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# A Review on Accommodation Processes in Non-Equilibrium Grain Boundaries

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**Abstract.** The grain boundaries in ultrafine-grained materials, including nanostructured ones, are in a specific non-equilibrium state, which is associated with extrinsic grain boundary dislocations trapped during plastic deformation. This grain boundary state plays a significant role in the stability and evolution of many mechanical and physical properties of nanocrystalline materials. In the present review, accommodation of different components of non-equilibrium grain boundary structure resulting in a formation of a more equilibrium structure and associated with a decrease in the internal stresses is analyzed. These are spreading of lattice dislocations trapped by grain boundaries, relaxation of disordered dislocation walls, relaxation of ensembles of sessile and glissile extrinsic grain boundary dislocations. The main advantages and limitations of the models describing accommodation processes are overviewed. Application of the obtained results to nanomaterials is discussed.

## 1. EFFECTS RELATED TO NON-EQUILIBRIUM GRAIN BOUNDARIES IN NANOMATERIALS

The physics of nanocrystals is one of the most important and intensively developing branches of nanotechnology. First outlined by Feynman in 1959 [1], it developed especially rapidly in the 80s and 90s of the last century [2-5]. Polycrystals with a grain size of less than 100 nm in one direction are called nanostructured or nanocrystalline materials. Interest in them from both researchers and industries is caused, first of all, by their unusual mechanical, structural, optical, electrical and magnetic properties [6]. These properties are mainly related to the large volume fraction of grain boundaries and triple junctions as compared to the coarse-grained counterparts of ultrafine-grained materials.

Since nature has not bothered to create nanomaterials, various processing methods are used. The most typical are worth highlighting: compaction of nanopowders, crystallization from the amorphous state, inert-gas condensation, severe plastic deformation methods, etc. A common feature of all nanocrystalline materials obtained by these methods is the non-equilibrium state of grain boundaries, which is primarily due to the non-equilibrium nature of the processing routes. Non-equilibrium grain boundaries are characterized by long-range elastic stress fields and excess elastic energy [4,7,8]. Depending on the processing method, nanocrystals can have a different type of non-equilibrium structure. The presence of porosity [9-12] as well as grain boundaries with so-called non-optimized rigid-body translation [13], that is, when one grain is shifted along the common boundary with respect to the other resulting in an increase in the grain boundary energy [14-17], is characteristic feature of nanomaterials obtained by the compaction method and crystallization from an amorphous state. For severe plastic deformation methods, the non-equilibrium structure of grain boundaries is due to extrinsic grain boundary dislocations, which are associated with the absorption of lattice dislocations by

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the boundaries during deformation [8]. The nature of mesodefects formed in grain boundaries due to this process was analyzed by Rybin and co-workers who showed that the plastic deformation resulted in the formation of disclinations at triple junctions and arrays of glissile dislocations in the boundaries, which determine the processes of grain subdivision and work hardening during deformation [18-20]. The stress fields and energies of junction disclinations were studied in detail by Romanov and co-authors [21-23]. In addition, in Ref. [8] it was shown that the disordered distribution of extrinsic dislocations also resulted in long-range stresses and excess energy and should be considered as a component of the non-equilibrium structure of grain boundaries. It seems quite natural that the different components of the non-equilibrium grain boundary structure mentioned above can coexist in one material.

The properties of nanocrystals are affected by the grain boundary state, their interaction with lattice defects, as well as their ability to relax upon deformation. At elevated temperatures, accommodation processes occur in non-equilibrium grain boundaries, leading to a formation of a more equilibrium structure associated with a decrease in the internal stresses and playing a significant role in the stability and evolution of both mechanical and physical properties of nanomaterials [2,4]. For example, the Young's modulus, as well as the ultimate strength, increase with an increase in the annealing temperature, which is associated with the relaxation of non-equilibrium grain boundaries and the transition to a more equilibrium state [24]. An increased strength and ductility during tensile testing after low temperature annealing of nanostructured Ti have been revealed in Ref. [25]. The changes in the mechanical properties have been associated with a recovery of non-equilibrium grain boundary structure. Thus, the importance of studying accommodation processes is primarily due to their influence on the properties of ultrafine-grained materials.

Tucker and McDowell [26], using atomistic simulations, investigated the influence of an excess free volume in the grain boundaries, which was taken as a measure of the degree of their non-equilibrium state, on the mechanical behavior of aluminum and copper bicrystals. In particular, it was revealed that the non-equilibrium grain boundary state resulted in a change in the observed deformation mechanism at an applied shear strain. Namely, for equilibrium grain boundary $\Sigma 11$ (113) in Al, emission of partial dislocations from the grain boundary at maximal shear strength has been observed, while for the same boundary but in non-equilibrium state, the grain boundary migration perpendicular to its plane has occurred. However, no change in the deformation mechanism during shearing for the same boundary $\Sigma 11$ (113) in Cu has been found.

Hasnaoui et al. [27] introduced the degree of non-equilibrium state via increasing the disorder in the interfaces by giving random displacements to interfacial atoms. The authors established that the non-equilibrium state of grain boundaries and triple junctions significantly affected the plastic deformation of a nanocrystalline Ni sample. At that, the annealed sample is characterized by a more structural order in the interfaces and triple junctions, which results in a reduced plasticity or equivalently increased strength.

Orlova and co-authors [28] measured the microhardness and electrical resistivity of ultrafine-grained commercially pure Al processed by high-pressure torsion followed by annealing. For the first time, they have demonstrated that the non-equilibrium strain-distorted grain boundary structure strongly affects electrical resistivity of ultrafine-grained Al. Namely, the resistivity of the material containing non-equilibrium grain boundaries has been found to be 50% higher as compared to the resistivity of the annealed one with a coarse-grained structure.

Recently, Nazarov and Murzaev [29,30] have studied an influence of oscillating tension-compression stresses on the non-equilibrium [112] tilt grain boundaries in Ni by means of molecular dynamics simulations. The non-equilibrium state has been created by introducing disclination dipoles into the grain boundaries. Application of oscillating stresses was accompanied with a generation of partial lattice dislocations from the grain boundaries, which led to a compensation of the stress fields of disclination dipole and the transition of grain boundaries to a more equilibrium state.

Thus, there are a number of effects related to the changes in the properties of nanostructured materials due to the non-equilibrium structure of grain boundaries and its relaxation during annealing or other external influences such as cyclic straining established recently by experimental studies and molecular dynamics simulations. Therefore, the knowledge of the kinetics of grain boundary recovery consisting of the accommodation of extrinsic grain boundary dislocations, is important for understanding these effects.

## 2. ACCOMMODATION PROCESSES IN NON-EQUILIBRIUM GRAIN BOUNDARIES

Non-equilibrium ensembles of grain boundary dislocations, formed during low-temperature deformation, are unstable at increased temperatures and can relax forming equilibrium systems with a lower energy. In the ideal limiting case, the dislocations trapped by the boundaries are completely assimilated by them so that a new

equilibrium grain boundary structure is formed, which differs from the initial one, at least, due to the fact that the total Burgers vector of the absorbed dislocations in general differs from zero. In this final equilibrium state, the long-range elastic stresses associated with the trapped dislocations are completely screened, and the boundary satisfies the Frank criterion [31]. Thus, the extrinsic grain boundary dislocations annihilate or transform into intrinsic grain boundary dislocations. The processes occurring during the absorption of lattice dislocations trapped by the grain boundaries do not include a significant migration of the boundaries and are called accommodation processes within the grain boundaries or grain boundary recovery.

Generally speaking, when a trapped lattice dislocation splits, sessile dislocations with the Burgers vector equal to the Burgers vector of intrinsic dislocations, as well as gliding dislocations are formed at the boundary. The latter are mobile at any temperature and therefore, gliding extrinsic grain boundary dislocations formed by different trapped lattice dislocations interact, annihilate or form clusters at triple junctions. Thus, these dislocations can leave the region of the core of the absorbed dislocation rather quickly. However, they are unable to quit the boundary quickly due to the presence of barriers, triple junctions (see below in Section 2.5) and will be accumulated in the grain boundary. Sessile extrinsic grain boundary dislocations disturb the periodic distribution of the intrinsic grain boundary dislocations. This perturbation at high temperatures can relax by a climb of intrinsic grain boundary dislocations into the new equilibrium positions and formation of a new periodic network, while the former extrinsic grain boundary dislocations are its integral part.

The ability of grain boundaries to act as sinks for lattice dislocations and to recover them has a strong effect on the mechanical properties of polycrystalline materials. During high-temperature deformation, a certain dynamic balance is established between the formation and recovery processes of extrinsic grain boundary dislocations, which determines the stationary deformation rate. This review paper examines the models describing the mechanisms of accommodation processes in the non-equilibrium grain boundaries with an emphasis on nanomaterials processed by severe plastic deformation methods.

## 2.1. Experimental studies of grain boundary accommodation processes

Ishida et al. [32], carrying out *in situ* electron microscopic observations of annealing of deformed metal foils, were the first to discover the phenomenon of dislocation spreading: when the foils were heated to a certain temperature, images of lattice dislocations trapped by grain boundaries gradually spread and weakened until their diffraction contrast disappeared completely. Since the diffraction conditions in the experiments were kept constant, this indicated physical changes in the structure of the boundary, i.e., the absorption of dislocations by the grain boundaries.

In numerous subsequent works, the phenomenon of spreading was studied in detail in different materials and under different conditions, and the following key features were revealed. In pure metals, the kinetics of the spreading depends on the melting temperature. In low-melting metals (Al, Mg), the images of extrinsic dislocations are widened and disappear within a reasonable time (about tens of seconds) already at room temperature [33, 34], and in Ni when heated to a temperature of about 500 K [35]. The spreading of the extrinsic dislocations with a noticeable rate occurs at temperatures of $0.2\text{-}0.5T_m$, where $T_m$ is the melting point. In alloys, lattice dislocations trapped by grain boundaries are much more stable in comparison with pure metals [34,36,37], which indicates the influence of impurities and alloying atoms on the kinetics of the process and, consequently, on its diffusion-controlled nature. The stability of trapped lattice dislocations also strongly depends on the structure of a grain boundary: in special boundaries, spreading occurs at higher temperatures as compared to arbitrary ones; in twin boundaries, trapped lattice dislocations are the most stable [38, 39]. In special and near-special grain boundaries, the splitting of trapped dislocations into extrinsic grain boundary dislocations is often observed [40-42], and the latter can be incorporated into the networks of intrinsic grain boundary dislocations [41,43].

Spreading of trapped lattice dislocations is an indicator of the grain boundary recovery, however, it should not be identified with it. Experimental studies show that even after the dislocations in grain boundaries have disappeared, the boundaries are still in non-equilibrium state. In this state, the yield stress is higher than in a well-annealed polycrystal [44]. In a number of experiments [38,39,45], it was observed that the spreading time in grain boundaries, that have already absorbed dislocations as a result of preliminary deformation and moderate annealing, is noticeably shorter than in grain boundaries of well-annealed polycrystals. Hence, the mobility of atoms in non-equilibrium grain boundaries is higher than in equilibrium ones, that is, the absorption of lattice dislocations leads to an increase in the diffusion coefficient. In Refs. [46,47], a correlation between the onset of intensive grain growth and the relaxation of trapped dislocations was found, which suggests that there is an accelerated migration of non-equilibrium grain boundaries. Detailed studies of grain

boundary sliding in bicrystals demonstrate that the presence of intragranular sliding significantly (more than 50 times in comparison with "pure" grain boundary sliding) increases the rate of this process [48-50]. The revealed features of non-equilibrium grain boundaries are extremely important for understanding the mechanisms of recrystallization and high-temperature deformation of polycrystals, but their nature has not yet been fully elucidated.

Thus, on the basis of experimental data, the process of grain boundary recovery can be conditionally divided into two stages. At the first stage, local restructuring of the grain boundary structure occurs in the region surrounding the trapped lattice dislocations, which is visible as their spreading. The second stage of relaxation includes the ordering of the arrays of extrinsic grain boundary dislocations and the annealing of the excess density of dislocations of the same sign, i.e., wedge disclinations and ensembles of tangential extrinsic grain boundary dislocations.

## 2.2. Spreading of lattice dislocations trapped by grain boundaries

Three types of models have been proposed for spreading of lattice dislocations trapped by grain boundaries: (i) the delocalization model, (ii) the dissociation model, and (iii) the incorporation model. Below they will be briefly discussed.

(i) The model of delocalization of trapped grain boundary dislocations was proposed by Lojkowsky and Grabsky [51]. The authors considered, for simplicity, a sessile extrinsic grain boundary dislocation with a Burgers vector $\vec{b}$ = ($b$,0,0) normal to the grain boundary plane. This dislocation is described with the help of a continuous displacement field $u(x,t)$. The derivative of this function represents the distribution of the Burgers vector and has a maximum at the center of the dislocation core. The stresses normal to the grain boundary plane cause the formation of vacancies in the tension regions, and their migration and sink in the compressed regions. Such a vacancy migration process leads to the spreading of the density distribution function $\partial u(x,t)/\partial x$. Solving the integro-differential equation for the displacement field, the authors obtained the following expression for the characteristic spreading time of the dislocation core [51]

$$t_{spr} = A\frac{kTS^3}{\delta D_b G V_a} = A\frac{kTS^3}{\delta D_{b0} G V_a}\exp\left(\frac{Q_b}{RT}\right), \qquad (1)$$

where the coefficient $A = 10$. Here $k$ is Boltzmann's constant, $T$ is the temperature, $\delta D_b$ is the grain boundary diffusion width times grain boundary self-diffusion coefficient, $Q_b$ is the grain boundary self-diffusion activation energy, $G$ is the shear modulus, $V_a$ is the atomic volume, and $S$ is the characteristic width of a dislocation core at which its diffraction contrast in an electron microscope disappears. Note that this width $S$ is approximately equal to 1-2 extinction distances [51, 52].

The main disadvantage of the presented model is the fact that $\underline{u}(x,t)$ does not accurately describe the solution of the integro-differential equation for the displacement field. Moreover, in a certain interval, the derivative $\partial u(x,t)/\partial x$ assumes negative values, which corresponds to the physically incorrect conclusion that in this interval there is a continuous distribution of dislocations with the Burgers vector opposite to that for the considered extrinsic grain boundary dislocation.

(ii) The most convenient way to accurately solve the problem of the spreading kinetics in the delocalization model is to consider this model as a limiting case of the dissociation model, in which the number of extrinsic grain boundary dislocations, the dissociation products of the grain boundary dislocations, tends to infinity, and the Burgers vector of these extrinsic grain boundary dislocations tends to zero.

The simplest dissociation model was proposed by Johannesson and Thölen [52]. The model considers the dissociation of the dislocations trapped by a grain boundary into two effective dislocations with the Burgers vector $\vec{b}$ /2, which, under the action of mutual repulsive forces, climb in the grain boundary plane in opposite directions (see Fig. 1a). The consideration of the kinetics of dissociation of a dislocation in the frames of diffusion transfer of matter gives the expression for the characteristic spreading time, which coincides with the expression (1), but with the coefficient of $A = 0.34$. Note, that in the original model of Johannesson and Thölen [52], the numerical coefficient in formula (1) was 1.5, and in the denominator, instead of the grain boundary width $\delta$, there was a half of the modulus of the Burgers vector of the dislocation trapped by a grain boundary.

A more general analysis of the spreading of dislocations trapped by a grain boundary in the dissociation model was undertaken in Ref. [53]. In the cited work, it is assumed that the dislocation trapped by a grain boundary is splitted into a large number of extrinsic grain boundary dislocations with small but finite Burgers vectors (see Fig. 1b). In the limit of infinitesimal Burgers vectors, the expansion of the dissociation products can be described as the expansion of the finite wall of continuously distributed dislocations. Calculating the change in the dislocation wall energy (which is supposed to be equal to the energy of the disclination dipole), the difference in chemical potentials and the number of vacancies produced similar to that in Ref [52], the authors [53] obtained formula (1) for the spreading time with the coefficient of $A = 0.7$. However, it should

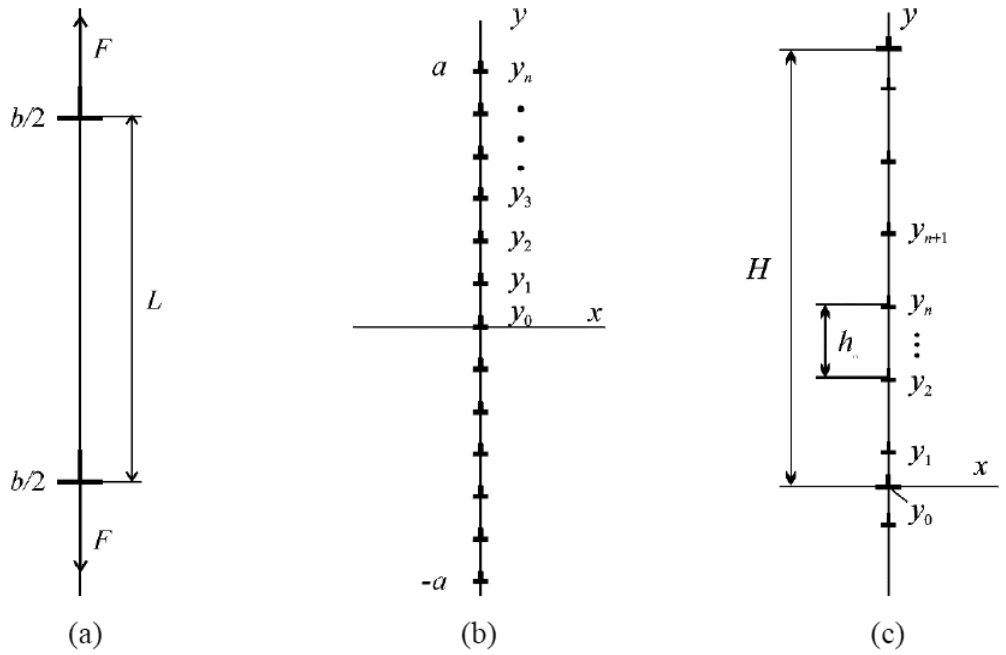


**Fig. 1.** Comparison of different spreading models of extrinsic grain boundary dislocations: (a) the delocalization model [23], where the dislocations trapped by a grain boundary splits into two effective dislocations, which are repel each other and climb along the grain boundary; (b) the dissociation model, where the expanding wall of *n* extrinsic grain boundary dislocations is obtained as a result of splitting of the trapped dislocation; (c) the incorporation model, which takes into account that the boundary has its own dislocation structure, i.e. intrinsic grain boundary dislocations. In (c), the small and large dislocation symbols denote the intrinsic and extrinsic grain boundary dislocations, respectively**.**

be noted that the analogy with the climb of two dislocations is inapplicable in this case, and the calculation of the chemical potential gradient given in Ref.[53] is incorrect, since both the vacancy flux and the chemical potential gradient turn out to be far from constant along the dislocation wall.

In Refs. [54,55], the kinetics of the spreading of the extrinsic grain boundary dislocations in the dissociation model was investigated by numerical solving of the equations of dislocations motion. Under the action of the $\sigma_{xx}$ component of the stress field, the dislocations climb, which results in an expansion of the wall. The climb velocity of the extrinsic grain boundary dislocation is determined by the gradient of the chemical potential, and the stress acting on the dislocation is calculated by a simple summing of the stresses induced by all other dislocations, with the exception of the self-stresses of any dislocation. Assuming that the contrast of the extrinsic grain boundary dislocations disappears, when the effective width is equal to *S*, the following expression for the spreading time was obtained:

$$t_{spr} \approx 0.036 \frac{kTS^3}{\delta D_b G V_a} \qquad (2)$$

which differs from formula (1) by a significantly smaller coefficient $A = 0.036$ and is valid for an arbitrary amount of dissociation products of the dislocations trapped by a grain boundary, including transition to the limit of continuous delocalization.

Thus, numerical calculations presented above demonstrate that, indeed there is practically no difference between the kinetics of the spreading of the dislocations trapped by a grain boundary in the dissociation (i) and delocalization (ii) models, both result in the same expression for the characteristic spreading time (2).

(iii) The incorporation model of the trapped lattice dislocations was proposed in Ref. [56]. The main feature of this model is the fact that it takes into account that the boundary, before absorption of the trapped lattice dislocations, has its own, intrinsic, dislocation structure. It should be emphasized that the idea of incorporation of extrinsic dislocations into the grain boundary structure was expressed earlier in Refs. [41,43], but it was extended only to the case of low-angle and near-special grain boundaries.

The kinetics of the spreading of extrinsic grain boundary dislocations in the incorporation model is controlled by the creep of the intrinsic grain boundary dislocations [56]. In contrast to the dissociation model, in which dislocations with small Burgers vectors can

climb over large distances, the climb of any dislocations in the incorporation model occurs at distances not exceeding the distance between the intrinsic grain boundary dislocations. It is assumed that in the initial state the tilt boundary contains a network of intrinsic grain boundary dislocations with the Burgers vector $\vec{b} = (b,0,0)$, and the extrinsic dislocations with the same Burgers vector are located at equal distances symmetrically relative to the intrinsic dislocations (see Fig. 1c). The location of the extrinsic grain boundary dislocations is assumed to be periodic insofar as it facilitates the numerical solution of the equations of motion allows avoiding boundary conditions. If number of extrinsic dislocations is large, then the obtained results will coincide with the kinetics of spreading of a single extrinsic dislocation. As a result of numerical solving of the equations of dislocations motion, the authors [56] obtained the following expression for the spreading time of the extrinsic grain boundary dislocations, i.e., the time during which the effective width of the dislocation becomes equal $S$:

$$t_{spr} \approx 0.03 \frac{kTS^3}{\delta D_b G V_a}. \qquad (3)$$

Thus, it turns out that all three models of the spreading of the dislocations trapped by a grain boundary lead to practically the same result. The numerical coefficients in the expressions for the spreading time (2) and (3) differ only by 20% and more than two orders of magnitude smaller than in the original formula of Lojkowsky and Grabsky [51].

Let us compare the obtained results with the experimental studies of the kinetics of spreading of trapped lattice dislocations. In Ref. [57], the results of calculating the spreading time within grain boundaries in Ni at $T = 493$ K obtained in different models are compared with each other and with experimental data [35], according to which at this temperature in Ni the spreading time is 30 s. The first two models lead to values of 4900 s (Johannesson and Töhlen [52]), 1400 s (Lojkowsky and Grabsky [51]), which are two orders of magnitude higher than the experimental value, while the formula (3), which is valid for all models, leads to value of 15 s, that is in very good agreement with the experimental result.

Let us also calculate the spreading time for stainless steel, taking the following values of the parameters [58,59]: $G = 7.74\times10^4$ MPa, $V_a = 1.16\times10^{-29}$ m$^3$, $S = 6\times10^{-8}$ m, $\delta D_{b0} = 1.5\times10^{-13}$ m$^3$/s and $Q_b = 184$ kJ/mol. Calculations using formula (3) for three temperatures lead to the following values of $t_{spr}$: 653 s at $T = 633$ K, 87 s at $T = 673$ K, and 22 s at $T = 703$ K. The experimental data for these temperatures are in intervals of 400-1200 s, 50-250 s, and 20-30 s, respectively [58]. Thus, a very good agreement with the experimental data is again achieved.

Let us now consider the limitations of the models of the spreading of trapped lattice dislocations considered above. The first limitation, common to all models, is that the formulas for spreading time are valid only for single extrinsic dislocation, that is, at low dislocation densities in comparison with $S^{-1}$. If the dislocation densities are higher than this value, their collective behavior has a strong influence on the spreading time. At higher dislocation densities, the spreading criterion should be changed. When the effective width of the dislocation wall is less than the extinction distance, but already approaching the distance between the extrinsic grain boundary dislocations, the stress field experiences the same screening as the stress of the periodic dislocation wall consisting of edge dislocations, and the image of extrinsic dislocation disappears. Thus, in this case, the spreading time will be determined by the recovery time, i.e., time of full relaxation of a system of extrinsic grain boundary dislocations, which will be discussed below. The numerical values of the extinction distance for metals are usually of the order of 100 nm [58], and therefore, formula (3) is valid up to dislocation densities of about $10^7$ m$^{-1}$, which is close to the maximum density of the trapped lattice dislocations during *in situ* observations [45]. Consequently, this limitation allows the use of the obtained expressions for the spreading time to the bulk of the experimental data. In addition, as was demonstrated in Ref. [60], in the boundaries close to special ones, the spreading of the trapped lattice dislocations occurs according to the incorporation mechanism, and in general grain boundaries - according to the delocalization mechanism. In periodic boundaries, which can be classified as general by their properties, but in which dislocations with a small but finite Burgers vector can exist, spreading will occur according to the dissociation mechanism.

## 2.3. Relaxation of a system of disordered dislocations

Disordered dislocation arrays can relax by the climb of dislocations to equilibrium positions with the following formation of uniform arrays with a period $h_0$ equal to the average distance between dislocations. The kinetics of this process in the frames of the discrete-dislocation approach was studied in Ref. [61]. The wall of chaotically distributed dislocations with the Burgers vector $\vec{b} = (b,0,0)$ was considered. The equation of motion of dislocations were solved starting from initial coordinates established using a random number generator for approximately 30 realizations of the initial coordinates of the extrinsic grain boundary dislocations. Calculations showed that the non-equilibrium parameter of the disordered walls, which was taken as the ratio of the disper-

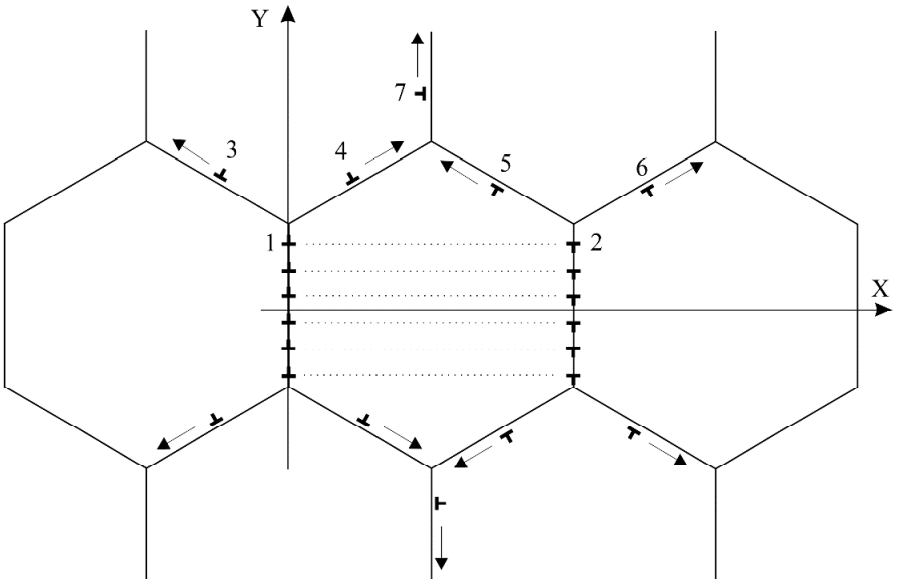


**Fig. 2.** A model for the relaxation of wedge junction disclination quadrupole, i.e., a system of discrete sessile extrinsic grain boundary dislocations. Arrows indicate the direction of motion of dislocations during relaxation.

sion of distances to the average distance between dislocations, decreased as

$$\Delta(t) = \exp\left(-1.18\sqrt{\frac{t}{t_r}}\right),$$

where the characteristic relaxation time $t_r$ is determined as follows

$$t_r \approx \frac{kTh_0^3}{\delta D_b G V_a}. \qquad (4)$$

Let us compare the relaxation time of disordered dislocation walls (4) with the spreading time for the lattice dislocations trapped by grain boundaries (3), assuming that the density of the latter is $10^7$ m$^{-1}$. For Ni, at a temperature of $T = 493$ K using formula (4), one obtains $t_r \approx 3.5\times10^3$ s, and the spreading time is 15 s [35]. For stainless steel, at a temperature of $T = 703$ K, one obtains $t_r \approx 3.4\times10^3$ s, while the spreading time is 22 s [58]. In both cases, the relaxation time of disordered dislocation arrays is more than two orders of magnitude longer than the spreading time of the extrinsic grain boundary dislocations. This confirms that fact, indeed, after the disappearance of the images of extrinsic dislocations, the grain boundaries are still in a non-equilibrium state.

## 2.4. Relaxation of wedge junction disclination quadrupole

Models for the relaxation of sessile components of trapped lattice dislocations were proposed in Refs. [62-64]. The relaxation of a disclination dipole at one boundary was considered in Ref. [62], while the relaxation of a quadrupole of disclinations formed at opposite grain boundaries was investigated in Refs. [63,64]. The results show that the relaxation kinetics in these two cases differ insignificantly. Both models are based on an assumption on the controlling role of grain boundary diffusion.

Let us consider the finite wall of sessile extrinsic grain boundary dislocations equidistantly distributed along boundaries, which is equivalent to a quadrupole of wedge junction disclinations illustrated in Fig. 2. It is assumed that both the strength and arms of the disclination quadrupole do not vary during relaxation. At elevated temperatures, under the forces of mutual repulsion, the dislocations begin to climb towards the junctions. In order to escape into neighboring grain boundaries, a leading dislocation must undergo a dissociation reaction at triple junctions. In a general case, if there are no dislocations of opposite sign near the junction in neighboring boundaries, the grain boundary dislocations at the junction should split into dislocations belonging to these boundaries. At obtuse dihedral angles between the adjacent boundaries, which the most often the case in real polycrystals, an energetically favorable splitting reaction is possible, as a result of which four dislocations 3, 4 and 5, 6 are formed from the sessile dislocations 1 and 2, respectively, and glide along the corresponding boundaries. These four dislocations 3, 4, 5, 6 can easily leave the triple junction by sliding and annihilate somewhere in the middle of the corresponding boundaries with dislocations of the opposite sign sliding from adjacent junctions. If dislocations 4 and 5 do not annihilate, they can reach the neighbouring junction, and an energetically favoured recom-

bination reaction results in a formation of a glissile dislocation 7. The latter can further glide along a vertical grain boundary unless annihilation with a dislocation of opposite sign occurs and thus can be excluded from the annealing of this disclination quadrupole. The same processes occur near the lower junction of the considered grain boundaries. As a result of the escape of one dislocation from each of the four triple junctions, the strength of the quadrupole $\Omega$ decreases. After the loss of these four head dislocations, the next dislocations approach the junctions, and the process is repeated. Hence, the process of the relaxation of the disclination quadrupole is controlled by the climb of grain boundary dislocations towards the triple junctions. At that, the arm of the quadrupole is kept constant and equal to the length of the boundary.

The kinetics of the relaxation of a disclination quadrupole were considered in a discrete-dislocation approach via solving the equations of motion of dislocations. The relative rate of change in the strength of the disclination quadrupole, $d\Omega/\Omega dt$, can be calculated from the time interval $\Delta$ in which two neighbouring dislocations successively approach the junctions. When dislocations approach the bottom and upper junctions, they are excluded from a consideration. It turned out that, after some short transient stage, the relative rate of decrease in the strength of the disclination quadrupole was constant and equal to 6.5 and did not depend on the number of dislocations remaining in the wall. For this steady-state stage, which is the stage with the longest duration, the strength of the quadrupole changes exponentially as $\Omega(t) = \Omega_0 \exp(-t/t_d)$ with the characteristic relaxation time proportional to the cube of the grain size:

$$t_d \approx \frac{kTd^3}{100\delta D_b G V_a}, \qquad (5)$$

where $\Omega_0$ is the initial strength of the disclination quadrupole. The modeling of the relaxation of the disclination dipole in the discrete-dislocation approach leads to the same equation, but with a coefficient of 125 instead of 100 [62]. Note that the relaxation of disclination dipole was also analyzed in the continuum model: the coefficients in the equations differ by about 1.5 times [62].

Detailed analysis of the kinetic of relaxation of disclination quadrupole shows that the process occurs in three stages [63, 64]. The first, transient stage is characterized by a high relaxation rate and has a duration determined by

$$t_t \approx \frac{kTd^3}{1600\delta D_b G V_a}. \qquad (6)$$

The second, steady-state stage is characterized by a constant relaxation rate (5). The third stage is characterized by a sharp decrease in the relaxation rate. It should be noted that the continuum analysis carried out in Ref. [62] is valid precisely for the second stage, i.e., when the distribution of diffusion fluxes along the boundary acquires a parabolic shape (for details see Ref. [62]). At this stage, the two approaches to the description of grain boundary recovery are practically equivalent. Consequently, the applicability of the continuum model is determined by the ratio of the total recovery time and duration of the second stage. It is obvious that the steady-state stage dominates over other recovery stages in the walls with a large number of dislocations.

The energy of a disclination dipole or quadrupole is proportional to the square of their strength, and therefore, the characteristic time during which the energy of the dipole or quadrupole decreases by a factor of $e$ is half the characteristic time for the strength. Direct calculations of the energy of the relaxing quadrupole confirm this fact [63,64].

## 2.5. Relaxation of a system of glissile extrinsic grain boundary dislocations

The kinetics of accommodation of a system of glissile (or tangential) extrinsic grain boundary dislocations was firstly analyzed in Ref. [65]. The authors assumed that the elementary relaxation mechanism of the system of glissile grain boundary dislocations is the climb of some effective sessile dislocation with the Burgers vector $b_t$ along the neighboring boundary from the triple junction towards a sink located at the center of this boundary. The driving force of the process is the stress of the system of gliding dislocations. However, one of the disadvantages of this model is its asymmetry. It assumes the creep of dislocations to the sink along only one neighboring boundary, while there are no restrictions to the sink along the other boundary.

A relaxation model symmetric with respect to neighboring boundaries was proposed in Ref. [62]. Fig. 3 shows a fragment of a hexagonal polycrystal, the horizontal boundary of which contains $N$ glissile extrinsic grain boundary dislocations. Under the mutual repulsion, the dislocations form a pile-up, locked at both ends at the triple junctions. This pile-up creates compressive stresses along the O$x$ axis and tensile stresses along the O$y$ axis. These stresses can relax by diffusion transfer of matter from the upper boundary to the lower one. Thus, the accommodation of glissile grain boundary dislocations can be described in the frames of the diffusion relaxation model. The equivalent discrete-dislocation description of this process is as follows. The head dislocation of a pile-up splits into two dislocations,

which, under the action of pile-up stresses and forces of mutual repulsion, climb to sinks located at the points *X* and *Y* (see Fig. 3). In this case, the sources of vacancies are dislocations climbing along the lower boundary, and the sinks are dislocations in the upper boundary.

Calculations performed according to a fairly traditional scheme [66] have shown that the decrease of the average density of the Burgers vector of tangential grain boundary dislocations occurs according to exponential law $\overline{\beta}(t) = \beta_0 \exp(-t/t_\tau)$, with a characteristic relaxation time [62]

$$t_\tau \approx \frac{kTd^3}{143\delta D_b G V_a}. \qquad (7)$$

Comparison of this expression with formula (5) suggests that the relaxation of the disclination component of non-equilibrium grain boundaries and systems of glissile extrinsic grain boundary dislocations obey the general equation and the characteristic relaxation times are practically the same.

The mechanisms of relaxation of systems of sessile and glissile extrinsic grain boundary dislocations considered above relate only to the processes occurring in one boundary. In the general case, the neighboring grain boundaries also contain extrinsic grain boundary dislocations, and the relaxation processes in different boundaries should be coordinated in a certain way. Unfortunately, for a time being, no models describing the accommodation processes of the spatial network of grain boundaries containing excess dislocations have been constructed. In both the continuous and discrete-dislocation models, such a calculation is a very challenging task. However, it can be assumed that taking into account the interaction of dislocations in different boundaries will not result in a qualitatively different kinetics of grain boundary recovery.

An indirect confirmation of the above said can be a recently discovered fact when considering the ultrasonic relaxation of disordered dislocation arrays in a columnar polycrystal containing non-equilibrium grain boundaries modelled be means of quadrupole of wedge junction disclinations [67]. It turned out that the presence of neighboring grains, which surrounds the central grain, does not have a significant qualitative effect on the kinetics of dislocation rearrangements in comparison with a single grain considered in Refs. [68-71], and all changes are of only quantitative character. It is because the quadrupole of wedge junction disclinations is a screened system and therefore it can be argued that all dislocations rearrangements are completely determined by long-range interactions within the individual grains.

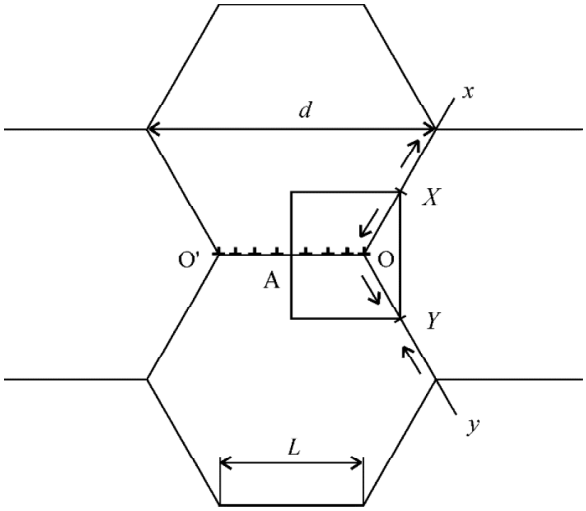


**Fig. 3.** A model for the relaxation of a system of glissile (or tangential) extrinsic grain boundary dislocations. Arrows indicate the direction of atomic diffusion during relaxation.

## 3. APPLICATION TO NANOMATERIALS AND CONCLUDING REMARKS

Grain boundaries in as-prepared nanostructured materials contain extrinsic grain boundary dislocations, which can be divided into the three types of non-equilibrium ensembles as said in Section 1 and considered in Sections 2.3-2.5: disordered systems of extrinsic grain boundary dislocations, junction disclinations, and tangential extrinsic grain boundary dislocations. The parameters of these ensembles of defects are determined by the ratio of the strain rate and the rate of relaxation, which can occur either by the climb of extrinsic grain boundary dislocations, or athermally by generating dislocations from grain boundaries, or by activating secondary slip in the grain, which lowers the level of internal stresses.

The most probable way of relaxation of disordered arrays of extrinsic grain boundary dislocations is diffusion-controlled rearrangement. Let us consider how this process can occur at room temperature. For this, it is sufficient to calculate the characteristic relaxation time using expression (4). Calculations carried out with the dislocation density of $\rho_0 = 10^8$ m$^{-1}$ for four metals (Al, Cu, Ni, and Fe) show that the disordered arrays of extrinsic grain boundary dislocations are extremely unstable at room temperature in Al and their relaxation time is 170 s. This is consistent with the fact that the spreading of images of extrinsic dislocations in Al occurs at temperatures much lower than room temperature [34,36,37]. These ensembles of dislocations are relatively stable in Cu: the relaxation time is of about one and a half months.

Researchers who have dealt with nanostructured Cu have noticed that these samples, which have been lying for a month, show significant signs of structural changes. The latter may be associated with the relaxation of this particular component of the defect structure of grain boundaries. In Ni, the density of disordered arrays of extrinsic dislocations, which are stable during one or two months, is much higher and equal to $4\times10^{8}$ m$^{-1}$, while the relaxation time at the dislocation density of $10^{8}$ m$^{-1}$ is $4.3\times10^{8}$ s. In Fe, this relaxation time is equal to $4.3\times10^{15}$s, i.e., disordered arrays of extrinsic grain boundary dislocations can persist for an almost unlimited time period.

Comparison of expression (4), on the one hand, and (6), (7), on the other hand, shows that the relaxation times of disclination quadrupoles and ensembles of tangential extrinsic grain boundary dislocations at room temperature, even in nanomaterials, are immeasurably longer than the relaxation time of disordered arrays of extrinsic grain boundary dislocations. Therefore, diffusion relaxation these components of non-equilibrium grain boundary structure are almost completely absent at room temperature.

At increased temperatures, relaxation processes in non-equilibrium grain boundaries occur relatively fast. The results obtained can be compared with the experimental data for submicrocrystalline Cu processed by severe plastic deformation method [72]. In the cited work, the authors observed a significant accommodation of the grain boundary structure and elastic moduli after annealing the samples during one hour at $T = 398$ K. These effects are related to relaxation of both components of non-equilibrium grain boundary structure: junction disclinations and tangential extrinsic grain boundary dislocations. Calculation of the characteristic relaxation times (5) and (6) using the following parameters for Cu: $\delta D_{b0} = 2.35\times10^{-14}$ m$^3$/s, $Q_b = 107.2$ kJ / mol [73], $G = 5\times10^{4}$ MPa, $V_a = 1.18\times10^{-29}$ m$^3$, gives circa 60 min. This is a very good agreement with the experimental observations.

It is interesting to compare the characteristic relaxation times for the first and second stages with each other and with the spreading time (3). From formulas (5) and (6) one obtains that $t_{spr}/t_t \approx 16$. Thus, the duration of the first transient stage is noticeably shorter than the duration of the second one. Taking into account expressions (3), (5), and (6), one derives: $t_t/t_{spr} > 1$, when $d > 230$ nm, $t_d/t_{spr} > 1$, when $d > 90$ nm. Considering that $t_d > t_t$, let us build a hierarchy of characteristic relaxation times depending on the grain size $d$. Thus, if $d < 90$ nm, then $t_t < t_s < t_{spr}$; if $90 < d < 230$ nm, then $t_t < t_{spr} < t_d$; if $d > 230$ nm, then $t_{spr} < t_t < t_d$. Thus, in the range of grain sizes of several tens of nanometers, the spreading time calculated by formula (3) turns out to be longer than the relaxation time of the disclination quadrupole. However, the duration of the relaxation process should always be no shorter than the spreading time, since, otherwise, it would turn out that the grain boundaries transformed into an equilibrium state before the delocalization of the nuclei of extrinsic grain boundary dislocations occurred. Therefore, in materials with the indicated grain size, spreading should take place in a shorter time and according to a different law, and, in this case, formula (3) cannot be used. Under these conditions, it should be assumed that the spreading time coincides with the relaxation time. The latter means that at $d \le 90$ nm, the observed spreading time of lattice dislocations trapped by the boundaries should depend on the grain size: the smaller is $d$, the faster is the spreading of images of extrinsic dislocations.

Presently, in the scientific literature there are many experimental data on the study of kinetics of spreading of the extrinsic grain boundary dislocations. However, unfortunately, there are no such data concerning the entire process of grain boundary recovery. In addition, there were also no studies on the kinetics of recovery for any property of a polycrystal, the relaxation time of which could be directly compared with the relaxation time of the non-equilibrium grain boundary structure. The influence of relaxation on the yield point during annealing of a deformed polycrystal is not direct, since in this case the yield point is affected by dislocation processes occurring in regions close to the grain boundaries.

The results presented in this review paper have important applications for high-temperature plastic deformation of polycrystals and, in particular, for superplastic deformation. During plastic deformation, the accumulation of extrinsic grain boundary dislocations occurs, which form the unscreened systems, such as quadrupoles of junction disclinations. The stress fields of these disclinations act on dislocations approaching the grain boundaries in such a way that this leads to hardening. The complete accommodation of extrinsic grain boundary dislocations results in a reduction of these stresses. Thus, the equilibrium between these two competing processes will lead to a stationary strain rate that will depend on temperature. Therefore, the characteristic relaxation time of the disclination quadrupole can be included in the most natural way in the rate equation for high-temperature deformation.

In summary, in the present paper, accommodation processes in non-equilibrium grain boundaries in nanostructured materials processed by severe plastic deformation methods have been reviewed. The results predicted by the models are in a good agreement with experimental data and allow us to describe the evolution of mechanical properties of nanomaterials associ-

ated with relaxation of non-equilibrium grain boundary state. In addition to the accommodation of different components of non-equilibrium grain boundary structure, their application to analysis of recovery of various mechanical properties for nanocrystalline and ultrafined-grained materials is undertaken.

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