Grain Structure Refinement Description in the Two-Level Statistical Crystal Plasticity Model

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Abstract. As both self-consistent and direct multilevel models (suggesting solution of boundary value problems at the meso-level) are extremely resource intensive, nowadays statistical crystal plasticity models are supposed to be the most promising ones for modeling technological processes of thermo-mechanical treatment of materials. The statement of a boundary value problem at the current configuration in the rate form is preferable, as it is convenient for applying numerical methods. In this case, step-by-step solution with redefining the computational domain configuration (including contacting surfaces) is possible. The two-level (macro- and meso-level) statistical constitutive model for describing deformation of polycrystalline metals and alloys, being formulated in terms of the actual configuration in the rate form, is proposed. The flexible coordinate system at the meso-level is connected with the symmetry elements of the crystallites, which determines appropriate choice of the corotational derivative in the constitutive relation. The approximate model for describing grain structure refinement on the basis of considering the amount of accumulated inelastic deformation as an integral characteristic of the defect structure state is included into the model. The results of the test calculations for describing loading processes, being relevant for equal-channel angular pressing, are given.

1. Introduction

In recent decades, processing by intensive plastic deformation have been increasingly used in various branches of engineering. This is due to significant improvement in performance characteristics of materials and products during the materials' grain structure refinement in these processes [1], [2] and etc. For example, in the works [3], [4] it is noted, that decrease in the grain size below a certain threshold value can lead to a drastic change in the properties. Firstly, the microhardness of such materials can be 2-6 times higher than the microhardness of the coarse-grained analogues. Secondly, yield strength and tensile strength are also increased significantly. The possibility of optimal combination of mechanical properties in metals and alloys with a nanosubmicron structure opens up broad prospects for their usage as new structural and functional materials.

At low homologous temperatures, when recrystallization processes can be ignored, the key factor determining the course of grain structure refinement process is (localized) accumulation of defects. As a result of it, the polycrystalline grains are firstly divided into a multitude of related microareas (fragments), where misorientations is increased in the deformation process [5, 6, 7, 8, 9, 10]. When the misorientations between the fragments reach the values being characteristic for the high-angle boundaries of the intergranular type, division of the grain into the separate parts (that is, loss of perfect connectivity) may occur (in particular, a shift along the formed border becomes possible). In a sense, the process of grain fragmentation into separate parts resembles the process of viscous fracture, but with preservation of coherence between the resulting parts of the original crystallite. Thus, grain structure refinement is manifested at the mesoscale level (the grain level) and is due to implementation of the defect structure changing processes at the microscale level.

The most suitable apparatus to describe the changing internal structure of metals and alloys is multilevel models based on crystal plasticity [11, 12, 13, 14, 15, 16, 17]. In the models of that class, the internal variables [18, 19, 20, 21] are explicitly introduced to describe the structure elements and
individual deformation mechanisms. To describe their changing, equations based on the known information from the solid-state physics, are formulated. There are three main groups of models of that class: statistical, self-consistent and direct ones. In statistical models [22, 23, 16] the meso-level elements (crystallites) are considered to be relatively independent on each other. Integration of meso-level elements into the macro-level element is carried out for a part of the characteristics based on the accepted kinematic or static hypotheses. The other characteristics are statistically averaged. In self-consistent models [24, 25, 26, 27] at the meso-level, the behavior of individual meso-level elements in the environment of the material matrix with effective characteristics is determined. These characteristics are defined iteratively by the properties of the meso-level elements using a particular averaging procedure for the last ones. In the direct models [28, 17, 29] the solution of boundary-value problems at the mesoscale level is implemented (in the vast majority of papers, the finite element method is used). Application of self-consistent and especially direct models is associated with extremely large computational costs, therefore, statistical models are the most promising ones for modeling real technological processes of the materials' thermo-mechanical treatment in the near future.

The two-level statistical model of polycrystalline metals and alloys, supplemented by correlations for describing grain structure refinement, is proposed.

2. Structure of the two-level statistical model

The two-level statistical model of polycrystalline metals and alloys [30] has been taken as a base constitutive model. The mechanisms of the intra-grain dislocation sliding and the crystallites' lattices rotation are taken into consideration in the model.

For the meso-level element (crystallite) the elastic law in the rate relaxation form in the actual configuration terms is as follows:

\[
\kappa^\varepsilon = \Pi : (\varepsilon^\varepsilon)^{\varepsilon} = \Pi : (z - z^0) = \Pi : \left(1 - \bar{\sigma} - \sum_{k=1}^{K} \gamma^{(k)} b^{(k)} n^{(k)}\right),
\]

where \(\kappa = 0/\hat{\rho} \sigma\) is the weighted Kirchhoff stress tensor, \(\sigma\) is the Cauchy stress tensor, \(\hat{0}\) is density of the crystallite's material in the initial (unloaded) and the actual configurations, \(\kappa^\varepsilon = d\kappa / dt + \kappa \cdot \bar{\sigma} - \bar{\sigma} \cdot \kappa\) is the corotational derivative of the Kirchhoff tensor, \(\bar{\sigma}\) is the spin tensor of the movable coordinate system, \(\bar{\kappa}\) is the tensor of elastic properties (which components are constant in the basis of the flexible coordinate system), \((\varepsilon^\varepsilon)^{\varepsilon}\) is the elastic deformations' rate, being fixed by the observer in the flexible coordinate system, \(I\) is the rate gradient, \(z = (1 - \bar{\sigma})\) is the full strains velocity tensor, being defined by the observer in the flexible coordinate system, \(z^{\text{in}} = \sum_{k=1}^{K} \gamma^{(k)} b^{(k)} n^{(k)}\) is the inelastic strains rate, \(\gamma^{(k)}\), \(b^{(k)}\), \(n^{(k)}\) are the shear rate, the shear direction and the normal to the shear plane in the actual configuration for the k-th intra-grain slip system (of the edge dislocations; the doubled quantity of the slip systems is used for convenience).

To define \(\bar{\sigma}\), the rotation model, described in [30, 31], is used. According to this model, the flexible coordinate system is connected with symmetry elements of the crystallites, which determines the appropriate choice of the corotational derivative. In this case, the tensors, being a part of the constitutive model formulation, would change as indifferent ones for the observer in the fixed laboratory coordinate system, which allows satisfying the principle of the constitutive relation independence on the reference frame choice. In [32] the comparison results of using the specified spin and the alternative formulations, including classical models of constrained rotation by Taylor and rotation with \(R^e\) (orthogonal tensor from decomposition of the strain gradient elastic component \(F^e\)), are described. The improvement in description of crystallites' lattice rotation by the including the force (moment) factors, appearing due to interaction of the neighboring grains' (subgrains') defects, into equations, can be noted as a development direction for the crystal plasticity models [33].
To determine the shear rates, the viscoplastic relation is used:

\[
\dot{\gamma}^{(k)} = \dot{\gamma}_0 \left( \frac{\tau^{(k)}}{\tau_c^{(k)}} \right)^m \mathcal{H}(\tau^{(k)} - \tau_c^{(k)}),
\]

where \( \tau^{(k)} \) and \( \tau_c^{(k)} \) are shear and critical shear stresses on the \( k \)-th slip system, \( \tau^{(k)} = \mathbf{e}^{(k)} : \mathbf{b}^{(k)} \mathbf{n}^{(k)} \), in common case \( \tau_c^{(k)} \) is a function of the shifts in the slip system accumulated up to the current moment and history of their changing, \( \dot{\gamma}_0 \) is the shear rate in the slip system when the shear stress reaches the critical shear stress, \( m \) is the indicator of material rate sensitivity (in the calculations, the parameter values are assumed as follows \( \dot{\gamma}_0 = 0.001 \text{s}^{-1} \), \( 1/m = 0.012 \)), \( \mathcal{H}(\cdot) \) is the Heaviside function. The evolution relation for critical stresses \( \tau_c^{(k)} \) and its parameters are supposed to be as in [34] and correspond to the technical copper.

To determine the impact at the meso-level the generalized Taylor hypothesis is used \( \mathbf{L} = \mathbf{L} \), where \( \mathbf{L} \) is the rate gradient at the macro-level.

The macro-scale variables are determined by averaging the meso-scale variables using the procedure of the constitutive relations' consistency [33]. Note, that taking temperature into consideration should be added into the problem formulation for the common case. Here, consideration is limited by a test isothermal case.

Note, that for simulation of technological processes, the boundary value problem statement in terms of the actual configuration in the rate form is more preferable, being convenient for applying numerical methods. In this case, the step-by-step solution with redefining configuration for the calculated area (including the surfaces being in contact) is possible. The proposed formulation of the two-level constitutive model is organically incorporated into such a statement.

To describe the possible grain structure refinement, the model is supplemented by the following relationships.

3. The description of grain structure refinement within the multi-scale constitutive model

The process of grain structure refinement is determined by localized accumulation of defects. Grain refinement is supposed to be realized by analogy with viscous destruction as a result of high defect density accumulation [35, 36]. As a result, a large angle boundary appears between the grain parts, but with preservation of their connectivity. Within the two-level statistical model the accumulated shears by slip systems are integral characteristics of the defects' densities [37, 29]. Within the framework of the basic statistical model the grain deformation is supposed to be homogeneous. An explicit consideration of the defective substructures at the micro level requires large computational resources due to introduction of an additional level into the constitutive model and a significant number of internal variables. Therefore, in the developed model, planned to be used in simulating the real technological processes of mechanical treatment, a simplified description of refinement is proposed to be used in a first approximation. For this, the separation criterion described below and based on consideration of accumulated shifts in slip systems is proposed to be applied. A simplifying hypothesis has been adopted that two ellipsoidal grains of the same size and shape are formed as a result of the original grain fragmentation. The maximum size of a new grain corresponding to a part of the initial grain is equal to the half of the maximum linear size of the initial grain and corresponds to the perpendicular original direction. The dimensions in the transverse direction are proportional to the original transverse dimensions. The proportionality coefficient is determined from the condition of equality for the total volume of the new grains to the volume of the original one. The axes of the new grains are disoriented at sufficiently small angles according to a random law (the distribution can be established using experimental data).

In the fragmentation criterion formulation based on consideration of the accumulated inelastic deformation amount, a large dislocation density along the slip system is assumed to be increasing the probability of separating the grain along this plane. The fragmentation criterion is taken as \( f = f_c \), where \( f_c \) is a model parameter, determined when identifying the model from the experimental data on the
average grain size changing in deformation processes \( f_c \) depends on the average grain size, it is assumed to be equal \( f_c = 0.7 \) in the test calculations), where a significant grains fragmentation occurs. The function \( f \) is defined as follows \[ f = \max_{n, \tau} \left( \frac{h_u}{h_e} \cdot \tau \cdot E^n \cdot n \right). \] (3)

In the relation (3) \( n, \tau \) are the normal to the shear plane and the direction of the shift in it (they are determined as a result of solving the optimization problem for ensuring the maximum value of the function), \( h_u, h_e \) are the maximum grain-ellipsoid sizes in the directions \( \tau \) and \( n \), \( E^n \) is the plastic strain accumulated in the grain. Thus, (3) determines the maximum shear strain at the current time, but taking into consideration the grain elongation. The amount \( E^n \) is determined by integrating the equation \[ \dot{E}^n = \bar{\omega} \cdot E^n + E^n \cdot \bar{\omega} = z^n, \] where \( \bar{\omega} \) is the spin of the flexible coordinate system, connected with the crystalline lattice [30], \( z^n = \sum_{k=1}^K \gamma^{(k)} b^{(k)} n^{(k)} \) is the grain inelastic deformations rate due to the intragranular dislocation sliding, the shear rates in the slip systems are determined by (2).

In a more general formulation, an explicit consideration of individual grain fragments misorientations [38] can be included into the refinement submodel by taking into consideration the moment factors and disclinations, but implementation of this model requires significantly more computational resources.

4. Results
To simulate equal-channel angular pressing, the analytical relation for the rate gradient given in [39] is used, according to which the \( L \) tensor components in the basis of the laboratory coordinate system \( OX_1X_2X_3 \) can be written as follows:

\[
[L] = [\nabla v^T] = L_0 \begin{bmatrix} -\sin \theta \cos \theta & \cos^2 \theta & 0 \\ -\sin^2 \theta & \sin \theta \cos \theta & 0 \\ 0 & 0 & 0 \end{bmatrix},
\] (4)

where \( L_0 \) is a (negative) shear rate, \( \theta \) is a half angle of articulation for the channels (the output channel is located along the axis \( OX_1 \), the entrance channel is angled at \( 2 \theta \) in the plane \( OX_1X_2 \)). Thus, emulation of equal-channel angular pressing is a multiple repetition of the cycle: shear deformation (4) and unloading (the turn of the workpiece before the next pass is possible; in the calculations, which results are presented here, the turn was not considered).

In the initial state, all crystallites were assumed to be equal balls with the size 50 mkm. During the deformation, significant refinement of the grain structure is observed. The characteristics of its state are shown in figure 1 and figure 2.
Figure 1. The histogram of distribution for the average grain semiaxis length, mkm (the left one is the result after the first pass, the right one is the result after the second pass)

Figure 2. The histogram of distribution for the ratio of the greatest grain semiaxis to the smallest one, mkm (the left one is the result after the first pass, the right one is the result after the second pass)

It can be noted that after the second pass the structure is more fined, the shape of the grains becomes closer to the equiaxial one. It qualitatively corresponds to the data on the grain structure changing in the process of the equal-channel angular pressing [8, 9].

5. Conclusion
The two-level constitutive model of polycrystalline metals and alloys allowing taking into consideration the grain refinement process as a first approximation is developed. The obtained simulation results indicate the corresponding capabilities of the model. The proposed approach can be used for modeling the structure evolution of a polycrystalline material when describing the technological processes of mechanical treatment for metals and alloys being based on severe plastic deformations.

6. Acknowledgments
The work was supported by the Russian Science Foundation (grant No. 17-19-01292).

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