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SOLID STATE

Model of Formation of Broken Dislocation Boundaries at Joint Disclinations

V. V. Rybin, V. N. Perevezentsev*, and Yu. V. Svirina

Mechanical Engineering Research Institute, Russian Academy of Sciences, ul. Belinskogo 85, Nizhny Novgorod, 603024 Russia

**e-mail: pevn@uic.nnov.ru*

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Abstract—We propose a physical model of formation of broken dislocation boundaries (partial disclinations of deformation origin) at the joints of large-angle grain boundaries. The model explains why and how rotational-type defects are necessarily formed in polycrystals in which plastic deformation at the microscopic level occurs exclusively via translational slips for strains $\varepsilon > 0.2$.

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INTRODUCTION

At the stage of developed plastic deformation, uniformly oriented grains of polycrystals are fragmented (i.e., split into a large number of strongly disoriented microscopic regions, viz., fragments) [1]. The transverse sizes d_m of the fragments range on the average from 0.2 to 0.3 μm, and disorientation angles Θ between them are distributed statistically in the interval from minimal value $\Theta_{\min} \approx 2°$ to the maximal value

$$\Theta_{\max} = \Theta_{\min} + \alpha(\varepsilon - \varepsilon_0). \quad (1)$$

Here, ε and ε_0 are the current and threshold values of strain,[1] and α is a coefficient describing the intensity of the process. It is usually assumed that the minimal disorientation angle Θ is equal to the average value of the Frank vector ω of partial disclinations of deformation origin. These specific mesodefects of rotational type play a very important part in fragmentation because it is these defects generated and moving over the crystal that cause relative rotations of crystal lattices of adjoining microscopic volumes.

The fragmentation phenomenon was detected for the first time in a neck directly under the surface of the fracture of a polycrystalline molybdenum cylindrical sample ($D \approx 40$ m) deformed at room temperature by uniaxial tension to $\varepsilon \approx 1$ with strain rate $\dot{\varepsilon} \approx 10^{-2}$ s^{-1} [2, 3]. It was found later that fragmentation is not exhausted by this particular case. It turned out that metals and alloys with different crystal lattices, different chemical and phase compositions, different initial structures and previous histories of preparation exhibit fragmentation. Fragmentation is observed in a wide range of temperature and strain-rate regimes ($T \leqslant 0.4T_m$, 10^{-3} s^{-1} $\leqslant \dot{\varepsilon} \leqslant 10^5$ s^{-1}) and technological schemes of plastic straining [1, 4–10]. These and other experimental facts convincingly prove that fragmentation is not at all a peculiar phenomenon. On the contrary, it should be considered as a natural and objectively existing stage in a chain of evolutionary transformations of structures of deformational origin that has not been studied comprehensively as of yet.

Fragmentation is manifested at a late stage of developed plastic deformation[2] ($\varepsilon \geqslant \varepsilon_0 \approx 0.2$), where it replaces the stages of formation of irregular non-disoriented and/or weakly disoriented cellular structures that have been studied comprehensively by the methods of dislocation physics.

The explanation of the nature of fragmentation can be reduced to the answer to the following question: how and why rotational-type mesodefects (partial disclinations of deformation origin) are nevertheless formed for $\varepsilon \geqslant \varepsilon_0$ in crystals the plastic deformation of which occurs on a microscopic level exclusively due to translational slips of the lattice? Here, we propose a model that makes it possible to analyze this problem at qualitative and quantitative levels, including the kinetics of formation and growth of partial disclinations of deformation origin, as well as the relation between the basic parameters of fragmentation physics ($\Theta_{\min}$ and ε_0).

[1] Here and below, ε and $\dot{\varepsilon}$ denote the true (logarithmic) strain and its rate.

[2] The structural feature of the beginning of the developed plastic deformation stage is the formation of partial disclinations of deformation origin, which is followed by fragmentation of the crystal [1].

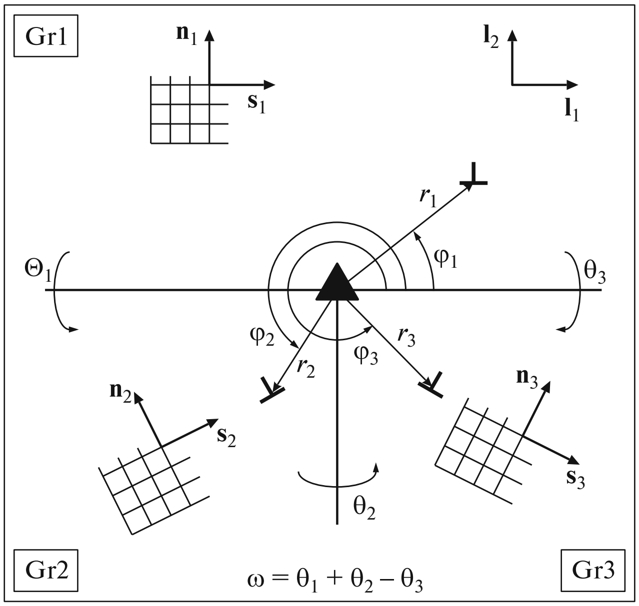

Fig. 1. Schematic representation of triple joint of grains.

1. MODEL

Numerous experimental data obtained using diffraction transmission electron microscopy show that partial disclinations of deformation origin observed at the stage of developed plastic straining have a number of common qualifying features [1, 11, 12]. These are dense broken dislocation boundaries (a) with predominant component of inclination; (b) with disorientation angle Θ exceeding disorientation of the boundaries of the (background) cellular structure formed earlier in the crystal; and (c) generated at joints, kinks, and ledges of large-angle grain boundaries[3] [1–3].

The latter distinguishing feature plays the key role in understanding the origin of partial disclination of deformation origin.

1.1. Joint Disclination of Deformation Origin

It was proposed in [1, 13, 14] that in the course of plastic deformation, special rotational-type mesoscopic defects that have not been described earlier in the literature appear at grain boundaries. These defects were called joint disclinations of deformation origin. It was assumed that these theoretically predicted mesodefects[4] generate in the surrounding space elastic stress fields σ_j of the disclination type with the power increasing monotonically with ε. At the stage of developed plastic deformation (for $\varepsilon \geqslant \varepsilon_0$), these fields attain critical values and begin to relax. Since joint disclinations are stationary, such a relaxation can only be due to a local redistribution of dislocations surrounding it. As a result, a broken dislocation boundary is generated at the joint with minimal disorientation angle $\Theta_{\min}$. In terms describing the evolution of mesodefects, this should be interpreted as the reaction of detachment of an elementary partial disclination of power ω_0 from the joint disclination. The relation between the micro- and mesolevels of description is established by the obvious equality $\Theta_{\min} = \omega_0$. The experimentally estimated power of such a partial disclination is $\omega_0 = 1°–2°$ [1].

1.2. Joint Disclination of Deformation Origin and Classical Taylor's Model

The above model of formation of partial disclinations of deformation origin required additional explanation because joint disclinations of deformation origin are absent in the classical dislocation model. To verify this, let us consider the joint of large-angle boundaries oriented along unit vector **j** (Fig. 1). We traverse it over a close contour in accordance with the right-hand screw rule, label the boundaries and grains adjoining them from i = 1 to k (k = 2, 3, ...), and denote by $\mathbf{N}_i$ the normals to these boundaries. In accordance with Taylor's model, plastic strain of each grain considered at the microscopic level is the result of uncorrelated motion of a large number of individual lattice dislocations belonging to different slip systems under the action of external stresses σ^{ext}. These dislocations emerging at a boundary produce on it additional disorientation Θ_i^{def} of deformation origin, which (other conditions being the same) depends on orientation $\mathbf{N}_i$ of the boundary. We denote by $\boldsymbol{\omega}^j$ the nullity vector of disorientations of deformation origin at the boundaries forming the jth joint. According to [13, 14], it is given by

$$\boldsymbol{\omega}^j \equiv -\sum_i \Delta\boldsymbol{\Theta}_i^{\text{def}} = -\sum_i \mathbf{N}_i \times (\varepsilon_i - \varepsilon_{i-1}) \cdot \mathbf{N}_i. \quad (2)$$

Let us calculate vector $\boldsymbol{\omega}^j$ using the classical Taylor's model [17], which is known to be based on the following postulates.

P1. Within a grain, the plastic strain is assumed to be spatially uniform.

P2. At the microscopic level, plastic strain tensor of the ith grain can be written in the form

$$\varepsilon_i = \frac{1}{2}\sum_s \rho_s \lambda_s (\mathbf{nb} + \mathbf{bn})_s, \quad (3a)$$

where **n** and **b** are the normal vector to the slip plane and the Burgers vector of lattice dislocations; ρ_s and λ_s are the density and average path length of lattice dislocations, and s is the number of effective slip system.

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[3] Henceforth, we will refer to all above-mentioned linear defects as joints of large-angle grain boundaries.

[4] The existence of joint disclinations of deformation origin was experimentally proved much later [15, 16].

P3. Tensors ε_i' and E_i written in the same system of coordinates are identical:

$$\varepsilon_i = E_i. \tag{3b}$$

P4. To satisfy condition (3b), simultaneous loading up to five dislocations slip systems in a grain is permitted.

P5. Plastic strain tensors are equal to the macroplastic strain tensor of the polycrystalline aggregate at the point of location of the ith grain:

$$\varepsilon_i = E_i = E(r_i). \tag{3c}$$

Substituting this relation into Eq. (2), we can easily see that nullity vector $\boldsymbol{\omega}^j$ of disorientations of deformation origin in the classical dislocation model of plastic deformation of polycrystals is identically equal to zero at all joints and kinks of grain boundaries without any exception (at least, for a uniformly deformed polycrystal).

1.3. Mesolevel of Plastic Strain

The reason for such a strange (at first glance) conclusion is that the postulates underlying the Taylor model describe the actual process of plastic deformation occurring with conserved continuity of a polycrystalline aggregate only approximately. Indeed,

(i) the continuity condition requires that not the plastic deformation tensor as in relation (3c), but total deformation tensors (i.e., the sum of its elastic and plastic components [18]) be equal at grain boundaries; for this reason, the mismatch of plastic strains of neighboring grains by the mismatch of their elastic strains is permissible;

(ii) plastic straining of a crystal is an inertial process; i.e., leveling of plastic strain tensors of neighboring grains requires a finite time; for this reason, plastic strain tensors ε_i of neighboring grains are necessarily different at any instant;

(iii) plastic deformation of a grain occurs nonuniformly over the volume because with increasing ε_i, grain boundaries become 2D sources of long-range stresses, the structure and intensity of which depending on ε_i and facet orientation $\mathbf{N}_i$. For this reason, grain regions belonging to different facets experience different strains, which ultimately leads to splitting of the initially uniformly oriented grain into an aggregate of disoriented mesovolumes.

Other reasons for violation of basic conditions (3c) also exist, but their analysis is beyond the scope of this article. It is sufficient to assume for further analysis that joint disclinations of deformation origin exist and their Frank vector is defined by Eq. (2).

2. FIELDS OF ELASTIC STRESSES GENERATED BY JOINT DISCLINATIONS OF DEFORMATION ORIGIN

In the general case, the Frank vector of a joint disclination of deformation origin can have wedge component ω_w^j as well as twist component ω_{tw}^j. If the latter component differs from zero, the joint disclination of deformation origin has a complex structure and includes, in addition to the linear source of internal stresses located along the joint line, at least one planar source located along one of the joining boundaries. Bearing this in mind, we will confine our analysis here only to a wedge joint disclination of deformation origin and a will analyze the forces exerted by the wedge joint disclination on the surrounding lattice dislocations using the simplest 2D model.

Let us place a wedge joint disclination at the origin of the laboratory system of coordinates with unit vectors ($\mathbf{l}_1$, $\mathbf{l}_2$, $\mathbf{j}$). We denote the most loaded (acting) slip systems of dislocations in the ith grain by unit vectors $(\mathbf{n}, \mathbf{s})_i$ ($i = 1, 2, 3$), where $\mathbf{s} = \mathbf{b}/b$. Let us consider a test dislocation placed at the tip of radius vector r_i with polar coordinates (r, φ), where r_i is the distance to the joint disclination and φ_i is the polar angle measured from unit vector $\mathbf{l}_1$ in the laboratory system of coordinates. For convenience of calculations, we direct $\mathbf{l}_1$ along $\mathbf{s}_1$. The corresponding geometry is shown in Fig. 1. In the same figure, symbols Θ_i denote relative rotations of crystal lattices of neighboring grains. The positive and negative values of angle Θ_i correspond to the lattice rotation in the direction of the right-hand and left-hand screw, respectively.

In the notation adopted here, force f_{nb}^i exerted by the joint disclination on the test lattice dislocation in the ith grain can be written in the form

$$f_{nb}^i = -\frac{G_w}{4\pi(1-\nu)} b_i \sin 2(\varphi_i + \Theta_i), \tag{4}$$

where G is the shear modulus and ν is the Poisson ratio. It is independent of the distance to the joint and is determined exclusively by the observation angle, being positive in the first and third quadrants and negative in the second and fourth quadrants. The distribution of this force expressed in the units of $\frac{G\omega b}{4\pi(1-\nu)}$ in the vicinity of the joint under investigation is shown in Fig. 2.

Apart from the force exerted by the joint disclination, test dislocations experience the action of forces associated with external stresses σ^{ext}. The total force acting on a test dislocation in the it grain is given by

$$F_{nb}^i = \left(\mathbf{n}_i \cdot \sigma^{\text{ext}} \cdot \mathbf{s} - \frac{G\omega}{4\pi(1-\nu)} \sin 2(\varphi_1 + \Theta_i)\right) b_i. \tag{5}$$

It follows from this expression and Fig. 2 that the emergence of a joint disclination leads to the formation of large mesoregions in the initially uniform force field of a grain in which the forces acting on slip lattice dislocations can differ significantly in both directions from the forces averaged over the grain. Since these forces determine the velocities and densities of dislo-

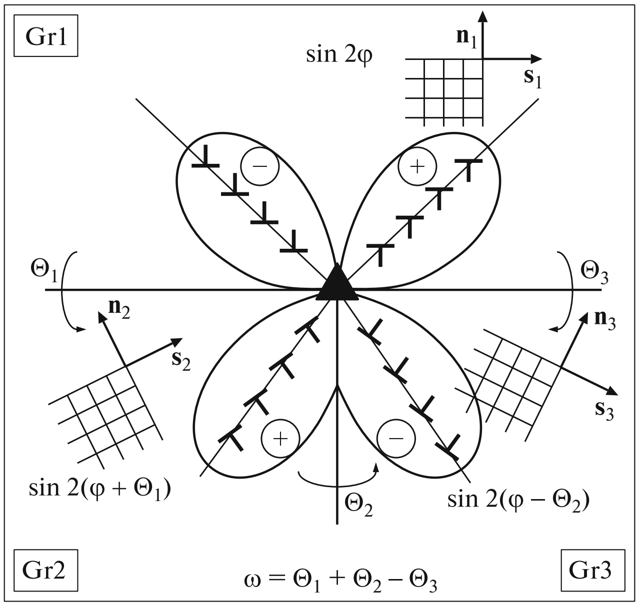

Fig. 2. Diagram illustrating the distribution of forces exerted by a joint disclination on a test dislocation in different grains forming a triple joint.

cation flows, plastic strains in adjacent mesovolumes are also different. With increasing plastic strain, these differences increase, and for

$$\omega \geq \omega_c = 4\pi(1-\nu)\left(\frac{\sigma^{\text{ext}}}{G}\right) \approx 8.4\left(\frac{\sigma^{\text{ext}}}{G}\right) \tag{6}$$

a wall of edge dislocations will align along ray $\varphi_i + \Theta_i \approx \frac{\pi}{4}$ in the ith grain because for ω defined by condition (6), the decelerating field from a joint disclination of deformation origin attains and exceeds the external field.

The estimate obtained for ω_c is obviously exaggerated because there is no need in stopping the dislocation flow completely for producing a tilted wall of edge dislocations emerging from the joint. Such a wall can also appear in a softer dynamic regime.

To verify this hypothesis, we performed computer simulation.

3. COMPUTER SIMULATION OF THE CRITICAL POWER OF A JOINT DISCLINATION OF DEFORMATION ORIGIN

3.1. Computer Experiment

Analysis of the dislocation flow dynamics in the total field of external stresses σ^{ext} and the elastic field of wedge joint disclination was carried out for a rectangular grain[5] (elastically isotropic medium) of size $(d \times d)$, where $d = 2$ μm. The joint disclination is at the center of the lower boundary of the grain. In our calculations, we used the method of dynamics of discrete dislocations [19] modified in [20–23] for analyzing the kinetics of a dislocation ensemble in the elastic field of the disclination.

[5]Upper grain in Figs. 1 and 2.

Each dislocation was characterized by Burgers vector $\mathbf{b}$ parallel to the direction of dislocation slip, coordinates $(x^{(k)}, y^{(k)})$, and velocities $(\nu^{(k)})$, $k = 1,..., N$, where N is the number of dislocations. The contribution of inertial terms to the equation of motion of the dislocation is assumed to be much smaller than from the terms associated with dynamic friction. In this case, the equation for the velocity of the kth dislocation in the quasi-viscous approximation has the form

$$\nu^k = M^{(s)}\mathbf{n}_s \cdot \sigma_\Sigma \cdot \mathbf{b}, \tag{7}$$

where $M^{(S)}$ is the mobility of dislocations in the sth slip system, $\mathbf{n}_s \cdot \sigma_\Sigma \cdot \mathbf{b}$ is the force acting on the kth dislocation in slip plane $\mathbf{n}_s$, and $\sigma_\Sigma = \sigma^{\text{ext}} + \sigma^{\text{int}}$, σ^{int} being the internal stress tensor defined as the total elastic field produced by the joint dislocation and other dislocations.

In this model, we assume that the plastic deformation in a grain begins when the shear stress attains critical value σ_c. Multiplication of dislocations in the bulk of the grain is characterized by a certain rate of generation of dislocation pairs of opposite sign in slip planes separated by distance $x_c = Db/\sigma_c$ from each other (σ_c is the threshold stress of actuation of a source of the Frank–Read type [24], $D = G/2\pi(1-\nu)$; at stress $\sigma_\Sigma < \sigma_c$, the dislocations of the generated pair annihilate). The coordinates of the dislocation pair were generated at random in the domain under investigation in accordance with the uniform distribution law. The recombination processes are taken into account in the model. The annihilation of dislocations of opposite signs moving towards each other is characterized by the capture cross section $S_a = \pi x_a^2/4$, where $x_a = 0.25x_c$. The sink is taken into account as the disappearance of dislocations reaching the lateral surfaces of the upper grain. In our calculations, we used the values of parameters $\sigma_c \approx 2.5 \times 10^{-3}\, G$, $b = 0.25 \times 10^{-9}$ m, and dislocation mobility $M^{(s)} \sim 10^{-4}$ Pa^{-1} s^{-1}, which ensure the plastic strain rate $\dot{\varepsilon} = 10^{-3}$ s^{-1} averaged over the grain volume.

4. RESULTS OF SIMULATION

For the chosen value of external stress from the interval $(10^{-3}$ to $2 \times 10^{-3})G$, the evolution of the dislocation ensemble was investigated for increasing joint disclination power. At a low disclination power (smaller than the critical value), regions of excess density of short-term dislocations with the same sign ("loose" subgrain boundaries) are formed. However, these formations are unstable and are periodically dis-

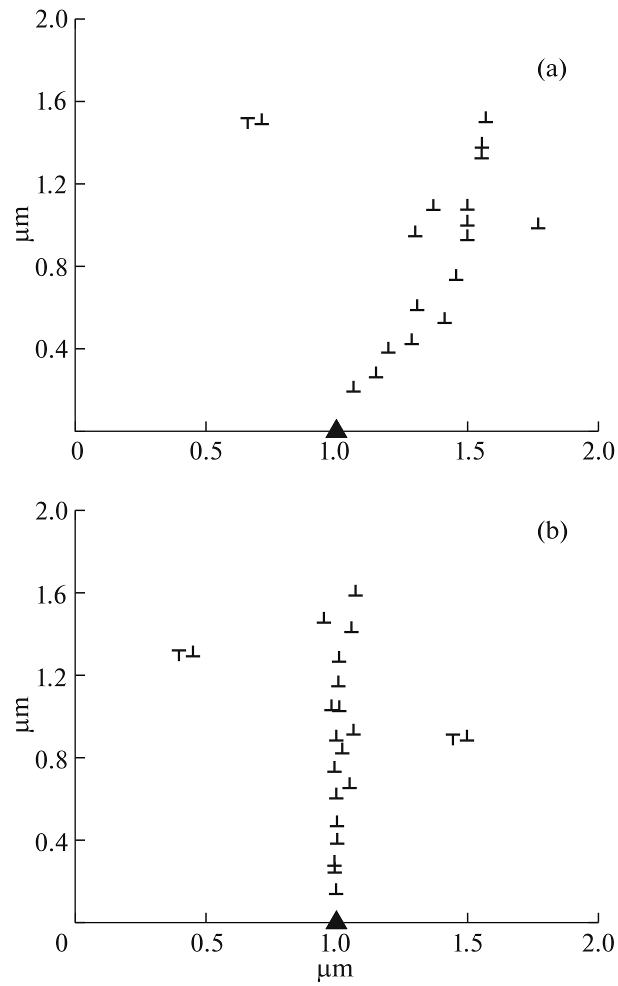

Fig. 3. Typical dislocation structures formed near a joint disclination in the field of external stresses $\sigma^{ext}/G = 10^{-2}$: (a) $\omega < \omega_c$; (b) $\omega > \omega_c$.

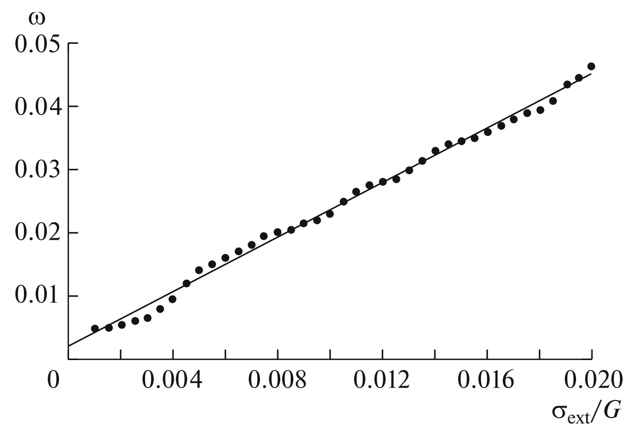

Fig. 4. Calculated and approximation dependences of the critical power ω_c of joint disclination on the reduced external shear stress σ^{ext}/G.

rupted by the external field (Fig. 3a). With increasing joint disclination power ω, its critical value ω_c is attained, at which the spatial distribution of dislocations statistically changes insignificantly, being localized in the vicinity of the disclination in the form of a narrow broken subgrain boundary (Fig. 3b).

The steady-state nature of the subgrain boundary is manifested in the fact that it looses and absorbs on the average the same number of dislocations per unit time.

The dependence of the critical value of disclination power ω_c on the reduced external shear stress σ^{ext}/G is shown in Fig. 4. Each point on this curve is the average value of ω_c obtained from the results of five computer experiments.

It can be seen from Fig. 4 that the dependence of ω_c on σ^{ext} is close to linear,

$$\omega_c = 2.2\frac{\sigma^{ext}}{G} + 0.002 \tag{8}$$

(approximation by the least squares method). Slight deviations from linearity are due to the statistical nature of formation of dynamic walls of dislocations. As expected, dependence (8) corresponds to the available experimental data much better than dependence (6). It shows that for stresses $\sigma^{ext}/G \sim 10^{-2}$ to 2×10^{-2} typical of the temporal limit of ultimate strength of bcc materials, the critical power of the joint disclination is $\omega_c \sim 1.4°–2.8°$. This result is in good agreement with available experimental data [1].

CONCLUSIONS

The above analysis makes it possible to draw several conclusions important for understanding the nature of fragmentation.

1. Fragmentation is a consequence of anisotropy of plastic flow of crystalline solids; in plastically deformed amorphous media, it must be absent in accordance with the above model.

2. Fragmentation of polycrystals is a consequence of the difference in macroplastic strains of adjacent grains.

3. The sequence of cause-and-effect relations leading to fragmentation of crystalline solids and to the formation of plastic strain mesolevel in them can be described as follows. The difference in macroplastic strains of joining grains (plastic strain macrolevel) leads to the emergence of disorientations of deformation origin (planar rotational-type mesodefects) at joining large-angle grain boundaries. In turn, misalignment of these disorientations leads to the formation of joint disclination (linear mesodefects of the rotational type) and to an increase in its power in the course of plastic deformation The elastic field of joint disclination caused a perturbation of the laminar flow of lattice dislocations (plastic strain microlevel), leading to the emergence and evolution of broken disloca-

tion boundaries, viz., partial disclinations of deformation origin (plastic strain mesolevel).

These interrelations can be observed quite clearly using the simplified model proposed here. The description of the initial stage of fragmentation in real polycrystals is a much more complicated problem. It is necessary to take into account multiple slips, a more complex geometry of joint boundaries, and the effects associated with the formation of planar sources of internal stresses on joining boundaries. These questions will be investigated in subsequent publications.

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