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Formation of subboundaries in cellular structures during plastic deformation of mono- and polycrystals

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ABSTRACT

The mechanisms of the formation and evolution of dislocation cellular structures in single crystals and polycrystals are investigated using correlation instability in a dislocation ensemble. It is shown that at the nonlinear stage of the system evolution, a cellular structure develops, characterized by both total and excess dislocation densities. At a certain stage in the dislocation ensemble evolution, equilibrium configurations form: configurations with excess density represent sub-boundaries, and those with total density represent dislocation dipole configurations that annihilate via the dislocation climb mechanism. It is shown that the occurrence of sub-boundaries is associated with rotational instability caused by the formation of walls in the regions of maximum values of excessive dislocation density in a cellular dissipative structure. Upon unloading, the dissipative structure is destroyed, and the remaining dislocations migrate into sub-boundaries, leaving behind an equilibrium "framework" of the subgrain structure.

KEYWORDS

dislocation ensemble • excess dislocation density • cellular structure • disclinations • subboundaries

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Introduction

Plastic deformation of crystalline materials is accompanied by a significant restructuring of their internal structure, which directly affects mechanical properties such as yield strength, ductility, and fatigue resistance. One of the most characteristic manifestations of this evolution is the formation of heterogeneous fragmented structures, including cellular structures with sub-boundaries [1,2]. Understanding the regularities governing the formation of such structures is an important task of physical mesomechanics and materials science.

At the initial stages of deformation, the dislocation distribution can be considered relatively homogeneous; however, as plastic strain accumulates, the system loses stability, and spatial correlations arise [3,4], leading to the formation of various heterogeneous structures, among which the cellular structure remains the least studied theoretically.

In recent years, the formation of cellular structures has been associated with the nonlinear dynamics of dislocations [5]: as the dislocation density ρ increases (typically at $\rho > \rho_c \approx 10^{14}\ m^{-2}$), the system tends to minimize elastic energy by forming quasi-

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ordered configurations — dislocation walls bounding regions with a relatively low dislocation density. Based on experimental data, the papers [2,6] postulate the existence of a universal relationship between the average cell size d and the dislocation density ρ, described by the relation $d = K\rho^{-1/2}$, where $K = 2 - 16$ is a certain constant [6]. However, this relationship is somewhat violated under conditions of severe plastic deformation, when an ultrafine-grained structure is formed [7,8].

Cellular structures are observed in a wide range of materials — from pure metals (copper, aluminum, nickel) to engineering alloys (steels, titanium and aluminum alloys) — and significantly affect mechanical properties, in particular strength, ductility, and fatigue life [9–11]. To describe the processes of cellular structure formatio, in [12,13], it was proposed to interpret the evolution of dislocations as reaction-diffusion-type processes within the framework of the general theory of self-organization [14,15]. However, this modeling approach has not received significant development, since it could not explain the formation of misorientations in the cellular structure.

An alternative is provided by continuum phase-field models, which effectively describe the evolution of boundaries and domains [16]. Nevertheless, most existing models of this type focus on the interaction of dislocations with grain boundaries, while the process of sub-boundary formation inside the grain volume is not considered.

An attempt to solve this problem for polycrystals was proposed in [17,18] within the framework of the fragmentation theory, in which the formation of sub-boundaries was considered as the nucleation and motion of partial disclinations [18]. However, in this theory, as in the previous ones, the cellular structure was not theoretically considered as an object of a fragmented structure, i.e., a structure divided by sub-boundaries [19,20].

At the same time, if we assume that the formation of sub-boundaries is associated exclusively with grain boundaries, then how to explain the fact that the process of formation of sub-boundaries and subgrains during plastic deformation also occurs in single crystals [21,22]? Consequently, the question of the criteria for the transition from a cellular structure to a fragmented one with well-defined sub-boundaries remains unclear [23].

The aim of the present work is to develop, investigate, and analyze a nonlinear model of cellular structure formation in monocrystals, for which the subgrain structure develops from the cellular one.

Basic equations

Let us consider the main aspects of the nonlinear theory of cellular structure formation for an ensemble of parallel dislocations [24], based on correlation (fluctuation) instability [3,4]. The evolution equations for the dynamics of edge dislocations, taking into account their local, elastic, and correlation interactions, can be written in the general form as follows [24]:

$$\frac{\partial \rho_a}{\partial t} + \mathrm{div}(\boldsymbol{J}_a + \boldsymbol{J}_a^{\mathrm{corr}}) = F_a(\rho_a), \tag{1}$$

$$\boldsymbol{J}_a(\boldsymbol{r},t) = \rho_a(\boldsymbol{r},t)V_a - M\rho_a(\boldsymbol{r},t)\sum_c \int \rho_c(\boldsymbol{r}',t)\nabla W_{ac}(\boldsymbol{r}'-\boldsymbol{r})d\boldsymbol{r}', \tag{2}$$

$$\boldsymbol{J}_a^{\mathrm{corr}}(\boldsymbol{r},t) = -M\rho_a(\boldsymbol{r},t)\sum_c \int \rho_c(\boldsymbol{r}',t)G(\mathbf{r}'-\boldsymbol{r})d\boldsymbol{r}'. \tag{3}$$

Here V_a is the constant component of the dislocation velocity due to the flow stress σ_e in the slip plane; M is the dislocation mobility in the slip planes; $a = \pm$ is the index determining the direction of the Burgers vector in the slip system; $G(r) = g_{ac}(\boldsymbol{r})\nabla W_{ac}(\boldsymbol{r})$

is the Green's function, where $g_{ac}(\boldsymbol{r})$ is the two-particle correlation function, $W_{ac}(\boldsymbol{r})$ is the elastic interaction energy of dislocations [25]; $F_a(\rho_a)$ is a nonlinear function determined by the mechanisms of dislocation generation and recombination.

Let us consider a situation where the dislocation motion occurs along a certain slip system (for example, along the $0x$ axis) under conditions of symmetric multiple slip. Let us choose the function F_a in the form:

$$F_a(\rho_a) = \delta(\rho_+ + \rho_-) - \kappa\rho_+\rho_-, \quad (4)$$

where δ is the dislocation multiplication coefficient, $\kappa = 2Vh$ is the annihilation coefficient, $h = D_e b/(2\sigma_e)$ is the characteristic capture radius of dislocations into dipole configurations, $D_e = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is Poisson's ratio.

In this case, the system of equations (1)–(3) for the total $\rho = \rho_+ + \rho_-$ and excess $I = \rho_+ - \rho_-$ dislocation densities, after several simplifications, takes the form [24]:

$$\frac{\partial\rho(\boldsymbol{r},t)}{\partial t} + V\frac{\partial I(\boldsymbol{r},t)}{\partial x} + \nabla\boldsymbol{J}^{\mathrm{corr}}(\boldsymbol{r},t) = \frac{\rho-\rho_0}{\tau} - \frac{\kappa(\rho-\rho_0)^2}{2}, \quad (5)$$

$$\frac{\partial I(\boldsymbol{r},t)}{\partial t} + V\frac{\partial\rho(\boldsymbol{r},t)}{\partial x} = -\frac{I(\boldsymbol{r},t)}{\tau_i}, \quad (6)$$

$$\boldsymbol{J}^{\mathrm{corr}}(\boldsymbol{r},t) = M\rho(\boldsymbol{r},t)\frac{D_e b^2}{2\rho_0}\sum_{n=1}^{\infty}\frac{1}{n}(r_d^2\Delta/2)^{n-1}\nabla\rho(\boldsymbol{r},t), \quad (7)$$

where $\tau = (2\delta)^{-1}$ and $\tau_i = (1-\nu)/(\rho_0 MGb^2)$ are the relaxation times to the equilibrium state:

$$\rho = \rho_0 = \frac{4\delta}{\kappa}, \quad I = 0, \quad (8)$$

for the total and excess dislocation densities, which is determined from the equality of the right-hand sides of Eqs. (5) and (6) to zero.

From the analysis of Eqs. (5)–(7) it follows that the criterion for the instability of the homogeneous state is the fulfillment of the condition

$$\rho_0 > \rho_c = \frac{8\pi e(1-\nu)^2}{b^2}\left(\frac{\sigma_e}{G}\right)^2. \quad (9)$$

For typical values of the parameters ($b = 3\cdot10^{-10}\ m$, $\nu = 1/3$ и $\sigma_e/G = 10^{-3}$) the critical density is $\rho_c \approx 10^{14}\ m^{-2}$.

In this case, in the instability region, a one-dimensional (since $k_y = 0$) periodic dislocation structure is formed with a characteristic spatial scale $L_c = 2\pi/k_c = 2\pi r_d/\sqrt{2(e-1)}$. Assuming the correlation radius r_d to be of the order of the average distance $\bar{r} = \rho_0^{-1/2}$ between dislocations [4], we obtain the characteristic scale of the cellular structure $L_c \approx 8\rho_0^{-1/2}$.

Nonlinear solutions of the system of equations (5)–(7) can be obtained by standard methods [15,24]. As a result of the corresponding transformations, we obtain an approximate solution for the total

$$\rho(r) = \rho_0 + 2\rho_0\sum_{n=1}^{N}[A_n\cos(\boldsymbol{k}_n r + \varphi_n) + C_n\cos 2(\boldsymbol{k}_n r + \varphi_n)], \quad (10)$$

and excess dislocation densities:

$$I(r) = 2\rho_0\sum_{n=1}^{N}[A_n\sin(\boldsymbol{k}_n r + \varphi_n) + C_n\sin 2(\boldsymbol{k}_n r + \varphi_n)], \quad (11)$$

where N is the number of equivalent slip systems during crystal deformation (in one plane), $A_n \approx 1.5\sqrt{\rho_0/\rho_c - 1}$ is the amplitude of the main unstable mode (order parameter), C_n are the amplitudes of small (in the vicinity of the bifurcation point) decaying modes.

Formation of sub-boundaries in a one-dimensional structure

Let us consider, according to the solutions (10), and (11), the simplest type of heterogeneous dislocation structure ($N = 1$) — periodic. Let us assume that the structure formation occurs along a certain direction, for example, along the x axis.

The spatial distribution of dislocations is shown for two cases: at the moment of the dislocation structure nucleation (Fig. 1(a)) and after additional deformation (Fig. 1(b)). In case (*a*), the structure amplitude $A_n \propto \sqrt{\rho_0 - \rho_c}$ is small and the solution is close to a sinusoidal shape. As we move away from the bifurcation point, the decaying modes cease to be small, and an increasing number of harmonics falls into their spectrum. This leads to the distortion of the sinusoidal profile and the emergence of a more contrast structure.

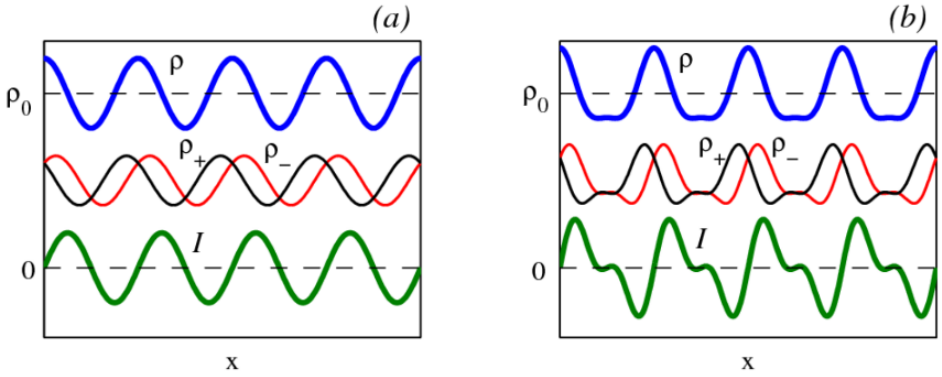


Fig. 1. Dependences of the dislocation distribution on the variable x for the cellular structure at the initial moment of its formation (a) and at a subsequent moment (b)

The obtained structure is a purely dynamic formation, i.e., upon unloading, it should relax to a homogeneous distribution. The fact that this does not happen is due to the fact that in the cellular structure, dislocations in the regions of increased density at a certain stage of evolution form equilibrium formations: in the structure with excess density — sub-boundaries (which remain after unloading), in the structure with total density — dipole and multipole configurations of dislocations, which partially annihilate with increasing strain due to climb. Therefore, in what follows, we will investigate the structure with excess dislocation density, which creates a continuous (Fig. 2(a)) and discrete (Fig. 2(b)) misorientation of the crystal regions.

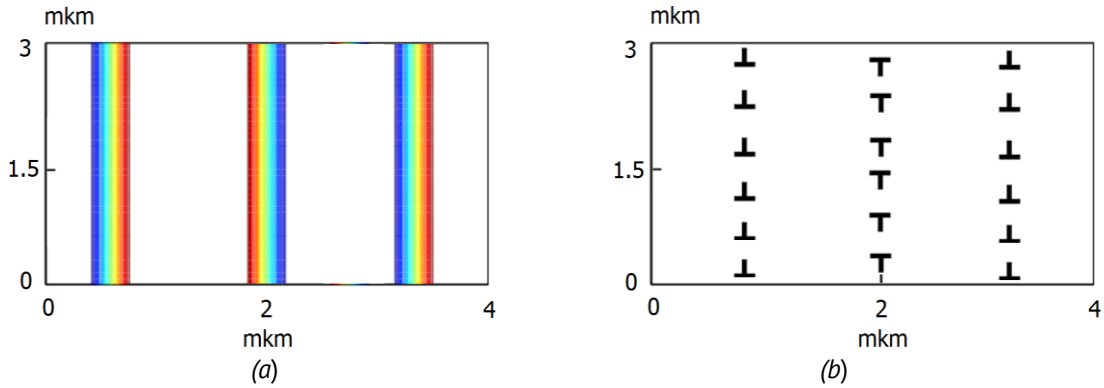


Fig. 2. Periodic structure for the excess dislocation density $I(r)$ (a) and its schematic dislocation representation (b)

For the interaction force of two dislocations lying in parallel planes with similarly directed Burgers vectors, we have [25]:

$$f_x = D_e b^2 \cdot \frac{x(x^2-y^2)}{(x^2+y^2)^2}. \quad (12)$$

Let us consider the expression for the force (12). The equality of this force to zero corresponds to an equilibrium dislocation configuration. It is easy to see that this is achieved at $x = 0$ and $x = |y|$. In the first case, a stable configuration is realized for dislocations of the same sign. In this case, for small x and a fixed value $y = y_0$, the force component acting in the slip system is $f_x \approx -kx$ (where $k = D_e b_1 b_2 / y_0$), i.e., two dislocations of the same sign located in the same plane perpendicular to the slip system at a certain distance y_0 form a stable dipole. This configuration is also stable for more than two dislocations. Therefore, straight edge dislocations tend to gather in one plane perpendicular to the slip plane and form so-called walls (sub-boundaries).

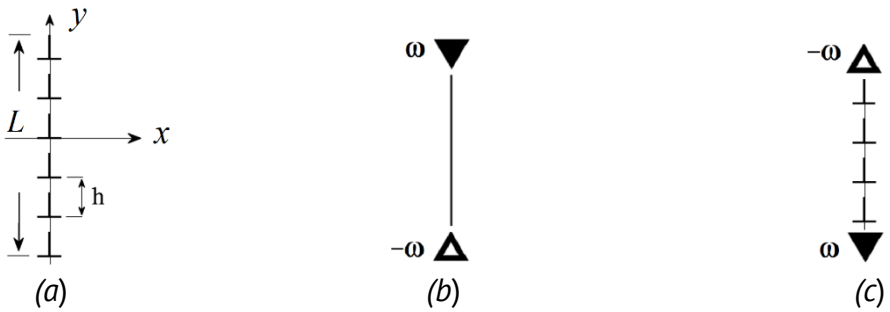


Fig. 3. Dislocation wall (a) and the corresponding disclination dipole (b). The wall after the completion of its development in a single crystal (c)

Let us consider this process for a wall of length L, shown in Fig. 3(a), in which the dislocations are at an equal distance h. Let us find the force in the slip direction with which such a wall acts on a test similar dislocation at $L >> h$. This force can be found using the formula (12):

$$F_x = \frac{D_e b^2}{h} \int_{-L/2}^{L/2} \frac{x-(y-\eta)^2}{[x^2+(y-\eta)^2]^2} d\eta = \frac{L D_e b^2}{h} \cdot \frac{x[x^2-y^2+(L/2)^2]}{[x^2-y^2+L/2)^2]^2+4x^2y^2}. \quad (13)$$

According to Eq. (13), the attraction region is bounded by a hyperbola $x^2 - y^2 + (L/2)^2 = 0$ (dislocations located in the regions above the upper or below the lower branch of the hyperbola are attracted to the Oy axis). Consequently, a dislocation wall that has appeared in the crystal automatically creates conditions for its further growth. Thus, in the dissipative structure, a rotational instability arises, which leads to the misorientation of regions in this structure. The considered wall of excess dislocation density (sub-boundary), formed in a certain slip system and having a misorientation $\theta = b/h$, is equivalent to a disclination dipole (Fig. 3(b)) of power $\omega = \theta$.

If the wall formation ends at a free boundary (as in a single crystal), then in the configuration shown in Fig. 3(b), the disclinations should disappear in accordance with the boundary conditions [18]:

$$\sigma_{ik} n_k|_S = 0, \quad (14)$$

which means that on the free surfaces S of an elastic body, the internal stresses generated by a finite wall (sub-boundary) or other stresses (for example, from disclinations) cannot lead to the appearance of surface forces. In this situation, the stress field of the wall can

be considered as a field screened by a system of disclinations of opposite signs (Fig. 3(c)). In fact, this means that the wall increases its size to infinity and, accordingly, the stress field in the region $y \in (-L/2, L/2)$ is the same as from an infinite wall [25]:

$$\sigma_{xy} \approx 4\pi^2 D_e \frac{bx}{h^2} e^{-2\pi x/h} \cdot cos(2\pi y/h). \quad (15)$$

Thus, the dislocation flux will interact with the wall locally in a region of the order of the distance between dislocations h in the wall. In this case, the flux of positive dislocations in the dissipative structure will prevail over the negative ones, given the fact that the considered wall is formed in the region of increased density of excess dislocations $I = \rho_+ - \rho_- > 0$.

As follows from Eq. (15), the stress σ_{xy} can take a negative value on the scale of h. Consequently, positive dislocations will be incorporated into the wall due to climb, and negative ones will annihilate. But since the flux of positive dislocations in the vicinity of the wall is greater ($I > 0$), the misorientation of the wall θ will increase during plastic deformation. A similar process will occur in neighboring walls, except that dislocations of the opposite sign will accumulate there.

The misorientation of sub-boundaries will increase until the condition (9) is violated, i.e., when the density of mobile dislocations due to the outflow to sub-boundaries becomes less than the critical value ρ_c. In this case, the dissipative structure will be destroyed, the dislocation flux will become homogeneous and, accordingly, in the cell bodies the condition $\rho_+(r,t) = \rho_-(r,t)$ will be fulfilled.

Formation of sub-boundaries in a cellular structure

The process of cellular structure formation is due to the action of several slip systems. Let us consider, according to solution (12) for the excess dislocation density at $N = 2$, the simplest type of cellular dislocation structure — rhombic (Fig. 4(a)). The structure is formed by dislocations moving in two mutually perpendicular slip systems under the condition $\rho >> \rho_c$, when the dissipative dislocation structure acquires a contrast appearance.

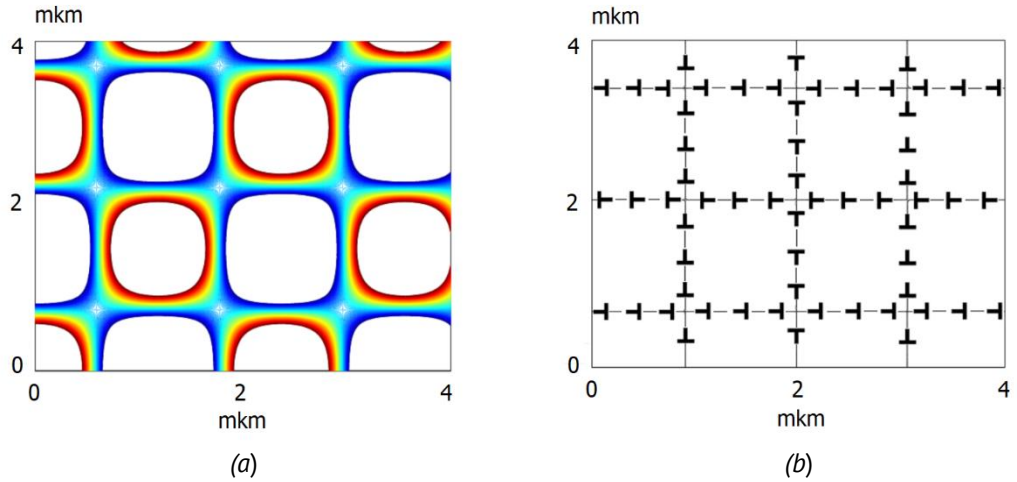


Fig. 4. Cellular structure for the excess density $I(r)$ of dislocations (a) its schematic dislocation representation (b)

As a result of rotational instability and polygonization processes, i.e., the formation of dislocation walls at the maxima of excess density in the cellular structure, a system of sub-boundaries with a misorientation θ is formed, which has a cellular shape (Fig. 4(b)). At the internal nodes of this structure, the total value of the disclination power is zero. In this case, at the outer free boundary of the single crystal, to take into account the boundary conditions (14), disclinations of the corresponding sign ($\omega = \pm\theta$) must be placed, screening the stress field from each wall.

Estimate the magnitude of the characteristic misorientation θ of subboundaries shown in Fig. 4(b). Misorientation can be determined assuming that in an arbitrary cell all excess dislocations N_0 of a certain Burgers vector gather into a wall. Accordingly, we have $\theta = bN_0/L_c$, where $L_c \approx 8\rho_0^{-1/2}$ is the period of this structure according to the previous analysis. The number of excess dislocations is approximately $N_0 \approx 0.5 I_{max} L_c^2$, where $I_{max} = 2\rho_0 A_n = 3\rho_0\sqrt{\rho_0/\rho_c - 1}$ according to (11). Thus, for example, at $\rho_0 = 2\rho_c$, the maximum value of excess density is $I_{max} = 3\rho_0$. As a result, for typical values $b = 3 \cdot 10^{-10}$ m, $\rho_0 \approx 10^{14}$ m^{-2}, we obtain $\theta \approx 0.04$, i.e., on the order of 2 degrees, which corresponds to experimental data [17]. (The same results hold for the one-dimensional periodic structure).

As the crystal is deformed, the misorientation of sub-boundaries increases. The misorientation of sub-boundaries will increase as long as the condition $\rho > \rho_c$ is fulfilled for the density of mobile dislocations. Otherwise, the dissipative structure will be destroyed, the dislocation flux will become homogeneous, and the misorientation of sub-boundaries will reach a stationary level.

In polycrystals, in relatively large crystallites, the occurrence of cellular structures also takes place. The grain boundary is not free. But even in this case, the elastic fields from sub-boundaries in the grain relax through the formation of broken low-angle boundaries in the neighboring grain [26], which have a screening effect on the sub-boundary fields. This issue requires additional research.

Conclusion

In this work, a structure with ideal symmetry was considered. However, as experimental studies show, the formation of a cellular dislocation structure in both polycrystals and monocrystals generally proceeds heterogeneously and gradually: the process begins in local zones of increased energy (boundaries, elastic inhomogeneities) and propagates into the volume [27]. In polycrystals, cells predominantly nucleate in near-boundary regions [17,28]. In monocrystals, heterogeneity may be caused by the influence of the free surface, etc. [29]. All this leads to geometric diversity of cellular structures [22,30].

However, it should be noted that the construction of a theory of complex phenomena usually begins with simple models, preferably self-consistent and without invoking numerous phenomenological assumptions. Therefore, in this work, the emergence of subboundaries is considered based on a consistent theory of cellular structure formation, related to correlation (fluctuation) instability in a dislocation ensemble. The main results of the study can be formulated as follows:

1. It is shown that the uniform dislocation distribution loses stability when exceeding the critical density ρ_c, determined by relation (9). In the instability region, a periodic dissipative structure forms with a characteristic scale $L_c \approx 8\rho_0^{-1/2}$, which agrees with known empirical dependencies.
2. At the nonlinear stage of evolution, the cellular structure is characterized by both total and excess dislocation densities. As one moves away from the bifurcation point, decaying modes cease to be small, leading to distortion of the sinusoidal profile and formation of a contrasted cellular structure.
3. Within the one-dimensional and two-dimensional (rhombic) approximations, it is demonstrated that with increasing plastic deformation, the structure contrast grows, and excess dislocations gather into subboundaries, creating misorientation of adjacent regions.
4. It is established that subboundary formation is caused by rotational instability associated with the formation of dislocation walls in regions of maximum excess density within the cellular dissipative structure. Straight edge dislocations of the same sign tend to gather in a plane perpendicular to the slip plane, forming stable walls (subboundaries).
5. It is shown that the growth of subboundary misorientation is driven by the prevailing flux of dislocations of the corresponding sign in the dissipative structure. The misorientation magnitude is estimated as $\theta \approx 0.04$ ($\approx 2°$), which is in good agreement with experimental data.
6. It is established that subboundary misorientation increases until the mobile dislocation density ρ exceeds the critical value ρ_c. When this condition is violated, the dissipative structure breaks down, the dislocation flux becomes uniform, and subboundary misorientation reaches a stationary level, forming an equilibrium subgrain framework.
7. It is shown that in a monocrystal, satisfying boundary conditions on the free surface during subboundary formation leads to the necessity of screening the subboundary stress field by a system of disclinations of opposite signs.

Thus, within the proposed model, it is demonstrated that the subgrain structure naturally develops from the cellular dislocation structure, and subboundary formation is a consequence of rotational instability in the dissipative structure, which in turn is caused by correlation interaction in the dislocation ensemble. The obtained results allow establishing criteria for the transition from a cellular structure to a fragmented one with well-defined subboundaries and can be used to describe the evolution of crystalline material microstructure during plastic deformation.

CRediT authorship contribution statement

Georgy F. Sarafanov : writing – review & editing, writing – original draft.

Conflict of interest

The author declares that he has no conflict of interest.

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