

# Multilevel model of polycrystalline materials: grain boundary sliding description

**E Sharifullina, A Shveykin and P Trusov**

Department of Mathematical Modeling of Systems and Processes, Perm National Research Polytechnic University, 29 Komsomolsky prospekt, Perm, 614990, Russia

E-mail: elvira16\_90@mail.ru

**Abstract.** Material behavior description in a wide range of thermomechanical effects is one of the topical areas in mathematical modeling. Inclusion of grain boundary sliding as an important mechanism of polycrystalline material deformation at elevated temperatures and predominant deformation mechanism of metals and alloys in structural superplasticity allows to simulate various deformation regimes and their transitions (including superplasticity regime with switch-on and switch-off regimes). The paper is devoted to description of grain boundary sliding in structure of two-level model, based on crystal plasticity, and relations for determination the contribution of this mechanism to inelastic deformation. Some results are presented concerning computational experiments of polycrystalline representative volume deformation using developed model.

## 1. Introduction

There are different approaches within the framework of multilevel and multiscale modeling of material inelastic deformation, based on crystal plasticity, in relation formulation for polycrystal inelastic behavior in the case of large deformation gradients. These models have two main aspects [1]: crystallite behavior description (crystal plasticity model is the basis of this level) and description of transition from crystallite level to macroscopic level. The last aspect is one of the important tasks, which solution could be achieved by different ways.

The most popular Taylor – Bishop – Hill models [2] (or Full Constraints (FC) models) are classical statistical models, based on relatively independent consideration mesolevel elements (crystallites, grains, subgrains); integration of mesolevel elements into macrolevel element (representative macrovolume or representative volume of macrolevel) is carried out by using the hypothesis about plastic strain homogeneity (plastic strain rate homogeneity) assumed a priori in all crystallites. It is noted in [1], that more common assumption – generalization of Voigt (Taylor) hypothesis about equality the velocity gradient in each crystallite of polycrystal to macroscopic velocity gradient ( $\hat{\mathbf{V}}^T = \hat{\mathbf{V}}^T$ ) could be performed. In a number of papers it is proposed Relaxed Constraints (RC) models, which don't strictly enforce condition about velocity gradient equality and «relax» it for some components. In these models the internal structure of a polycrystalline material is modeled as lamellar structure consisting of elongated grains. The assumption about homogeneity of velocity gradient is used not for each crystallite but for stacks of two crystallites, other relations are formulated for these stacks too. Different models (Pancake, Lath, Lamel and ALamel models) exist depending on hypothesis about possible directions of relative crystallite displacements along a common boundary,



shears are defined using these displacements, which act as additional ones with respect to shears from Taylor model. Other type of models are viscoplastic self-consistent (VPSC) [3, 4, 5], which consider crystallites in a representative macrovolume as inhomogeneous inclusions interacting with some homogeneous effective medium with characteristics weighted averaged over all the crystallites from this representative volume. Cluster model is another common type of models [6, 7] (above-mentioned models, considering interactions between crystallite pairs, can be classified as cluster models, in which the cluster consists of two crystallites). In [7] it is pointed out that introduction of additional (intermediate) scale level between macrolevel and mesolevel (level of individual grains) comprising of cluster of several crystallites provides the possibility to come close to physics of their interaction.

The description of statistical model modification is performed in this paper including grain boundaries along with grains to take into account the mechanism of grain boundary sliding (GBS). We focus on description of GBS mechanism in the structure of two-level model, relationships between levels and equations for determination the contribution of this mechanism to inelastic deformation.

## 2. Grain boundary sliding description within two-level model

The structure of basic two-level model and its general relations are presented in detail, for example, in [8]. The developed model unlike the last one includes on macro- and mesolevel not only stress state measure (and its objective rate) and strain rate measure, but temperature and grain structure state (in view of GBS description in wide range of influence changes included superplastic deformation regime) as process characteristics. Besides, it is used a new method of motion decomposition, proposed by the authors of paper [9]: Cartesian orthogonal coordinate system with quasi-solid motion (moving coordinate system) [9, 10] is introduced for each crystallite and is associated with its symmetry elements – crystallographic direction and plane, containing this direction.

In accordance with modifications, noted above, the constitutive mesolevel model for each crystallite assumes the following form (crystallite index is omitted):

$$\mathbf{\kappa}^{\text{cor}} \equiv \dot{\mathbf{\kappa}} - \bar{\mathbf{\omega}} \cdot \mathbf{\kappa} + \mathbf{\kappa} \cdot \bar{\mathbf{\omega}} = \bar{\mathbf{\Pi}} : (\mathbf{z} - \mathbf{z}_s^{\text{in}} - \mathbf{z}^{\text{th}}) = \bar{\mathbf{\Pi}} : (\hat{\mathbf{V}}\mathbf{v}^T - \bar{\mathbf{\omega}} - \mathbf{z}_s^{\text{in}} - \mathbf{z}^{\text{th}}), \quad (1)$$

$$\theta = \Theta, \dot{\theta} = \dot{\Theta}, \quad (2)$$

$$\hat{\mathbf{V}}\mathbf{v}^T = \hat{\mathbf{V}}\mathbf{V}^T - \mathbf{z}_{\text{gb}}^{\text{in}}, \quad (3)$$

$$\mathbf{z}_s^{\text{in}} = \sum_{i=1}^K \dot{\gamma}^{(i)} \mathbf{b}^{(i)} \mathbf{n}^{(i)}, \quad (4)$$

$$\dot{\gamma}^{(i)} = f_1(\tau_c^{(i)}, \tau_c^{(i)}, \theta), i = 1, \dots, K, \quad (5)$$

$$\dot{\tau}_c^{(i)} = f_2(\dot{\gamma}^{(i)}, \gamma^{(i)}, \theta), i = 1, \dots, K, \quad (6)$$

$$\mathbf{q} = f_3(\mathbf{\kappa}, \mathbf{z}_s^{\text{in}}), \quad (7)$$

$$\mathbf{z}^{\text{th}} = \alpha \dot{\theta}, \quad (8)$$

$$\bar{\mathbf{\omega}} = f_4(\hat{\mathbf{V}}\mathbf{v}^T, \dot{\gamma}^{(i)}, \boldsymbol{\mu}), \bar{\mathbf{\omega}} = \dot{\mathbf{r}} \cdot \mathbf{r}^T, \quad (9)$$

$$\mathbf{r} \cdot \mathbf{g} \cdot \mathbf{r} = 1, \mathbf{g} = \mathbf{f}^{-T} \cdot \mathbf{g}_0 \cdot \mathbf{f}^{-1}, \quad (10)$$

where (1) is constitutive relation in terms of actual configuration (hypoelastic law),  $\mathbf{\kappa}$  is Kirchhoff stress tensor of mesolevel,  $\mathbf{\kappa} = \overset{\circ}{\rho}(\hat{\rho}\boldsymbol{\sigma})^{-1}$ ,  $\boldsymbol{\sigma}$  is Cauchy stress tensor,  $\overset{\circ}{\rho}$  is material density of crystallite in reference configuration,  $\hat{\rho}$  is material density of crystallite in actual configuration,  $\mathbf{\kappa}^{\text{cor}} = \dot{\mathbf{\kappa}} - \bar{\mathbf{\omega}} \cdot \mathbf{\kappa} + \mathbf{\kappa} \cdot \bar{\mathbf{\omega}}$  is objective rate (corotational derivative) of stress state measure on mesolevel,

$\bar{\omega}$  is spin tensor, which defines rotation rate of crystallite moving coordinate system,  $\bar{\mathbf{n}}$  is elastic modulus tensor of crystallite (its components are constant in the basis of moving coordinate system),  $\hat{\nabla} \mathbf{v}^T = \dot{\mathbf{f}} \cdot \mathbf{f}^{-1}$  is transposed velocity gradient, which is transmitted from macrolevel with extended Voigt hypothesis (3) taking into account the implementation of some forcing due to GBS mechanism  $\mathbf{Z}_{\text{gb}}^{\text{in}}$ ,  $\mathbf{z} = \bar{\nabla} \mathbf{v}_r^T = \hat{\nabla} \mathbf{v}^T - \bar{\omega}$  is strain rate measure, determined as transposed relative velocity gradient  $\mathbf{v}_r$  (relative to moving coordinate system of mesolevel),  $\bar{\nabla}$  and  $\hat{\nabla}$  are nabla-operators in moving and actual Lagrangian coordinate systems respectively,  $\mathbf{z}_s^{\text{in}}$  and  $\mathbf{z}^{\text{th}}$  are inelastic and thermal components of transposed relative velocity gradient. Inelastic component  $\mathbf{z}_s^{\text{in}}$  is defined by relation (4), in which  $\mathbf{b}^{(i)}$  and  $\mathbf{n}^{(i)}$  are unit vectors of slip direction and normal to slip planes in actual configuration, intragranular shear rates  $\dot{\gamma}^{(i)}$  (relation (5)) in each crystallite describe the contribution to inelastic deformations due to intragranular dislocation sliding in terms of crystallographic slip planes for this material ( $K$  is number of slip systems) using Arrhenius-type relation. Strengthening law (6) is used to describe the evolution of critical shear stresses  $\tau_c^{(i)}$ , rates of critical shear stresses  $\dot{\tau}_c^{(i)}$  are generally a function of accumulated shears and shear rates on slip systems as well as temperature [8]. Relation (7) includes internal heat source capacity  $q$ , which is determined due to energy dissipation on inelastic strains in crystallite and transmitted to macrolevel. Thermal component  $\mathbf{z}^{\text{th}}$  is defined by relations (8), in which  $\alpha$  is thermal expansion tensor,  $\dot{\theta}$  is temperature rate (from relation (2)). To determine  $\bar{\omega}$  (relation (9)) the rotation model from [9] is used. Orientation change of moving coordinate system for each crystallite during deformation process is described with orthogonal tensor  $\mathbf{r}$  established by integrating the rotation rate  $\dot{\bar{\omega}} = \dot{\mathbf{r}} \cdot \mathbf{r}^T$ . The first relation in (10) determines surface of crystallite (its shape is assumed to be ellipsoidal),  $\mathbf{g}$  is second rank tensor defining both crystallite geometry (shape and dimensions using the lengths of three semi-axes) and its spatial orientation; the second relation in (10) characterizes form change using applied kinematics (strain gradient  $\mathbf{f}$ ), change of tensor form can be also formulated taking into account realization of fragmentation and breaking (more detail in [11]).

System of equations on macroscale level assumes the following form:

$$\mathbf{K}^{\text{cor}} \equiv \dot{\mathbf{K}} - \bar{\Omega} \cdot \mathbf{K} + \mathbf{K} \cdot \bar{\Omega} = \bar{\Pi} : (\mathbf{Z} - \mathbf{Z}_{\text{gb}}^{\text{in}} - \mathbf{Z}_s^{\text{in}} - \mathbf{Z}^{\text{th}}) = \bar{\Pi} : (\hat{\nabla} \mathbf{V}^T - \bar{\Omega} - \mathbf{Z}_{\text{gb}}^{\text{in}} - \mathbf{Z}_s^{\text{in}} - \mathbf{Z}^{\text{th}}), \quad (11)$$

$$\bar{\Omega} = \langle \bar{\omega} \rangle, \quad (12)$$

$$\bar{\Pi} = \langle \bar{\mathbf{n}} \rangle, \quad (13)$$

$$\mathbf{Z}_s^{\text{in}} = \langle \mathbf{z}_s^{\text{in}} \rangle + \bar{\Pi}^{-1} : \langle \bar{\mathbf{n}}' : \mathbf{z}_s^{\text{in}'} \rangle + \bar{\Pi}^{-1} : (\langle \mathbf{\kappa}' \cdot \bar{\omega}' \rangle - \langle \bar{\omega}' \cdot \mathbf{\kappa}' \rangle), \quad (14)$$

$$\mathbf{Z}^{\text{th}} = \langle \mathbf{z}^{\text{th}} \rangle + \bar{\Pi}^{-1} : \langle \bar{\mathbf{n}}' : \mathbf{z}^{\text{th}'} \rangle, \quad (15)$$

$$\mathbf{k} \dot{\theta} = \langle q \rangle, \quad (16)$$

where constitutive relation (11) is also formulated in actual configuration,  $\mathbf{K}$  is Kirchhoff stress tensor of macrolevel,  $\mathbf{K}^{\text{cor}} = \dot{\mathbf{K}} - \bar{\Omega} \cdot \mathbf{K} + \mathbf{K} \cdot \bar{\Omega}$  is objective rate (corotational derivative) of stress state measure on macrolevel. Spin tensor  $\bar{\Omega}$  of moving coordinate system (relation (12)) and elastic modulus tensor  $\bar{\Pi}$  (relation (13)) are transmitted from mesolevel to macrolevel using the averaging operation over a representative macrovolume. Tensors  $\mathbf{Z}_s^{\text{in}}$  (relation (14)) and  $\mathbf{Z}^{\text{th}}$  (relation (15)) are defined from mesolevel model with consistency conditions [12], the following notations are used:  $\langle \rangle$  as in relations (12) and (13) is for averaging operation over a representative macrovolume, line quantities  $\mathbf{a}'$  are for deviation of tensor characteristic  $\mathbf{a}$  in crystallite (to reduce notation the crystallite

index is omitted) from the mean value ( $\mathbf{a}' = \mathbf{a} - \langle \mathbf{a} \rangle$ ), averaging operation has a property:  $\langle \mathbf{a}' \rangle = 0$  for any characteristic  $\mathbf{a}$ . Temperature rate on macrolevel  $\dot{\Theta}$  in relation (16) is defined due to averaging of internal heat source capacity  $q$  over a representative macrovolume,  $k$  is heat capacity (generally temperature and temperature rate are defined from boundary value problem for temperature). We will have more to say below about inclusion of GBS mechanism in structure of performed two-level statistical model and description of inelastic component  $\mathbf{Z}_{gb}^{in}$  due to realization of this mechanism.

The following modification of model is proposed. Two structural levels are distinguished by mechanisms: one of them is associated with description of intragranular dislocation sliding (this structural level refers to the scale of mesolevel), the other – with description of GBS (this structural level refers to the scale of macrolevel). The level of GBS description is introduced as a separate structural level, and the model is modified into a three-level one: macrolevel – structural level of GBS description (it is considered as a macrolevel submodel) – mesolevel. Relative displacements of crystallites (grains, subgrains) along the common boundary during GBS are observed in bicrystals and polycrystals [13]. In polycrystalline materials GBS is limited by neighboring crystallites, which is modeled in grain boundary hardening law [12]. It is assumed that grain boundary of each crystallite is a set of flat facets with zero thickness, each pair of neighboring crystallites in a representative macrovolume has a common boundary facet, and relative displacements of crystallites occur along a common facet by moving grain boundary dislocations (however the last one is not modeled in explicit form). Basis of vectors  $\mathbf{n}_{gb}$ ,  $\mathbf{b}_{gb}^{(1)}$  and  $\mathbf{b}_{gb}^{(2)}$  in three-dimensional space is introduced to determine GBS for each intergranular facet:  $\mathbf{n}_{gb}$  – normal to the facet plane,  $\mathbf{b}_{gb}^{(1)}$  and  $\mathbf{b}_{gb}^{(2)}$  – sliding directions in the facet plane. The transition from displacements to deformation characteristics is carried out for model construction: both for intragranular dislocation sliding and GBS displacement or set of displacements (velocities) is approximated by shear (shear rate) on a certain volume.

Now we formulate the relation for shear rate due to GBS using analogy with Orowan equation for intragranular shear rate [14]. The following model description of real kinematics during GBS is adopted: the relative velocity of two crystallites along the common boundary is approximated by shear rate of the entire representative macrovolume, this procedure is repeated for each pair of neighboring crystallites. Representative macrovolume contains, in general case, differently oriented boundaries with various directions of displacement vectors of grain boundary dislocations, that makes it impossible to define slip systems for GBS by analogy with slip systems for intragranular dislocation sliding. Each boundary facet is considered as a separate slip plane with its orientation and directions of displacement vectors in it, therefore it can be assumed that in this slip plane (boundary facet)  $N_{gb}$  grain boundary dislocations move (i.e. in this case each slip system of GBS is represented by one slip plane). Then the value of shear rate in a representative macrovolume as a result of displacement of  $N_{gb}$  grain boundary dislocations in direction  $i$  in boundary facet with using relation for  $\bar{v}_{gb}$  [15, 16] can be written:

$$\dot{\gamma}_{gb}^{(i)} = \frac{1}{h} K_V^{(i)} v_{gb0}^{(i)} \left( \frac{\tau_{gb}^{(i)}}{\tau_{cgb}^{(i)}} \right)^{\frac{1}{n}} \exp \left( -\frac{\Delta F}{k\theta} \right), i = 1, 2, \dots, 4K_{gb}, \sum_i \quad (17)$$

where  $h$  is crystallite size–height (the average crystallite size in a representative macrovolume), coefficient  $K_V^{(i)} = h l_{gb} d_{gb} (\text{HLD})^{-1}$  is ratio of crystallite volume to representative volume of macrolevel,  $l_{gb}$  is boundary length,  $v_{gb0}^{(i)} = b_{gb}^{(i)} \rho_{gb}^{(i)} v_0 \Delta l_{gb} A$  is initial velocity of grain boundary dislocations in boundary facet,  $b_{gb}^{(i)}$  is displacement vector module of grain boundary dislocations,  $\rho_{gb}^{(i)} = N_{gb} d_{gb} (l_{gb} d_{gb})^{-1}$  is density of grain boundary dislocations (dimension is 1/m) as a ratio of total length of grain boundary dislocations in boundary facet to the boundary facet area [17], the absence of a model description of breaking processes (changes in crystallite size during deformation) allows to

combine the quantities into one parameter  $(h)^{-1} K_V^{(i)} v_{gb0}^{(i)} \equiv \dot{\gamma}_{gb0}^{(i)}$ ,  $\dot{\gamma}_{gb0}^{(i)}$  is initial shear rate in boundary facet,  $n$  is rate sensitivity parameter,  $\Delta F$  is magnitude of the energy barrier (activation energy of GBS),  $k$  is Boltzmann constant,  $4K_{gb}$  is total number of sliding directions for all boundary facets in a representative macrovolume.

The inelastic component of transposed relative velocity gradient  $\mathbf{Z}_{gb}^{in}$  due to GBS realization is determined from the shear rates (17) as follows:

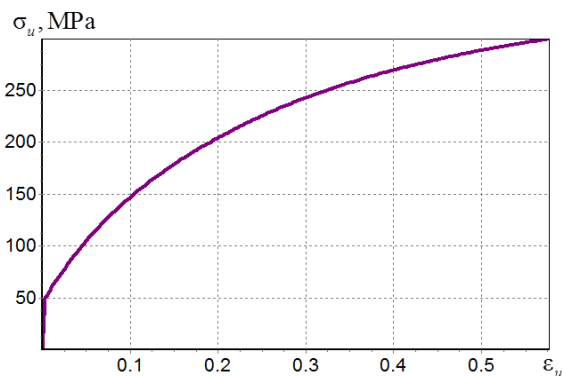
$$\mathbf{Z}_{gb}^{in} = \sum_{i=1}^{4K_{gb}} \dot{\gamma}_{gb}^{(i)} \mathbf{b}_{gb}^{(i)} \mathbf{n}_{gb}^{(i)}. \quad (18)$$

### 3. Results of modelling

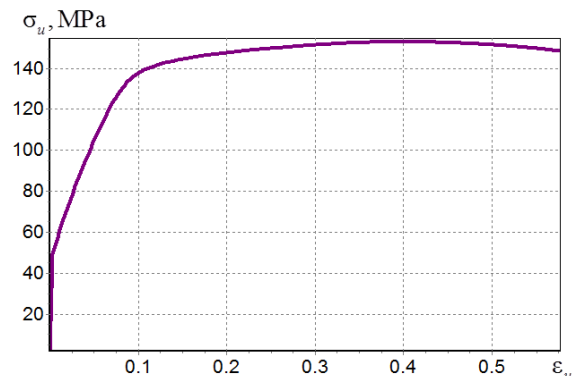
The results for simple shear of polycrystalline representative macrovolume (343 crystallites) in isothermal case using parameters of material model close to copper are performed below. Intragranular hardening law (6) with parameters is from [18]. Relation for critical stress evolution of grain boundary shears  $\tau_{cgb}^{(i)}$  is taken as in the work [11], submodel for GBS description includes following parameters:

$$\dot{\gamma}_{gb0} \exp(-\Delta F(k\theta)^{-1}) = 10^{-4} s^{-1}, \quad n = 0.02, \quad \tau_{cgb}^{(i)}(0) = 80 \text{ MPa}, \quad h = 3000 \text{ MPa}, \quad g = 0.01, \\ g_i^k = 1000 \text{ MPa} \quad \forall k, i, \quad c(S_i)^{-1} \exp(-U_d(k\theta)^{-1}) = 0.0005 s^{-1}.$$

Figure 1 and figure 2 show macrolevel stress intensity – strain intensity diagrams when process of simple shear of polycrystal using two-level model (without GBS) and three-level model (with GBS) is considered.



**Figure 1.** Stress intensity – strain intensity diagrams, obtained in calculations with two-level model without GBS.



**Figure 2.** Stress intensity – strain intensity diagrams, obtained in calculations with three-level model with GBS.

The obtained curve in figure 2 has lower flow stress and flattened form compared with curve in figure 1. It means that after reaching a certain amount of strain intensity (in this case at about 0.1) GBS mechanism switches on and becomes dominant. The presented results demonstrate model capabilities in description of GBS and transitions to deformation regimes with reduced flow stresses, particularly, regime of structural superplasticity, when GBS is important mechanism.

### 4. Conclusion

Modification of statistical model – three-level constitutive model of polycrystal, which takes into account intragranular dislocation sliding and GBS as main mechanisms of inelastic deformation, is developed. The model also includes temperature, characteristics of grain structure and relationship between the levels. Special attention is given to description of GBS within two-level model and relations, which determine the contribution of this mechanism to inelastic deformation. The results of numerical experiments on the modeling of a simple shear of polycrystal copper sample are presented.

They demonstrate significant role of GBS and characterize the model as promising from the point of view of its capabilities for describing different deformation regimes (depending on the temperature-rate conditions and the state of grain structure) and transitions between them.

### Acknowledgements

The work was supported by the Russian Federation Ministry of Education and Science (basic part of the state task PNRPU, project №9.7434.2017/8.9), RFBR (grants Nos. 15-08-06866-a, 17-41-590694-r\_a).

### References

- [1] Van Houtte P, Delannay L and Samajdar I 1999 *Textures and Microstructures* **31** 109
- [2] Taylor G 1938 *J. Inst. Metals* **62** 307
- [3] Lebensohn R 1999 *Modelling Simul. Mater. Sci. Eng.* **7** 739
- [4] Molinari A, Canova G and Ahzi S 1987 *Acta metall* **35** 2983
- [5] Tomé C 1999 *Modelling Simul. Mater. Sci. Eng.* **7** 723
- [6] Eisenlohr P, Tjahjanto D, Hochrainer T, Roters F and Raabe D 2009 *International Journal of Materials Research* **100** 500
- [7] Xie Q, Van Bael A, Sidor J, Moerman J and Van Houtte P 2014 *Acta Materialia* **69** 175
- [8] Trusov P, Shveykin A, Nechaeva E and Volegov P 2012 *Physical Mesomechanics* **15** 155
- [9] Trusov P and Shveykin A 2016 *Physical Mesomechanics* **19** 25
- [10] Pozdeev A, Trusov P and Nyashin Yu 1986 *Large elastoplastic deformations: theory, algorithms, applications* (Moscow: Nauka) p 232
- [11] Shveykin A and Sharifullina E 2015 *Nanomechanics Science and Technology: An International Journal* **6** 281
- [12] Trusov P, Sharifullina E and Shveykin A 2015 *IOP Conf. Series: Materials Science and Engineering* **71** 012081
- [13] Gleiter H and Chalmers B 1975 *High-angle grain boundaries* (Moscow: Mir) p 375
- [14] Orowan E 1940 *Proc. Phys. Soc.* **62** 8
- [15] Asaro R and Needleman A 1985 *Acta metal* **33** 923
- [16] Kocks U, Argon A and Ashby M 1975 *Prog. Mater. Sci.* **19** p 291
- [17] Orlov A, Perevezentsev V and Rybin V 1980 *Grain Boundaries in Metals* (Moscow: Metallurgiya) p 156
- [18] Anand L 2004 *Comput. Methods Appl. Mech. Engrg.* **193** 5359