PACS: 61.63.Bn

A.A. Nazarov[1,2], N.A. Enikeev[1], A.E. Romanov[3], T.S. Orlova[3], I.V. Alexandrov[1], I.J. Beyerlein[4]

MODELING OF GRAIN SUBDIVISION DURING SEVERE PLASTIC DEFORMATION BY VPSC METHOD COMBINED WITH DISCLINATION ANALYSIS

[1]Ufa State Aviation Technical University
Ufa, 450000, Russia

[2]Institute for Metals Superplasticity Problems, Russian Academy of Sciences
Ufa, 450001, Russia

[3]Ioffe Physico-Technical Institute, Russian Academy of Sciences
St. Petersburg, 194021, Russia

[4]Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Microstructure development during severe plastic deformation by simple shear is modeled using a combination of the visco-plastic self-consistent (VPSC) method and a disclination model. Strain incompatibilities between a homogeneous effective medium and a grain are calculated by VPSC. These are assumed to result in an accumulation of disclinations in the junctions of a grain that are relaxed by a growth of low-angle dislocation boundaries from the junctions. Predicted misorientation distributions between subgrains and their parent grains agree semi-quantitatively with experimental misorientation distributions for geometrically necessary boundaries. The texture after 100% simple shear was found to be insensitive to the presence of subgrains with misorientations less than 15°.

Introduction

Grain fragmentation and refinement is one of the most important consequences of dislocation substructure evolution during large plastic deformation common for crystals of different types [1,2]. Mechanisms and characteristics of microstructural refinement is a matter of great theoretical and practical importance, particularly in producing ultrafine grained materials using equal-channel angular pressing (ECAP) and other methods of severe plastic deformation [3]. In principle, the refinement process can be rigorously described in terms of dislocation dynamics, though full 3-*D* modeling is a challenging task due to the complex nature of dislocation multiplication, interaction and annihilation in real crystals. Recently, the disclination approach has been shown to be very helpful for the description of elementary processes of grain subdivision [1,4]. It has been proposed that grains subdivide by the growth of low-angle boundaries due to the motion of partial disclinations generated at grain boundaries and grain boundary junctions. In turn, this formalism alone cannot be used to analyze the whole process of grain subdivision, since it neglects the distribution of plastic deformation on slip systems and does not consider important crystallographic and geometric factors influencing grain refinement.

On the other hand, polycrystal models are successfully used to study the plastic deformation of polycrystals and texture formation. These models account for the distribution of strain among crystallographic slip systems and grains, albeit as an approximate continuum approach. The VPSC model is one such approach [5]. This model considers each grain as an ellipsoidal inclusion deforming in a homogeneous equivalent medium (HEM) representing the whole polycrystal. Very recently, this model has been applied to simulate the texture evolution during ECAP [6]. However, the one-site VPSC model used in the cited paper neglects the non-uniformities of the stress and strain within grains that lead to subdivison. Instead, a very simple geometric criterion of grain subdivision was used and thus internal grain microstructural development was neglected.

The joint use of disclination models with polycrystal modeling combines the advantages of both methods and makes a powerful tool for modeling microstructure development during large plastic deformation. In this combination, VPSC provides the data on the incompatibilities of strain between the HEM and a grain, while the disclination model predicts subgrain formation and characteristics. The aim of the present paper is to develop such a combined simulation scheme for severe plastic deformation. By modeling simple shear we will demonstrate that this scheme allows one to describe the main microstructural characteristics of grain subdivision, such as the evolution of misorientations and texture.

Description of the model

Following the basic ideas of the VPSC method, consider an ellipsoidal grain, Fig. 1,*b*, deforming in a HEM, representing the average behavior of the aggregate. Let the strain rate of the HEM be given by a tensor $\dot{\mathbf{E}}$. For the case of simple shear, Fig. 1,*a*, with a velocity gradient tensor in the 1, 2, 3 coordinate system

$$\mathbf{D} = \begin{pmatrix} 0 & D & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad (1)$$

the strain rate of the HEM is $\dot{E}_{12} = \dot{E}_{21} = D/2$, equal to the applied strain rate. The strain rate tensor of a grain is denoted as $\dot{\boldsymbol{\varepsilon}}$ and depends on its orientation. If the grain deforms differently than the HEM, strain incompatibilities will result in an accumulation of disclinations in the junctions of this grain that will force its splitting. Splitting occurs by redistribution of slip in different domains of the grain and formation of low-angle dislocation boundaries. To be able to introduce junction disclinations and obtain a criterion for the splitting, we approximate the grain by a parallelepiped circumscribing the corresponding ellipsoid (Fig. 1,*b*). Edges of this parallelepiped coincide with the axes of ellipsoid. The difference between the shear strain rates of the HEM and a grain, $\dot{E}_{12} - \dot{\varepsilon}_{12}$, are then transformed to the coordinate frame made by the axes of the ellipsoid (1′, 2′, 3′) (Fig. 1,*b*). Let ς_{ij} denote the components of this transformed tensor. Using the formulae in [7] one can calculate the rates of disclination accumulation on the edges of the parallelepiped as follows:

$$\dot{\Omega}_1 = [2\varsigma_{23}, \varsigma_{13}, \varsigma_{12}], \quad \dot{\Omega}_2 = [\varsigma_{23}, 2\varsigma_{13}, \varsigma_{12}], \; \dot{\Omega}_3 = [\varsigma_{23}, \varsigma_{13}, 2\varsigma_{12}]. \qquad (2)$$

If $\dot{E}_{12} - \dot{\varepsilon}_{12} > 0$ and when the maximum of Ω_1, Ω_2, Ω_3 exceeds the critical value of $\Omega_c = 1°$, it is assumed that a pair of dislocation boundaries with a misorientation vector $\boldsymbol{\theta} = \boldsymbol{\Omega}_1 + \boldsymbol{\Omega}_2 + \boldsymbol{\Omega}_3$ is formed along the diagonals of the parallelepiped as shown in Fig. 1,*b*. Full relaxation of junction disclinations and a rotation of two of the four subgrains formed with this misorientation vector result (Fig. 1,*c*). The sense of this rotation is chosen such that the subgrains rotate in a direction nearly opposite to that of the parent grain. Nucleation of subgrain boundaries as described above will be referred to as the *splitting* of a grain.

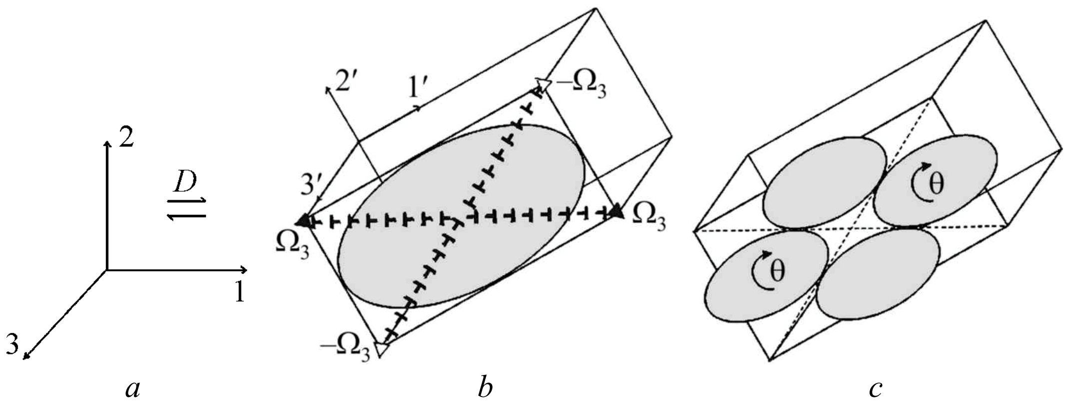

Fig. 1. A model of grain subdivision by a growth of a pair of subboundaries along the grain diagonals: *a* – coordinate frame: 1 – shear direction, 2 – normal direction, 3 – transverse direction; *b* – a junction disclination quadrupole and a mode of its relaxation; *c* – new grains (subgrains) formed due to subdivision

Further straining accumulates new disclinations on the junctions unless the strength of one of them exceeds Ω_c. These subsequent disclinations will relax by evolving along the initially formed low-angle boundaries causing a step-by-step increase in their misorientation angle. The rotation matrix for these stepwise subgrain rotations is accumulated unless the angle of rotation becomes larger than a value delimiting low- and high-angle grain boundaries (θ_0 = 10° to 15°). When this occurs, the grain is considered to *subdivide* into four grains, which are assigned corresponding orientations and further included into the aggregate simulated by VPSC. In turn, these new grains can split and subsequently subdivide during further straining thus leading to the formation of next-generation subgrains and new grains. Thus, the number of grains will progressively increase during deformation. Each time a grain can contain only one generation of subgrains; new generations will form when subgrains become independent grains and accumulate their own internal misorientation.

Results of simulations

To test the proposed simulation scheme simple shear of a polycrystalline aggregate containing initially 200 randomly oriented grains is modeled (Fig. 1,*a*). The evolution of the microstructure is described in terms of the calculated number of splitting/subdivison events per original grain, total number of split/subdivisions, misorientation distributions and texture for different values of applied strain. The low/high angle boundary limit is assumed to be 15°.

For the aggregate a simulated shear strain of E_{12} = 1.0 (equivalent von Mises strain E_{VM} = 1.12) resulted in 30 subdivisions; one grain subdivided 6 times, some grains 2 and 3 times, and others only once. The lower the strain rate of a grain, the more rapidly it divides into subgrains. Accumulation of a 15° misorientation sufficient for the first subdivision occurred after E_{12} = 0.36. Among 230 grains in the final aggregate, 152 grains are split into subgrains with misorientations less than 15°.

For each new grain and subgrain, the identity of their parent grain is recorded, which allowed a conditional misorientation distribution function $f(\theta)$ to be calculated. In calculating this function, misorientations θ of all new grains and subgrains with respect to the current orientation of their parent grain is taken into account. This function is calculated instead of the true distribution function, since in the 1-site VPSC neighborship of grains is not defined. Nevertheless, $f(\theta)$ can give semi-quantitative information on the distribution of misorientations of subboundaries. Histograms representing the distribution for three values of the shear strain are plotted in Fig. 2,*a*–*c*. In accordance with trends observed in experimental data [8–10], the distribution becomes wider and the average misorientation increases with increasing strain. The dependence of the average misorientation angle on the strain plotted in Fig. 2,*d* agrees quantitatively well with experimental data obtained on the substructure of cold-rolled metals [8–10].

Presented in Fig. 3 are the pole figures calculated for the polycrystal subjected to E_{12} = 1.0. Fig. 3,*a* has been calculated using output from the standard VPSC code, Fig. 3,*b* for the aggregate of 230 grains resulting from combined VPSC/disclination simulations, i.e. taking into account the orientations of only grains including those newly formed during deformation, while Fig. 3,*c* additionally includes all subgrains rotated to less than 15° with respect to their parent grains. Generally, during the simulation with grain subdivision texture develops in the same way as in the standard VPSC code. Maxima are located along the same

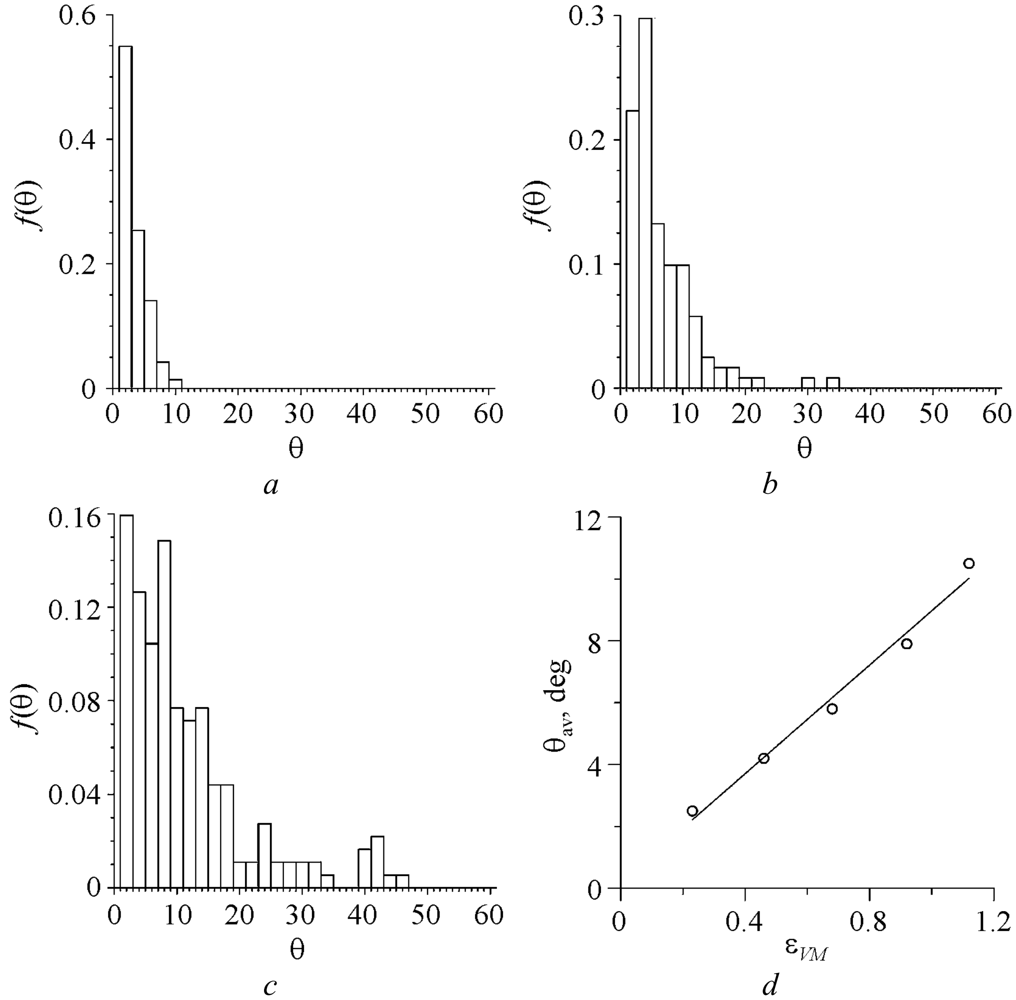

Fig. 2. Evolution of the conditional misorientation distribution function during simple shear strain up to E_{VM} = 0.23 (*a*), 0.68 (*b*), and 1.12 (*c*) and a plot of the average misorientation angle of subgrains with strain (*d*)

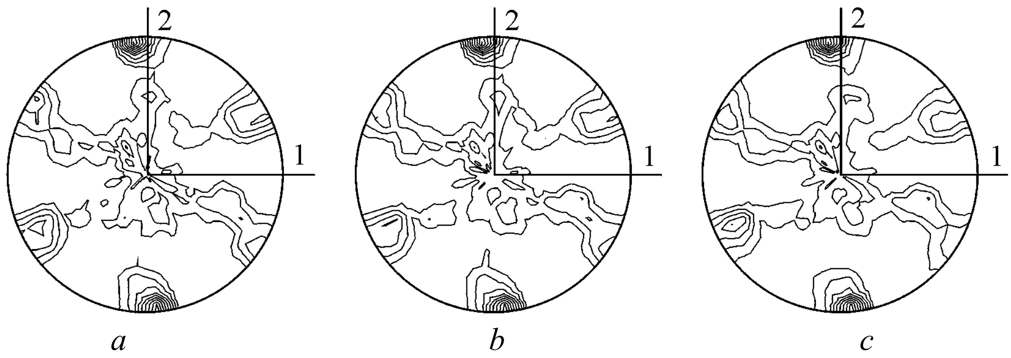

Fig. 3. Pole figures for a polycrystal with 200 initially random grains deformed by simple shear up to E_{VM} = 1.12: *a* – after a standard VPSC simulation (number of grains 200); *b* – after a VPSC/disclination simulation neglecting subgrains with misorientations $\theta < \theta_0 = 15°$ (final number of grains 230); *c* – as in *b*, additionally including subgrains (final number of grains and subgrains 382). Intensity level increment is equal to 0.95. Direction of shearing and axes are defined in Fig. 1,*a*

directions and have nearly the same value for all three cases (9.54, 9.64, and 9.56, respectively). It would be expected that the presence of low-angle misorientations of up to 15° inside grains would result in a significant spread of the texture. Surprisingly, however, only slight differences in the pole density in the vicinity of some maxima are observed in Fig. 3,*c* as compared to Fig. 3,*a*. Nevertheless, all the simulated pole figures are in a good qualitative agreement with well-known experimental data on standard textures for simple shear (see, for example [15]). This result may not be too surprising as standard VPSC has proven to predict well first ECAP pass textures in many materials (See [13] and [14] and references therein). However, the coupling between misorientation evolution and texture is expected to become stronger under larger strains and strain path changes, such as in ECAP.

Discussion

We have presented a simple model, which combines the advantages of both the VPSC polycrystal model and a disclination model for subgrain boundary nucleation and evolution and provides a possibility to study the substructure evolution during large plastic deformation. The key feature of this model is a splitting/subdivision criterion that is based on the disclination concept.

The relaxation of junction disclinations occurs by a complicated process of redistribution of slip near the junctions under the combined action of applied and internal stresses. This process has to be analyzed with a model that accounts for the non-uniformity of stress and strain inside grains. This can be done in terms of the n-site VPSC model [11] or a finite-element simulation. However for multiscale modeling, these methods would be computationally too expensive. Instead, physically-based models can be used to understand the modes of relaxation of disclinations. The model presented here is the simplest one of these. More sophisticated models can be put forward on the basis of an energetic analysis of disclination systems. The development of such models is under way [12]. Nevertheless, even with the simplest disclination subdivision criterion, this combined approach is capable of describing some important structural characteristics of heavily deformed polycrystals and thus can be used to simulate the ECAP process.

Recent electron microscope studies of cold-rolled polycrystals provided extensive data on the substructure evolution during large deformation. One of the important findings of those works is that geometrically-necessary boundaries (GNBs) form on two different scales [9]. The boundaries formed on a smaller scale slightly larger than the cell size have misorientations less than 6°, whereas the GNBs formed on a larger scale slightly smaller than the grain size can have misorientations exceeding 15°. It is the latter type whose average misorientation angle increases with strain in good accordance with the predictions presented in Fig. 2,*d* [9]. One can suggest that the first type of GNBs forms due to an inhomogeneity of strain inside grains, while the second type forms due to the incompatibility of strain of neighboring grains, by an accumulation and relaxation of junction disclinations.

Thus, the model presented in this paper describes well the formation and parameters of the largest-scale substructure in deformed metals, which is characterized by truly large-angle misorientations and most important for grain refinement by severe plastic deformation.

Finally, only slight differences of the final texture are found between the standard and modified VPSC codes for the case of simple shear up to 100%. However, for deformation with strain path changes, such as in multi-pass ECAP, a more significant influence of grain subdivision on texture can be expected.

This research is funded by a Los Alamos National Laboratory – Initiatives for Proliferation Prevention Project № T2-0197.

1. *V.V. Rybin*, Large Plastic Deformations and Fracture of Metals, Metallurgija, Moscow (1986).
2. *N. Hansen*, Scripta Metall. Mater. **27**, 1447 (1992).
3. *R.Z. Valiev, R.K. Islamgaliev, I.V. Alexandrov*, Prog. Mater. Sci. **45**, 103 (2000).
4. *A.E. Romanov, V.I. Vladimirov*, Dislocations in Solids, F.R.N. Nabarro (ed.), North-Holland, Amsterdam (1992), vol. 9, p. 191.
5. *R.A. Lebensohn, C.N. Tome*, Acta Metall. Mater. **41**, 2611 (1993).
6. *I.J. Beyerlein, R.A. Lebensohn, C.N. Tome*, Mater. Sci. Eng. **A345**, 122 (2003).
7. *V.V. Rybin, A.A. Zisman, N.Yu. Zolotarevsky*, Acta Metall. Mater. **41**, 2211 (1983).
8. *D.A. Hughes, Q. Liu, D.C. Chrzan, N. Hansen*, Acta Mater. **45**, 105 (1997).
9. *Q. Liu, D.J. Jensen, N. Hansen*, Acta Mater. **46**, 5819 (1998).
10. *D.A. Hughes, N. Hansen*, Acta Mater. **48**, 2985 (2000).
11. *R.A. Lebensohn*, Acta Mater. **49**, 2723 (2001).
12. *T.S. Orlova, A.A. Nazarov, N.A. Enikeev, I.V. Alexandrov, R.Z. Valiev, A.E. Romanov*, Phys. Solid State, submitted.
13. *S. Li, I.J. Beyerlein, C.T. Necker, D.J. Alexander, N.A.M. Bourke*, Acta Mater. **52**, 4859 (2004).
14. *S.C. Vogel, D.J. Alexander, I.J. Beyerlein, M.A.M. Bourke, D.W. Brown, B. Clausen, C.N. Tomé, R.B. Von Dreele, C. Xu, T.G. Langdon*, Mater. Sci. Forum **426–432**, 2661 (2003).
15. *U.F. Kocks, C.N. Tome, H.-R. Wenk*, Texture and Anisotropy, Cambridge Univ. Press, Cambridge (2000).