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THE INFLUENCE OF DIFFERENT TYPES OF MESODEFECTS ON THE FORMATION OF STRAIN INDUCED BROKEN DISLOCATION BOUNDARIES AT THE FACETED GRAIN BOUNDARY

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Abstract. In this paper we analyze mesodefects accumulating during plastic deformation on the faceted high angle grain boundaries. It is shown that the system of mesodefects can be represented as a set of linear mesodefects of the rotational type (junction disclinations), and planar mesodefects of the shear type (uniformly distributed dislocations with Burgers vector lying in the plane of the facet). The process of formation of broken dislocation boundaries in the elastic fields of various configurations of the abovementioned mesodefects is studied within the framework of computer simulation.

Keywords: fragmentation; broken dislocation boundaries; mesodefects; computer simulation.

1. Introduction

According to the modern concepts [1-2], the formation of misoriented structures at the initial stage of fragmentation of crystalline solids is caused by the accumulation of plastic incompatibilities on the boundaries and in the junctions of grains. Being relatively regular, they form the mesodefects (disclinations, dipoles of disclinations, planar mesodefects) that generate powerful nonuniform elastic stresses in grains of polycrystals [3-9].

These stresses disturb and redistribute the flows of lattice dislocations providing plastic deformation in the volume of grains and it leads to an unequal strain in the grain mesovolumes. As a consequence, spatially localized regions with an increased density of dislocation charge are formed near the mesodefects, which can be considered in the first approximation as broken dislocation boundaries separating mutually misoriented mesovolumes of the grain. Namely the strain induced broken dislocation boundaries are the most typical elements of the structure of materials at the early stages of fragmentation [1-2]. In recent years, a large number of papers have been devoted to the investigation of the formation of strain induced broken dislocation boundaries in the elastic field of isolated mesodefects [10-13]. It has been shown that the appearance of broken dislocation boundaries leads to a decrease in the elastic energy and to a decrease in the gradients of the internal stresses generated by mesodefects.

In fact, the systems of mesodefects appear on the grain boundaries of the plastically deformed polycrystal. Its configuration depends on the morphology of the grain boundary and the geometry of the lattice slip in the body of grains. In this paper, we analyze the influence of different mesodefect configurations on the formation of strain induced broken dislocation boundaries in case of a faceted tilt grain boundary.

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2. Analysis of mesodefects formed on the faceted grain boundary during plastic deformation

Different configurations of mesodefects can be formed on the grain boundary during plastic deformation depending on its geometry and orientation of the active slip planes. This is due to the fact that grain boundaries have morphological features in the form of ledges, facets and kinks existing in the initial state or arising during deformation [14-15]. In this paper, we consider mesodefects arising on a faceted tilt grain boundary consisting of identical structural elements, one of which is shown in Fig. 1. The normal components of Burgers vectors of dislocations accumulating during plastic deformation on the $j^{\text{-th}}$ facet of the grain boundary in the course of its interaction with the lattice dislocations flows (Fig. 1a) cause an additional misorientation $\vec{\theta}_j$.

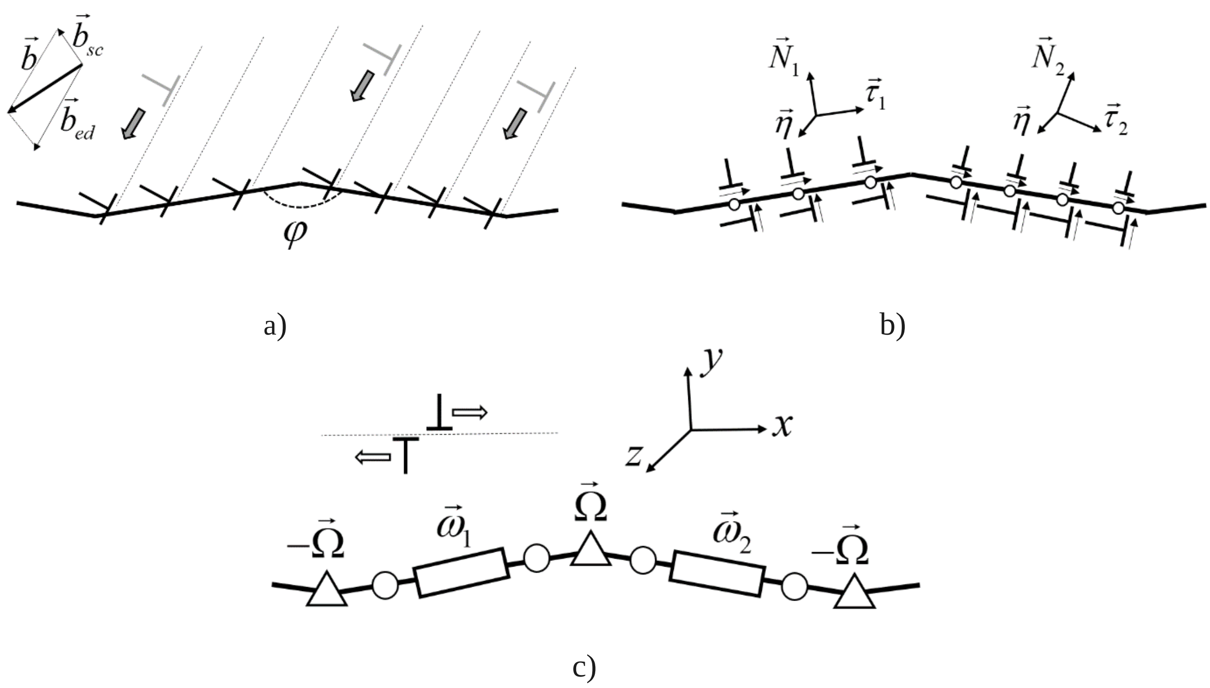


Fig. 1. Schematic plot of the system of mesodefects accumulating on a faceted tilt grain boundary during plastic deformation: (a) dislocations accumulating on the grain boundary due to its interaction with the flow of lattice dislocations; (b) representation of the dislocations in the form of edge and screw dislocations systems with normal and tangential components of the Burgers vector (the ○ symbols denote screw components); (c) the equivalent configuration of mesodefects: △ - junction disclinations, ○ - planar mesodefects, consisting of screw components, ▭ - planar mesodefects, consisting of edge components.

The linear mesodefects of the rotational type (i.e. unlike strain induced junction disclinations (Fig. 1c) with the strength $\vec{\Omega}_{j,j-1}$) appear at the tops of the joining facets as a result of a mismatch of additional plastic rotations $\vec{\theta}_j$ and $\vec{\theta}_{j+1}$,:

$$\vec{\Omega}_{j,j+1} = \vec{\theta}_j + \vec{\theta}_{j+1}. \tag{1}$$

The tangential components of Burgers vectors form a planar mesodefect with the strength $\vec{\omega}_j = [\omega_\tau \vec{\tau} + \omega_\eta \vec{\eta}]_j$ on the j^{th} facet. Here, $\omega_{\tau,j}$ and $\omega_{\eta,j}$ are the densities of Burgers vector of edge and screw of dislocations correspondingly. Thus, generally, the system of mesodefects on the faceted boundary is a combination of junction disclinations and planar mesodefects (Fig.1c). This general conclusion is valid for arbitrary geometry of lattice slip.

To calculate the mesodefects strength at the grain boundary with the normal $\vec{N}$ both in cases of discrete dislocations and its continual distribution with the given plastic distortion jump $\Delta\hat{\beta}$ it is necessary to find the tensor of Burgers vector density:

$$\hat{B} = \sum_k \left[\rho\left(\vec{\xi} \otimes \vec{b}\right)\right]_k = -\vec{N} \times \Delta\hat{\beta}, \tag{2}$$

where $\Delta\hat{\beta}$ is the difference of plastic distortion between joining grains, ρ_k is the linear dislocation density at the grain boundary and $\vec{\xi}_k$ is the unit vector of dislocation line for k[th] slip system. For the considered case of tilt grain boundary, the strengths of the abovementioned mesodefects are equal to:

$$\vec{\theta}_j = (\vec{\eta} \cdot \hat{B} \cdot \vec{N})\vec{\eta} = [(\Delta\beta_{xx} - \Delta\beta_{yy})N_x N_y + N_y{}^2\Delta\beta_{xy} - N_x{}^2\Delta\beta_{yx}]_j[\vec{l} \times \vec{N}], \tag{3}$$

$$\omega_{\tau,j} = (\vec{\eta} \cdot \hat{B} \cdot \vec{\tau})_j = [\Delta\beta_{xx}N_y{}^2 + \Delta\beta_{yy}N_x{}^2 - (\Delta\beta_{xy} + \Delta\beta_{yx})N_x N_y]_j, \tag{4}$$

$$\vec{\omega}_{\eta,j} = (\vec{\eta} \cdot \hat{B} \cdot \vec{\eta})_j = [N_y\Delta\beta_{xz} - N_x\Delta\beta_{yz}]_j. \tag{5}$$

Expressions for the fields of elastic stresses of junction disclination and the planar mesodefect consisting of the edge components of the dislocations are given in [9]. Calculation of the tensor of elastic stresses of planar mesodefect consisting of screw components of dislocations in the laboratory coordinate system (Fig. 1c) gives the following expressions:

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = 0,$$

$$\sigma_{xz} = \frac{G\omega_\eta}{2\pi}[arctg(\frac{x-a}{y}) - arctg(\frac{x+a}{y})],$$

$$\sigma_{yz} = \frac{G\omega_\eta}{4\pi}\ln[\frac{(x+a)^2 + y^2}{(x-a)^2 + y^2}],$$

where G is the shear modulus.

3. Description of the model

The simulation was carried out for 2D approximation in the framework of the approach described in [10,16-19]. To analyze the dynamics of a dislocation ensemble, we used the equation of dislocation motion in a quasi-viscous approximation [11, 16]:

$$v_k^i = M\left(\vec{n} \cdot \left(\hat{\sigma}^{ext} + \hat{\sigma}^{\text{int}}\right) \cdot \vec{b}\right)_k^i, \tag{6}$$

where v_k^i is the velocity of i^{th} dislocation in k^{th} slip system, $\left(\vec{n} \cdot \left(\hat{\sigma}^{ext} + \hat{\sigma}^{\text{int}}\right) \cdot \vec{b}\right)_k^i$ is the force acting on the dislocation in the slip plane, $\hat{\sigma}^{\text{int}}$ is the internal stresses tensor, defined as the total elastic field from the system of mesodefects and from the lattice dislocations ensemble, M is the dislocations mobility. Mobility, generation rate and radius of annihilation of dislocation are chosen to provide sufficiently high strain rate value $(10^{-3} - 10^{-2})\text{s}^{-1}$.

An analysis of the dynamics of the dislocation ensemble and the formation of the strain induced broken dislocation boundaries in the elastic fields of the considered mesodefects was carried out for the case of a faceted grain boundary with periodic arrangement of its structural elements. Let us consider separately the influence of boundary conditions on the results of the simulation. In order to reduce the influence of the size of the model crystal on the results of the calculation, the simulation of this process was carried out in the crystal central region containing only three structural elements of the faceted boundary (i.e. 6 facets), far from the edges of the model grain.

In this case, the total number of facets was chosen so that the difference in the values of the elastic stresses σ(x,y) from the mesodefects at neighboring "equivalent" points of the considered area, normalized to the value of averaged over these points stress value, did not exceed a certain value χ (<2%), characterizing the deviation from the periodic conditions. Results of the calculation of the value χ

$$\chi = \frac{1}{n}\sum_{i=1}^{n} abs(\frac{\sigma(x,y)-\sigma(x+x_p,y)}{\bar{\sigma}}), \tag{7}$$

performed for 400 different points from the considered area of the crystal depending on the number of facets n on each side of this region, are shown in Fig. 3. As can be seen from Fig. 4, a good approximation to periodic conditions is achieved even at a value n ≥ 20.

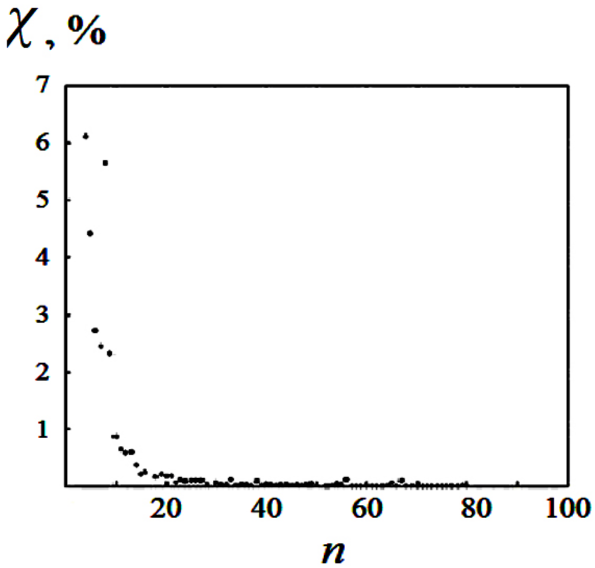


Fig. 2. Dependence of the value χ on the number of grain boundary facets.

Below, the crystal size for the computer simulation was chosen in such a way as to satisfy this condition.

4. Simulation results

The simulation was performed using the following parameters: the size of the considered region is 8 μm × 4 μm, the external stress is ~ 0.008 G, the loading axis is oriented perpendicular to the average orientation of the faceted boundary. The angle between the facets φ varied in the range of φ = 90° - 150°, the size of the facet x_p = 2 μm, the orientation of the accommodation slip plane of the dislocations α = 0° (Fig. 1). Various combinations of mesodefects induced by various plastic distortion jumps on the faceted boundary were considered.

The results of the research show that well-defined strain induced broken dislocation boundaries are formed in two limiting cases. The first one is realized when the influence of the elastic field of planar mesodefects on the motion of lattice dislocations in the accommodation slip plane can be neglected. In this case, broken dislocation boundaries are formed under the junction disclinations stress field and are mainly located perpendicular to accommodation slip plane.

For the selected deformation scheme at $\Delta\beta_{xx} = -\Delta\beta_{yy}$, $\Delta\beta_{xy} = \Delta\beta_{yx} = \Delta\beta_{xz} = \Delta\beta_{yz} = 0$ these conditions are satisfied for $|2N_x N_y| >> |N_y{}^2 - N_x{}^2|$ as follows from eq.(3, 4). As an example, the results of simulation of broken dislocation boundaries formation are shown in Fig. 3 for $\Delta\beta_{xx} = -\Delta\beta_{yy} = 0.02$, $\Delta\beta_{xy} = \Delta\beta_{yx} = \Delta\beta_{xz} = \Delta\beta_{yz} = 0$.

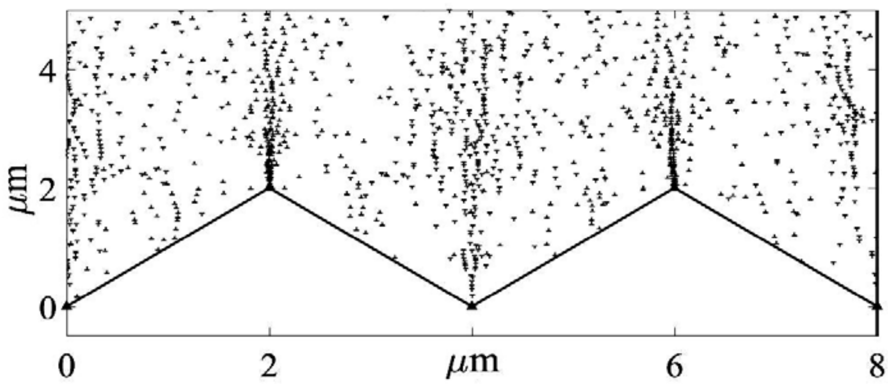
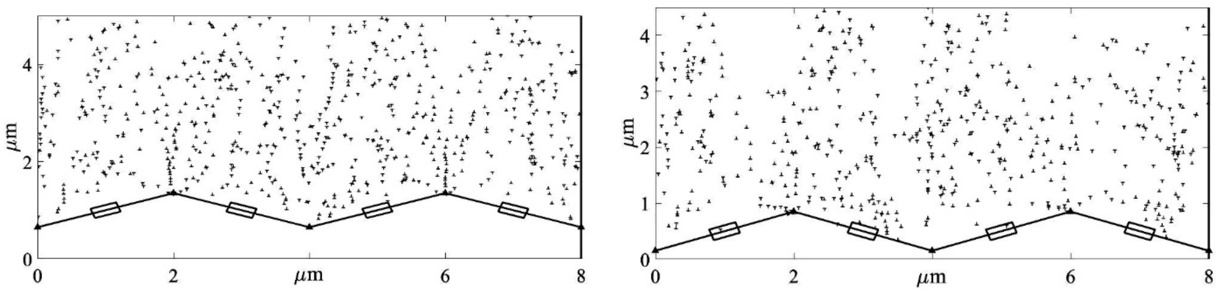


Fig. 3. Strain induced broken dislocation boundaries formed in field of elastic of junction dislclination's system.

In the second limiting case, with a small or zero strength of junction disclinations, a well-defined broken dislocation boundary is formed only in the case of a symmetrical arrangement of planar mesodefects, and accommodation slip plane parallel to the medium orientation of the faceted grain boundary. When deviation from the symmetrical arrangement of facets occurs, formation of such broken dislocation boundaries is suppressed.



a) b)

Fig. 4. Dislocation structure formed near grain boundary in the case of a) symmetric distribution of planar mesodefect (the strength of planar mesodefect is comparable to the strength of junction disclination) b) asymmetric distribution of planar mesodefect (the strength of planar mesodefect is comparable to the strength of junction disclination).

In the general case, the simulation shows that the presence of planar mesodefects suppresses the formation of broken dislocation boundaries. As an example, the results of simulation of dislocation structures formation near the facets tops are shown in Fig. 4 for a) $\Delta\beta_{xx} = -\Delta\beta_{yy} = 0.02$ $\Delta\beta_{xy} = \Delta\beta_{yx} = \Delta\beta_{xz} = \Delta\beta_{yz} = 0$ b) $\Delta\beta_{xx} = -\Delta\beta_{yy} = 0.02$ $\Delta\beta_{xy} = \Delta\beta_{yx} = 0.01$ $\Delta\beta_{xz} = \Delta\beta_{yz} = 0$.

5. Discussion

Discrete dislocation dynamics simulations have been used to investigate the formation of strain induced broken dislocation boundaries on the faceted grain boundary with the periodic arrangement of its structural elements. Despite this idealization, the broken dislocation boundaries morphology calculated by computer simulation methods is close to the experimentally observed boundaries, which appear near grain boundaries containing quasiperiodic facets with different sizes and orientations. It can be seen that broken dislocation boundaries are formed in the vicinity of the faceted high-angle grain boundary, growing from the tops of the joining facets into the body of grain.

As it follows from the simulation results, the field of elastic stresses created by the system of junction disclinations is responsible for their formation. The length of broken dislocation boundaries is comparable with the length of the facet. It can be shown that the broken dislocation boundaries are located along the zero-level stresses lines generated by a system of unlike junction disclinations.

As the simulation shows, well-defined broken dislocation boundaries are formed in the case when the strength of junction disclinations is much greater than the strengths of the planar mesodefects. For the given jump of plastic distortion tensor, this condition is satisfied only for a certain interval of orientations of the facets plane N_j and the interval of angles between the facets φ.

Nevertheless, it can be assumed that the formation of strain induced broken dislocation boundaries is possible in a more general case, when planar mesodefects and junction disclination have comparable strength. In our opinion, the process of broken dislocation boundaries formation may occur stepwise. At first, when a certain critical value of the planar mesodefect strength is reached, its relaxation occurs by plastic shear along the slip planes close to the facets plane.

This process should lead to the emission of lattice dislocations in the body of the grain. As a result, the strength of the planar mesodefect decreases, its elastic field relaxes and the conditions for the initiation of the accommodation process of junction disclination occurring by the formation of broken dislocation boundary are created. Such shear-rotational mechanism of relaxation of the elastic stress fields of mesodefects can explain the prevalence of strain induced broken dislocation boundaries near the facets and ledges of boundaries in plastically deformed polycrystals.

6. Conclusion

1. The computer simulation shows that well-defined strain induced broken dislocation boundaries are formed when the influence of the elastic field of planar mesodefects on the motion of lattice dislocations in the accommodative slip plane can be neglected. In this case, broken dislocation boundaries are formed under the effect of the elastic field of junction disclinations.
2. In the general case of comparable mesodefects' strengths, the formation of strain induced broken dislocation boundaries can be implemented by two sequentially occurring accommodation processes. The first one is associated with the relaxation of the planar mesodefect due to the emission of the plastic shear located on the facet into the body of the grain. The second one starts when the planar mesodefect strength decreases and is related to the broken dislocation boundaries formation.

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