect significantly the accuracy of predicting destruction.

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**Table 2.** Characteristics of the RMS obtained using the isotropic and anisotropic elastic properties of crystallites

|      | bcc     | fcc     | hcp     |
|------|---------|---------|---------|
| A–V  | $\|\Delta_{V}\|$, MPa | 89.14   | 67.42   | 114.18  |
|      | $\Theta_{V}$ | 0.61   | 0.72    | 0.68    |
|      | $\Theta_{A}$ | 0.52   | 0.64    | 0.55    |
|      | $(\Delta_{V})_{ij}$, MPa | (24.74 17.42 −19.57) | (14.18 12.94 −26.1) | (15.47 −31.27 16.62) |
| A–R  | $\|\Delta_{R}\|$, MPa | 98.57   | 78.57   | 120.23  |
|      | $\Theta_{R}$ | 0.58   | 0.58    | 0.49    |
|      | $\Theta_{A}$ | 0.52   | 0.64    | 0.55    |
|      | $(\Delta_{R})_{ij}$, MPa | (12.39 16.25 −21.62) | (24.91 13.4 −15.6) | (4.99 −50.63 −35.13) |
| A–H  | $\|\Delta_{H}\|$, MPa | 104.98  | 74.93   | 166.88  |
|      | $\Theta_{H}$ | 0.46   | 0.70    | 0.61    |
|      | $\Theta_{A}$ | 0.52   | 0.64    | 0.55    |
|      | $(\Delta_{H})_{ij}$, MPa | (28.13 19.9 −34.4) | (6.28 14.9 −18.1) | (9.31 −40.62 −3.18) |

When analyzing residual mesoscopic stress for materials with bcc and fcc lattices, the best approximation to an anisotropic body was obtained using the elastic relations of materials, the elastic moduli in which are determined using the Reuss hypothesis. For an hcp material, the best correspondence was obtained at isotropic elastic characteristics, obtained within the Hill hypothesis. Application of different approaches to determination of elastic properties of the corresponding elastically isotropic body affects significantly the results of calculating the residual mesoscopic stress: some approaches may lead to high errors in estimating the fatigue strength of a product. Residual mesoscopic stress allows one to assess the accumulated elastic energy in crystallites as a result of the previous elastoplastic deformation and forecast crack formation and propagation at the mesoscale, which should be taken into account when predicting strength properties of products. The processes of damage accumulation and destruction are also affected significantly by the form of the strained state; the triaxiality ratio is often used as the main characteristic of the strained-state form. The calculation results based on the two-level model showed that, when applying anisotropic and corresponding isotropic laws to describe elastic deformations, the triaxiality ratios for the RMS yield differences as large as 23%, which may also affect significantly the accuracy of predicting destruction.
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