Three-level modeling of fcc polycrystalline inelastic deformation: grain boundary sliding description

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Abstract. This paper considers three-level model of polycrystalline inelastic deformation based on crystal plasticity that allow describing the internal structure evolution of the material. It is assumed that crystallite inelastic deformation is realized by intragranular dislocation sliding with lattice rotation. The paper focuses on the problem of grain boundary sliding description. To solve this problem the additional scale level is introduced into the model, evolution and closing equations are formulated on the basis of physical analysis. To connect different scale levels the consistency conditions of constitutive relations are used. The results of computational experiments under uniaxial tension of a polycrystalline pure copper representative volume are obtained.

1. Introduction

Recently different methods of severe plastic deformation (for example, equal channel angular pressing, extrusion, rolling and their various combinations or modifications) are widely used in practice to obtain fine grain and ultra-fine grain metals with improved physical and mechanical properties. The possibility of material switching into superplastic state, producing of details with a complex shape by corresponding treatment and minimum cost, attracts to fine grain and ultra-fine grain materials [5]. Today there is increasingly more need for constructing mathematical models that allow describing integral characteristics of material processes mentioned above and internal structure evolution, which has an influence on physical and mechanical properties. Such mathematical models will define efficient process conditions to produce materials and details of the required quality. The multilevel models of inelastic deformation based on crystal plasticity [6,9] suggested to be the most suitable to achieve the goals indicated above (taking into account that influence on material in different parts of details and changing of internal structure caused by this can be essentially various). These models allow analyzing deformation processes at the macrolevel, to describe explicitly inelastic deformation mechanisms, material internal structure and it's evolution at lower scale levels. Up to this point it would seem that mentioned models have a high generality, allow description of both plastic (viscoplastic) and superplastic regimes within a common model. Brief review of multilevel models based on crystal plasticity is given in [1,6,9,10].

Three-level model of polycrystalline inelastic deformation is used in the paper. The model regards the temperature and includes the most important mechanisms: intragranular dislocation sliding, crystallite lattice rotations and grain boundary sliding, which are significant at elevated temperatures and fine grain structure of the material [2]. Special attention is devoted to description of critical stress...
changes for grain boundary sliding realizing due to different mechanisms of interaction between defects.

2. Description of three-level inelastic deformation model for polycrystalline

The three-level model is constructed on the base of two-level constitutive model previously developed [9]. It is a statistical model considered the deformation of single crystallites with different orientations, generalized Voigt's hypothesis is used to describe the influence on elements of lower scale levels, averaging procedure is applied to define the response of a representative volume [9]. Statistical models are computationally more efficient than the direct models and intensively used in the inelastic deformation modeling of real materials [7,8].

The scale level hierarchy is defined in this way (by descending scale): macroscale level, mesolevel I and mesolevel II. Mesolevel I is introduced for grain boundary sliding description. Crystallite inelastic deformation in mesolevel II model is assumed to be realized by intragranular dislocation sliding with crystallite lattice rotation. All macrolevel quantities are given by uppercase letters, quantities of mesolevel I are denoted by lowercase letters with the index I, mesolevel II quantities are denoted by lowercase letters with the index II.

The equation system of macroscale level is the following:

\[
\begin{align*}
\Sigma + \Omega^T \cdot \Sigma + \Sigma \cdot \Omega &= \Pi : (D - D^a - D^b), \\
\Pi &= \langle \mathbf{n}_f \rangle, \\
\Omega &= \langle \omega \rangle, \\
D^a &= \langle \mathbf{d}^a \rangle + \Pi^{-1} : \langle \mathbf{d}^a \rangle : \Pi^{-1} : \langle \sigma' \cdot \omega \rangle \approx \langle \sigma' \cdot \omega \rangle, \\
D^b &= \langle \mathbf{d}^b \rangle + \Pi^{-1} : \langle \mathbf{n}_f : \mathbf{d}^b \rangle, \\
\dot{\Theta} &= \langle \dot{\theta} \rangle.
\end{align*}
\]

Hooke's law in rate form (1) is the constitutive relation, \(\Sigma\) is Cauchy stress tensor. The explicit internal variables of macrolevel model are spin of movable coordinate system \(\Omega\), effective anisotropic elastic properties \(\Pi\), inelastic \(D^a\) and thermal \(D^b\) components of the strain rate tensor. These variables depend on behavior of lower scale levels at each time moment. They are determined from consistency conditions of scale levels (1)_2, (1)_3, (1)_4 and (1)_5 [9]. The hypothesis of process adiabaticity is adopted at macrolevel: the rate of temperature change at macrolevel \(\dot{\Theta}\) depends only on the rate of temperature change at mesoscale level due to grain boundary and intragranular shears; the hypothesis of temperature homogeneity is assumed at the initial moment at all scale levels.

Constitutive model at mesolevel I is presented by the following relation system:
Hooke’s law in rate form (2) is the constitutive relation of mesolevel I model. The explicit internal variables of mesolevel I model are elastic modulus tensor $\mathbf{p}_I$, inelastic $\mathbf{d}^{in}_I$ and thermal $\mathbf{d}^{th}_I$ components of the strain rate tensor, spin of movable coordinate system $\mathbf{o}_I$ defined quasi-solid motion. These variables depend on behavior of lower scale level at each time moment. They are determined from consistency conditions of scale levels (2)_2, (2)_3, (2)_13 and (2)_14 [9]. Inelastic strain rate is defined by sum of two components: the first one is determined by grain boundary sliding realizing (equations (2)_8, (2)_9, (2)_10, (2)_11), the second component is defined by inelastic deformation at mesolevel II (consistency condition of constitutive relations at scale levels (2)_13). Thermal component of the strain rate tensor is also defined by sum of two elements: temperature change occurs by grain boundary sliding (relations (2)_12) and inelastic deformation at mesolevel II (relation (2)_14). Here $\mathbf{a}$ is thermal expansion tensor, $\alpha_I$ is coefficient of heat eduction, $C_m$ is specific heat, $\rho$ is substance density. Velocity gradient (2)_4 is transmitted as forcing from macrolevel. In (2) notations are following: $< \beta >$ is the average value of $\beta$ in a representative volume of level considered, $\beta^I$ is deviation from the average value for element considered (the element index is omitted), $\alpha_{ij}$ is the volume fraction of boundaries.

Shears on slip systems of grain boundary sliding are described by elastoviscoplastic relation with regard to thermally activated motion of grain boundary dislocations (2)_8, in which $\mathbf{d}^{in}_{gb}$ is grain boundary shear rate under shear stress $\mathbf{r}_{C_gb}$ equal to critical shear stress $\mathbf{r}_{C_gb}$, $U_{gb}$ is the energy barrier (for grain boundary shear), $K_{gb}$ is total slip systems of grain boundary sliding.
The evolution equation for critical stress is proposed in the following form:

\[
\dot{\gamma}_{gb}^{(k)} = h \left(1 - \exp \left(-\frac{U_d}{k_b \theta_j}ight)\right) \gamma_{gb}^{(k)} - \sum_{i=1}^{K_g} \sum_{j=1}^{N_g} \left(g_{gb}^{(k)} \cdot y_{gb}^{(i,j)}\right) \dot{\theta}_j - \tau_{gb}^{(k)} \frac{c}{S_j} \exp \left(-\frac{U_d}{k_b \theta_j}\right).
\]

The first item describes increasing of critical stress by intrusion during grain boundary sliding, \(q\) is nondimensional model parameter defined due to model identification; \(\gamma_{gb}^{(k)}\) is cumulative shear on grain boundary sliding system, \(h\) is hardening coefficient. The second item describes the decreasing of critical stress by increasing boundary energy due to inflow of intragranular dislocations (the summation is assumed only for slip systems of two adjacent grains, dislocations from which are really going out to boundary), \(g_{gb}^{(k)}\) is hardening (softening) matrix due to intragranular dislocations which are out to boundary facet, \(\gamma_{gb}^{(i,j)}\) is shear rate on \(i\) slip system in grain \(j\), \(b_{gb}^{(i,j)}\) is unit vector in the direction of Burgers vector for \(i\) slip system in grain \(j\), \(N_g\) is outer normal to the boundary for grain \(j\), \(H(\cdot)\) is Heaviside function. The third item describes diffusion processes [3] on the base of Arrhenius law, \(U_d\) is activation energy of thermally activated (diffusion) processes, \(c\) is the diffusion coefficient, \(S_j\) is square of boundary facet \(j\).

Constitutive model at mesolevel II has the form:

\[
\begin{align*}
\dot{\mathbf{u}}_H &= \mathbf{u}_H : \left(\mathbf{d}_H - \mathbf{d}_H^w - \mathbf{d}_H^\theta\right) + \mathbf{\omega}_H \cdot \mathbf{\sigma}_H - \mathbf{\sigma}_H \cdot \mathbf{\omega}_H, \\
\mathbf{d}_H &= \mathbf{u}_H \dot{\theta}_H, \\
\dot{\theta}_H &= \mathbf{u}_H : \mathbf{\sigma}_H - C_m \rho, \\
\dot{\mathbf{V}}_H &= \dot{\mathbf{V}}_H - \dot{\mathbf{V}}_{gb}, \\
\mathbf{d}_H &= \frac{1}{2} \left(\dot{\mathbf{V}}_H + \left(\dot{\mathbf{V}}_H^*\right)^T\right), \\
\gamma_i^I &= \gamma_0 \left(\frac{\tau_i^I}{\tau_c^I}\right)^{\frac{1}{\nu}} H(\tau' - \tau_c^I) \exp \left(-\frac{U_d}{k_b \theta_j}\right), \\
\tau_c^I &= f(\gamma_i^I, \dot{\gamma}_i^I, \theta_j), \\
\mathbf{d}_H^w &= \frac{1}{2} \sum_{i=1}^{K_g} \beta_{ij} \gamma_i^I \left(\mathbf{d}_H^w b_{ij} + \mathbf{b}_i^w \mathbf{n}_j^I\right), \\
\text{relations for lattice spin } &\mathbf{\omega}_H, \dot{\mathbf{a}} \cdot \mathbf{a}^T = \mathbf{\omega}_H.
\end{align*}
\]

Hooke's law in rate form (3)\(_1\) is the constitutive relation of mesolevel II model. The explicit internal variables of mesolevel II model are elastic modulus tensor \(\mathbf{u}_H\), inelastic \(\mathbf{d}_H^w\) and thermal \(\mathbf{d}_H^\theta\) components of the strain rate tensor, spin of movable coordinate system \(\mathbf{a}_H\) defined quasi-solid motion. Thermal component \(\mathbf{d}_H^\theta\) is defined by relation (3)\(_2\), where \(\mathbf{a}\) is thermal expansion tensor. Relation (3)\(_3\) describes temperature change due to inelasticity, \(\alpha_H\) is coefficient of heat eduction, \(C_m\) is specific heat, \(\rho\) is substance density. The implicit internal variables are shear rates of intragranular dislocation sliding \(\dot{\gamma}_i^I\) and critical shear stress rates \(\dot{\tau}_c^I\): shear rate is determined by elastoviscoplastic relation (3)\(_4\) with regard to activation energy of inelastic deformation \(U\), hardening law (3)\(_7\) is used for describing the critical shear stresses [9]. Macrolevel velocity gradient \(\dot{\mathbf{V}}\) is transmitted as forcing to mesolevel II (3)\(_4\) with taking into account that some forcing is dedicated to grain boundary sliding.
realization $\hat{V}V_{gb}$ at mesolevel I. Schmid law as a criterion of shear activity (dislocation motion) is used to describe intragranular dislocation sliding [4]. Rotation model with regard to incompatibility of dislocation sliding in neighboring crystallites is suggested [9].

Introduction the tensor variable $\mathbf{z}$ for each crystallite as a characteristic of it's shape and boundary is proposed for grain structure description. The equation for this parameter evolution will be added to the relation structure at mesolevel II (3) on the base of forming, breaking and fragmentation consideration. In the future it is planned to connect the volume fractions of grain boundaries $\alpha_{ij}$ and grain interior $\beta_{ij}$ included in the kinetic equations of mesoscale levels with the representative volume averaging of parameter mentioned above.

3. Results of modelling
The computational experiment under uniaxial tension of polycrystalline pure copper (1000 crystallites) is conducted. Parameters for shear description are taken as in [9]. Parameters for grain boundary sliding description are as follows:

$$c \exp \left( \frac{-U_{gb}}{k\theta} \right) = 0.1 m^2 \cdot s^{-1}, \quad q = 1,$$

$$\tau_{gb}^i = \text{exp} \left( \frac{-10}{0.1 \cdot h \cdot \text{MPa}} \right), \quad g^i_0 = 0.33 \quad \forall k, i.$$.

The results are obtained for four different choices of parameters (Figure 1): (1) $h = 1$, $\tau_{gb}^i(0) = 15 \text{MPa}$ $\forall i$, (2) $h = 0.8$, $\tau_{gb}^i(0) = 14 \text{MPa}$ $\forall i$, (3) $h = 0.6$, $\tau_{gb}^i(0) = 14 \text{MPa}$ $\forall i$, (4) $h = 0.4$, $\tau_{gb}^i(0) = 13 \text{MPa}$ $\forall i$. The first set of parameters corresponds to coarse grain structure, the last one corresponds to fine grain structure, when grain boundary sliding is relieved.

![Figure 1](image)

**Figure 1.** Dependence of the stress intensity from the strain intensity for four different types of grain structure ((1) – coarse grain structure, (4) – fine grain structure).

The results obtained show the increasing role of grain boundary sliding during deformation process, fine grain structure is characterized by a lower flow stress in comparison with coarse grain structure.

4. Conclusion
Three-level constitutive polycrystalline model is developed taking into account main mechanisms of inelastic deformation: intragranular dislocation sliding, lattice rotation and grain boundary sliding. The model includes temperature and consistency conditions of constitutive relations at different scale levels. Special attention is devoted to grain boundary sliding description due to included various mechanisms of interaction between defects into evolution relations: it is assumed on the base of existing theoretical and experimental data analysis that grain boundary sliding is occurred by inflow of intragranular dislocations, change in the boundary structure under realization of grain boundary sliding and diffusion processes. The results of computational experiments under uniaxial tension of a
polycrystalline pure copper are obtained. They show model resources in description of increasing role the grain boundary sliding during deformation process.

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