

Polycrystals multilevel models using crystal plasticity: consistency of constitutive equations at different scale levels

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Abstract. Two-level models of different polycrystalline metal's inelastic deformation based on crystal plasticity and describing viscoplastic intragranular dislocations slip, lattice rotation with an explicit consider of dislocation slip incompatibility in neighboring grains, and fragmentation of crystallites are developed. The homogenization of constitutive equations at various scale levels is used, which allows to connect the same type of characteristics of different scale levels and leads to an unambiguous description of geometric nonlinearity on the macro level by specifying the corotational derivative of Cauchy stress tensor. An algorithm for solving boundary value problems in FEM package Abaqus with using proposed models to describe the behavior of the material is developed, corresponding computational modules are created. Numerical investigation of different loading of samples from various polycrystalline metals with a description of the evolving internal structure is done.

1. Introduction

Numerous theoretical and experimental studies show that the performance of the internal material structure determines the behavior of the material at the macro level and its performance characteristics. During intensive plastic deformation the internal structure of the material is significantly restructured: the grain and dislocation structures are changing, crystallites lattice is rotated; it is widely used to produce materials with unique properties: submicrocrystalline, nanocrystalline, textured materials and materials, which are capable of superplastic deformation.

At the time, the construction of models capable of describing the change of the internal structure of polycrystalline materials, a growing acceptance of the approach based on an explicit introduction to the structure of the constitutive relations parameters reflecting the state and evolution of meso- and microstructure evolution and the kinetic equations for these parameters (so-called internal variables) [1]. In particular, recent decades, a very wide development of crystal plasticity based models, which built in the framework of this approach and explicitly describing the material structure and the mechanisms of inelastic deformation at the crystallite level, is observed; this models allows a natural way to describe the structure evolution at deep plastic strain.

Based on the crystal plasticity models can be divided into three classes [2,3]: statistics, self-consistent and direct. Models of the last two classes require inaccessible currently computing resources, so for modeling of real processes statistical constitutive model are more popular.

The paper briefly discusses the general structure of the two-level models of polycrystalline metals inelastic deformation developed by the authors, explains how to homogenize the constitutive equations



on different levels of scale, describes the algorithm for applying models of the material in the boundary value problems solution and obtains the results.

2. Two-level constitutive model for inelastic deformations of polycrystals

In the simulation of polycrystalline metal's inelastic deformation scale levels hierarchy can be defined as follows: the macro level – meso level (the level of crystallite – grains, subgrains, fragment) – micro level (the dislocation structure) (Fig. 1).

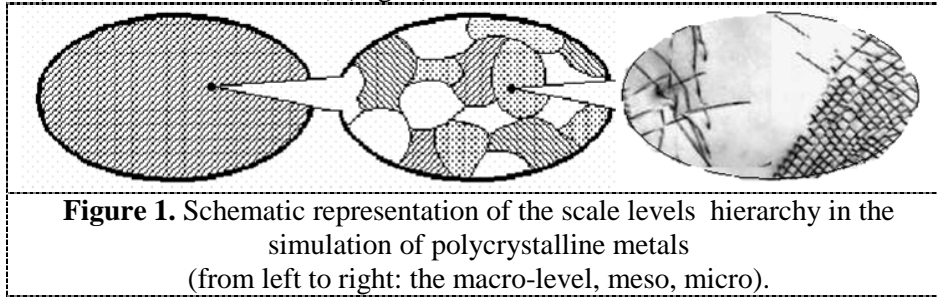


Figure 1. Schematic representation of the scale levels hierarchy in the simulation of polycrystalline metals (from left to right: the macro-level, meso, micro).

At the macro level considers a representative volume of a polycrystalline metal, consisting of a set of crystallites (meso-level elements). The constitutive equations system at the macro level is [1]:

$$\begin{cases} \dot{\Sigma}^r \equiv \dot{\Sigma} + \Omega^T \cdot \Sigma + \Sigma \cdot \Omega = C : D^e = C : (D - D^{in}), \\ \Omega = \Omega(w_{(i)}, c_{(i)}), i = 1, \dots, N, \\ C = C(c_{(i)}), i = 1, \dots, N, \\ D^{in} = D^{in}(d_{(i)}^{in}, c_{(i)}), i = 1, \dots, N, \end{cases} \quad (1)$$

where Σ – Cauchy stress tensor, C – elastic properties 4th-range tensor, D , D^e , D^{in} – the strain rate, its elastic and inelastic parts, the index «r» means derivative independent of the choice of reference system, Ω – tensor describing the motion of the moving coordinate system, which defines itself in relation to deformational movement [4] on the macro level. To determine Ω the homogenization condition for constitutive equations on different scale levels is proposed. Thus, the inelastic strain rate D^{in} , the effective anisotropic elastic properties C and describing the motion of the moving frame tensor Ω are explicit internal variables in the macro-level model, at any moment depends on the structure at the lower scale levels (and through it depends on the loading history) and determined by meso-level model, used for each crystallite (number of meso level items N should be sufficient for a statistical description of a representative volume at the macro level).

At the meso level the system uses the following relations (for the description of each crystallite, the index number of the crystallite is omitted):

$$\begin{cases} \sigma^r \equiv \dot{\sigma} - \omega \cdot \sigma + \sigma \cdot \omega = n : d^e = n : (d - d^{in}), \\ d^{in} = \sum_{i=1}^K \dot{\gamma}^{(i)} m_{(s)}^{(i)}, \\ \dot{\gamma}^{(i)} = \dot{\gamma}_0 \left| \frac{\tau^{(i)}}{\tau_c^{(i)}} \right|^{1/n} H(\tau^{(i)} - \tau_c^{(i)}), i = 1, \dots, K, \\ \dot{\tau}_c^{(i)} = f(\gamma^{(j)}, \dot{\gamma}^{(j)}), i, j = 1, \dots, K, \end{cases} \quad (2)$$

where σ – Cauchy stress tensor, c – fourth-rank elastic properties tensor of the crystallite, d , d^e , d^{in} – the strain rate, the elastic and inelastic strain rate, γ^i , τ_c^i – accumulated slip and the critical shear stress on the i -th slip system, m^i – the orientation tensor of i -th slip system, $m^i = 1/2(b^i n^i + n^i b^i)$, b^i , n^i – the unit vectors in the direction of the Burgers vector and the normal to the slipping plane;

bedding planes and orientation of the Burgers vector along the translational motion (slip) of edge dislocations are known, they are the most densely packed planes and directions, so, in fcc metals sliding edge dislocations are in the planes of $\{111\}$ in directions $\langle 110 \rangle$, $\dot{\gamma}_0, n$ – constants of the material: the characteristic shear rate and strain rate sensitivity of the material [1], τ^i – shear stress in the i -th slip system, $\tau^i = \mathbf{b}^i \mathbf{n}^i : \boldsymbol{\sigma}$, $H(\cdot)$ – Heaviside function, K – the number of slip systems for considered type lattice, \mathbf{o} – tensor current orientation of the crystallographic coordinate system relative to the fixed grain laboratory system.

As constitutive relation at the meso level Hooke's law in the speed form is used (2₁), the geometric nonlinearity is taken into account: quasi-solid movement [4] associated with the rotation of the lattice (in crystallographic coordinates); spin tensor $\boldsymbol{\omega}$ in corotation derivative Cauchy stress tensor $\boldsymbol{\sigma}^r$ characterizes the crystal lattice rotation. Thus, stress is characterized the elastic bonds in grain and determined by lattice distortions.

Equation (2₂) is kinematic equation, according to which the inelastic deformation of the crystallite is defined by sliding to slip systems. If other intragranular deformation mechanisms, such as grain boundary sliding or twinning in the (2₂) to the modes of intragrain dislocation glide mechanisms are added to the appropriate mode for shear rates that determine the kinetic equations.

To determine inelastic deformation rate of polycrystalline metals can be used [2,3]: elastoplastic model based on the Lin model [5], or the elastoviscoplastic model used here (2₃), where \mathbf{d}^{in} (and $\boldsymbol{\omega}$) associated with implicit internal meso-level variables characterizing dislocation slip – shear rates on slip systems $\dot{\gamma}^i$, the critical stress τ_c^i , tensor \mathbf{o} of the crystallographic orientation of the current coordinate system of grain relative to a fixed laboratory system coordinates. Specification of equation (2₄), describing the evolution of the critical shear stress on the slip system, is in the paper [6].

Taylor's hypothesis is applied for scale transition implemented at the macro level to the lowest levels in the scale model $\mathbf{d} = \mathbf{D}$.

Relations (2₅) for the determination of the spin system the following ratio are used:

$$\left\{ \begin{array}{l} \boldsymbol{\omega} = \boldsymbol{\omega}_1 + \boldsymbol{\omega}_2 \\ \boldsymbol{\omega}_1 = \frac{1}{2}(\hat{\nabla} \mathbf{v}^T - \hat{\nabla} \mathbf{v}) - \sum_{i=1}^K \frac{1}{2} \dot{\gamma}^i (\mathbf{b}^i \mathbf{n}^i - \mathbf{n}^i \mathbf{b}^i) - (\mathbf{B} : \boldsymbol{\sigma}) \cdot \mathbf{D}^{\text{in}} + \mathbf{D}^{\text{in}} \cdot (\mathbf{B} : \boldsymbol{\sigma}) \\ \boldsymbol{\omega}_2 = \begin{cases} \frac{1}{A} \boldsymbol{\mu}^r + \frac{1}{H} \boldsymbol{\mu}, & \text{if } \|\boldsymbol{\mu}\| = \mu_c \text{ и } \boldsymbol{\mu} : \boldsymbol{\mu}^r > 0 \\ \frac{1}{A} \boldsymbol{\mu}^r, & \text{otherwise} \end{cases} \\ \boldsymbol{\mu}^r = \sum_{m=1}^M (\boldsymbol{\mu}^r)^m \\ \mathbf{m}^r = \mu \mathbf{N} \times \left[\sum_i^K \dot{\gamma}^i \mathbf{n}^i \mathbf{b}^i - \sum_j^K \dot{\gamma}^{j(m)} \mathbf{n}^{j(m)} \mathbf{b}^{j(m)} \right] \cdot \mathbf{N}, \text{ for each neighboring grain } m \end{array} \right. \quad (4)$$

The first component $\boldsymbol{\omega}_1$ describes the rotation of the lattice with the grain material during the imposed kinematic effects (material associated with the orthogonal rotation tensor accompanying elastic deformation). The second component $\boldsymbol{\omega}_2$ describes the rotation of the actual crystallite lattice due to the interaction with the environment. To do this, the model (3) introduced the couple stresses $\boldsymbol{\mu}$ acting on the crystal, the critical moment stress μ_c and set the normal to the crystallite $\mathbf{q}^m, m = 1, \dots, M$ (M -

number of neighboring crystallites). Additivity velocity moments of interaction with all neighboring grains is assumed in (4₄). The evolution of the vector-momentum associated with the couple stress tensor and determines from the analysis of the incompatibility of dislocation motion on the boundary of the crystallites by equation (4₅). Based on the input of the couple stresses may be used for description of fragmentation [7].

3. The homogenization procedure of constitutive equations for scale transition

One of the keynote questions in the multilevel models construction is the issue of constitutive equations homogenization at various scale levels. The logical understanding of the problem is follows: macro level equations should be defining from meso level constitutive equations with a priori relations of the macro- and meso level parameters [1]; specific type of relations associated with the aggregation hypothesis (combining elements of meso level to the macro level element). For statistical crystal plasticity models a priori relation is the equality of velocity gradient, stresses and the effective elastic properties tensor at the macro level are average the corresponding meso level characteristics (for the velocity gradient this conditions are automatically done due Taylor's hypothesis).

The constitutive equations homogenization procedure for the proposed model is as follows:

1. Represent the quantities in the description of the stress-strain state at meso-level as the sum of average representative volume of macro-level variables and deviations from these averages.
2. Substitute this representation in the meso-level of the defining equation (2₁), the obtained relations are averaged.
3. Finding the form obtained in step 2 averaged meso-level constitutive equation running the macro-level (1₁), defining the necessary connections.

For the proposed models the connections are

$$\mathbf{\Omega} = \langle \mathbf{\omega} \rangle, \quad \mathbf{D}^{in} = \langle \mathbf{d}^{in} \rangle + \mathbf{C}^{-1} : \langle \mathbf{c}' : \mathbf{d}^{in'} \rangle - \mathbf{C}^{-1} : (\langle \mathbf{\omega}' \cdot \mathbf{\sigma}' \rangle - \langle \mathbf{\sigma}' \cdot \mathbf{\omega}' \rangle). \quad (5)$$

Thus, the proposed approach results in more focused form of the defining relations on the macro level (and in particular – the type of independent of the reference system choice derivative). Proposed method is easy to apply for other forms of constitutive relations for meso- and macro-levels for a wide range of constitutive models with internal variables.

4. Algorithm for solving boundary value problems using constitutive model and the simulation results

The algorithm to use developed model for solving boundary value problems in FEM package ABAQUS is made. To do this, we use standard package – implementation of the proposed models in the custom procedure UMAT, including the integration of the constitutive equations of the model (determination of the stresses and internal variables at the end of step in the UMAT) and the definition

of the current cutting modulus matrix $[\mathbf{C}^{ep}] = \frac{\partial\{\Delta\mathbf{\Sigma}\}}{\partial\{\Delta\mathbf{E}\}}$, where $\Delta\mathbf{\Sigma}$ – increment of stress on the step,

$\Delta\mathbf{E}$ - increment deformation step. The analyzes were carried out, resulting in an analytical expression for \mathbf{C}^{ep} connecting it with the internal meso-scale variables.

It should be note that many existing models [2,3] are not considered in the explicit level the constitutive equations at the macro level, but at numerical implementation in FEM-package Abaqus is the (implicitly) introduction is macro-scale level is done, there are Jauman derivative of Cauchy stress tensor is used in Abaqus, which violates the consistency of the two-level constitutive model. It is shown that this approach can lead to physically incorrect.

5. Numerical results

A brief analysis and comparison of the results of calculations using different conditions of scale levels coupling is described underneath:

- 1) the use of the proposed coupling conditions (5) to determine the quasi-solid motion and inelastic strain rate at the macrolevel;
- 2) the use of the Jaumann derivative at the macrolevel

$$\mathbf{\Omega} = \mathbf{W} = \frac{1}{2}((\hat{\nabla}\mathbf{v})^T - \hat{\nabla}\mathbf{v}), \quad (6_1)$$

and direct averaging of the inelastic strain rates (which corresponds with the Voigt's hypothesis direct stresses averaging $\mathbf{\Sigma} = \langle \mathbf{\sigma} \rangle$)

$$\mathbf{D}^{in} = \langle \mathbf{d}^{in} \rangle. \quad (6_2)$$

Fig. 2 present the modeling results of the simple shear with velocity gradient (components in fixed laboratory coordinate system): $(\nabla\mathbf{v})_{23} = -0.5 \cdot 10^{-5} \text{ s}^{-1}$, $(\nabla\mathbf{v})_{ij} = 0$, $(ij) \neq (23)$.

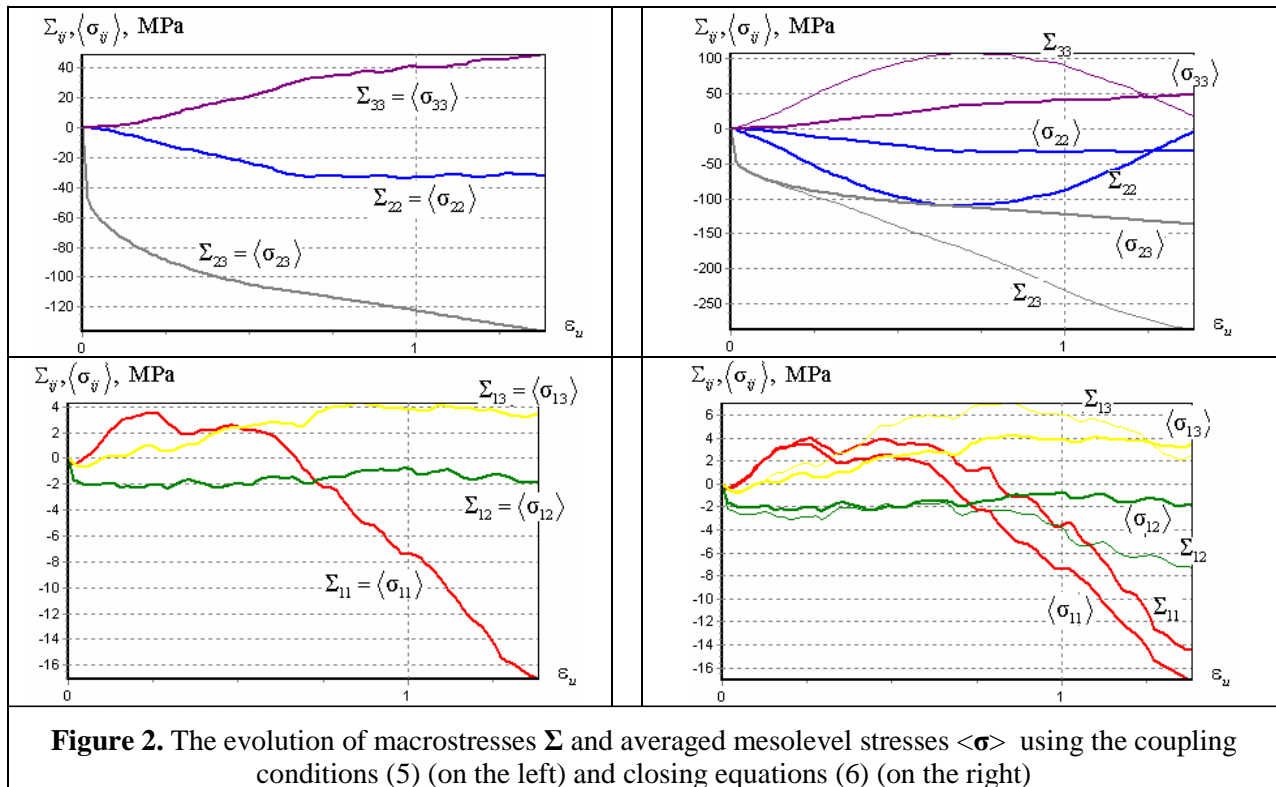


Figure 2. The evolution of macrostresses $\mathbf{\Sigma}$ and averaged mesolevel stresses $\langle \mathbf{\sigma} \rangle$ using the coupling conditions (5) (on the left) and closing equations (6) (on the right)

The results of Fig.2a,2c show that the coupling conditions provided a complete correspondence between the macrostresses and the averaged mesolevel stresses, while the use of the conventional closing conditions (6) of the deviations were significant and they were growing (Fig.2b,2d). Meanwhile there is a change in the sign of the stress tensor components at the macrolevel that is typical for the Jaumann derivative, which seems unphysical for the monotonic loading.

6. Conclusions

To describe the deformation processes of polycrystalline materials with the evolution of its meso-structure two-level constitutive model based on the crystal plasticity is created.

The method of different scale levels parameters coupling based on the agreement of the constitutive equations at these levels and providing consistency of the measures of stress and strain states on these levels is developed. Apart from that, the proposed approach leads to the concretization of the

constitutive relation form at the macrolevel (and the kind of the material frame indifferent derivative, in particular). In principle, the relations of the lowest level are “transported” to the top level solving the problem of their correct formulation for the geometrically and physically nonlinear problem. In this case it is surely not possible to completely avoid the phenomenological relations, however, for the lowest scale level they are written in the accepted hierarchical set; for this level it is possible to specify the physical mechanisms of deformation and their detailed description by using the known statements of solid physics (this is a much easier problem compared to the one for establishing macrophenomenological relations while taking the state of the multiscale internal structure into account and describing the variety of all the mechanisms of the inelastic deformation).

An algorithm for solving boundary value problems using the finite element method, implemented in the Abaqus package. With the use of modeling software system obtained results during loading of samples from various polycrystalline metals, including the evolution of the internal structure: the shape, size and orientation of the crystallographic axes of the structural elements of the polycrystalline aggregates (grains, subgrains, fragments), effective macroscopic elastic and plastic properties of polycrystalline materials. The results is in good agreement with experimental data.

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