NUCLEATION OF DISCLINATION DEFECTS AND DEVELOPMENT OF MISORIENTATION BANDS AT GRAIN BOUNDARY JUNCTIONS

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ABSTRACT

Grain boundary triple junctions and other faults in grain boundary geometry (i.e., steps, kinks and jogs) are strong concentrators of applied stresses. They also may serve as the sources of internal stresses when disclination defects are present at junctions or steps. In nanocrystalline materials the density of triple junctions and four-fold nodes of triple junctions is high. Therefore disclination defects show stronger impact on the properties of such materials. In the present report, the disclination models for misorientation band (MB) generation at grain boundary kinks and junctions are analyzed. The models consider wedge disclination dipole and quadrupole configurations and predict the value for critical external shear stress τ_c, above which the event of disclination nucleation takes place. The numerical estimates for τ_c give the values of $G/1000$ – $G/100$ (G being shear modulus). These values correspond to the level of deforming stress observed in the materials with ultrafine grain structure. Further evolution of disclination structure at an isolated grain boundary fault demonstrates two main regimes of MB development: stable and unstable propagation. Current results on computer simulations of dislocation-disclination interactions, which are the key-issues for the kinetics of MB nucleation and propagation, are also discussed.

KEYWORDS

Disclinations, misorientation bands, grain boundaries, nanocrystals, deforming stress.

INTRODUCTION

Under high degrees of plastic strain and other extreme deformation conditions, metals and alloys (especially those having nanocrystalline structure) reveal defect substructures, which are characterized in terms of disclinations [1-3]. Typical elements of such substructures are misorientation bands (MBs), which are observed as long straight strips of material having the crystallographic orientation different from that of neighboring areas of the material. The boundaries of such MBs, i.e., the misorientation boundaries, are often considered as low-angle dislocation tilt boundaries although they may have a finite thickness of about 0.1-0.5 μm depending on the deformation magnitude [1], and consist in fact of high-density dislocation arrangements. From the dislocation models of MBs follows that the edges of a misorientation boundary pair can also be viewed as lines of partial wedge disclinations of opposite signs, i.e., as a two-axes disclination dipole [1,2].

In 1978, Vladimirov and Romanov [4] developed a dislocation-disclination model to describe the mechanism of MB propagation. The main idea of the model is that the elastic stresses created by the disclination dipole, make a statistically arranged dislocation ensemble in front of the MB to be separated into “positive” and “negative” parts whose dislocations, “positive” or “negative”, are caught by the positive or negative disclinations, respectively. Every event of capturing of a dislocation dipole by the disclination dipole leads to an elementary act of the MB conservative motion. The mechanism proposed in [4] has been observed experimentally [1,2] and used in modeling the dislocation-disclination kinetics in metals under large deformation [2,5-8]. However, a number of questions still arises concerning the mechanisms of disclination defect nucleation. Until now, no theoretical model exist that would allow to describe the MB generation and predict appropriate critical conditions as well as regimes of MB propagation; no details of dislocation capture by disclination dipoles have still been known.

It is well documented [1,2] that possible sites for MB generation in conventional polycrystalline metals are various faults (defects) of grain boundaries (GBs) including kinks, double and triple junctions of GBs. In nanocrystalline solids, such GB faults often contain disclinations, even in an initial as-sintered state [3]. Below the models for initial disclination configurations at GB junctions are proposed and the mechanisms of their evolution leading to MB generation and propagation are investigated. Critical shear stresses are calculated, which are necessary for these processes. The limiting shear stress is also found which separates stable and unstable regimes of MB propagation. Corresponding MB equilibrium lengths are introduced for the stable regime of MB development. In conclusion, some current results on computer simulations [9] of dislocation-disclination interactions are reported and discussed.

MODELS FOR INITIAL DISCLINATIONS AT GRAIN BOUNDARY JUNCTIONS

Consider a simple scenario, shown in Fig.1, which may be applied to initial disclination configuration formation at a GB. Let a shear band consisting of some gliding dislocations with Burgers vectors $\vec{b}_1$ crosses a GB plane (Fig.1a) and moves into the neighboring grain where the gliding dislocations have Burgers vectors $\vec{b}_2$ (Fig.1b). As a result, a wall of difference dislocations having Burgers vectors $\delta\vec{b} = \vec{b}_2 - \vec{b}_1$ and interdislocation spacing l, appears at the crossing site together with the GB kink. On a mesoscale level, when the characteristic scale of consideration L is much larger than l, the geometry and resulting elastic fields for such difference dislocation wall may be effectively described as those of a two- axes dipole of wedge partial disclinations of strengths $\pm\omega = \delta b / l$ [2] (Fig.1c).

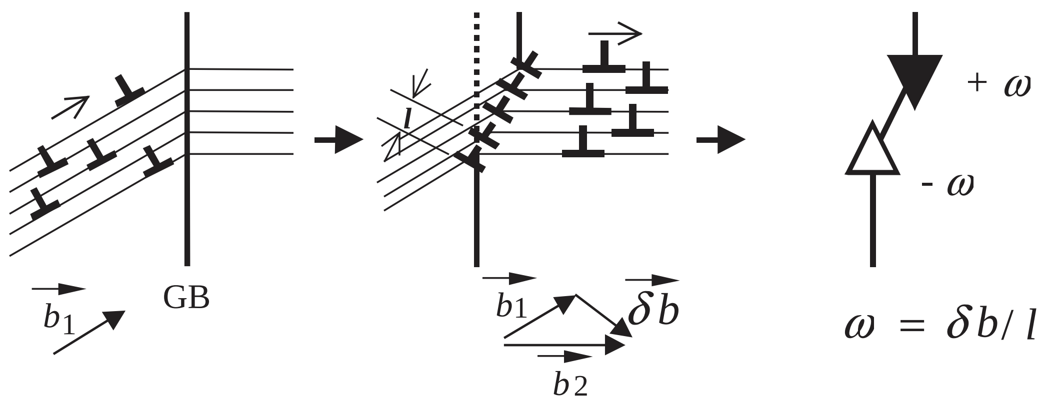


Figure 1. Formation of grain boundary disclination dipole of strength ω.

In reality, the initial disclination configurations at GBs result from more complicated processes which are typical for the stages at which translational deformation modes are replaced by rotational ones [1, 2]. For example it is known [1], that in the vicinity of GB kink or junctions the dislocation cells have smaller size than far from such sites. This means that within these areas, the density of GB difference dislocations must be much higher than at straight or smooth segments of GBs. As a corollary, one can assume the formation of initial quadrupole-like disclination configurations at GB kink or junctions (for more details, see [9]).

GENERATION OF MISORIENTATION BANDS

Consider the simplest initial GB disclination configuration that is a GB disclination dipole (GBDD) shown in Fig.2a. Let this GBDD be under an external shear stress τ. We also assume that around of the GBDD, there is typical cellular dislocation structure. Under the action of the internal shear stress (which is caused by the GBDD and external shear stress τ), the dislocations from the cell boundaries nearest to the dipole disclinations have to glide to them thus forming two dislocation walls, i.e., a new disclination configuration (Fig.2b). The latter may be considered as that produced by splitting of the initial GBDD. This new split configuration is characterized by the split distance d, the interdislocation spacing l, the dipole arm $2a$ and the disclination strengths $\pm\alpha$ and $\pm\beta$ satisfying the relationships $\beta = b/l$ and $\omega=\alpha+\beta$, where b is the magnitude of Burgers vector for lattice dislocations and ω is the initial strength of the GBDD. In fact, the new split disclination configuration represents a model for a MB of finite length, which consists of a new immobile GBDD having the strength α (α-dipole), a new mobile disclination dipole with the strength β (β-dipole), and two misorientation boundaries of the length d.

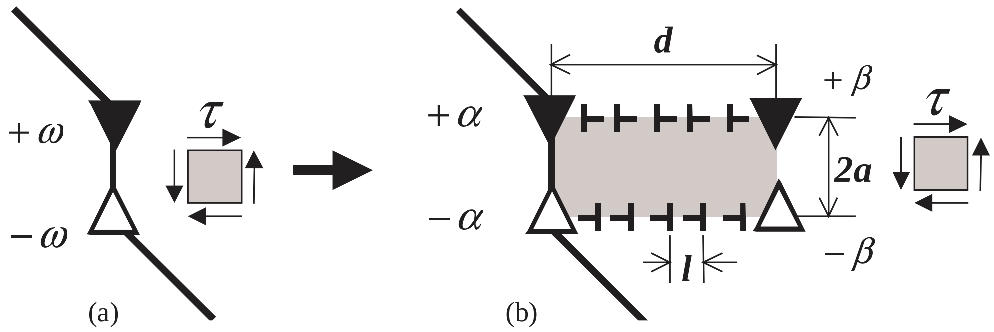
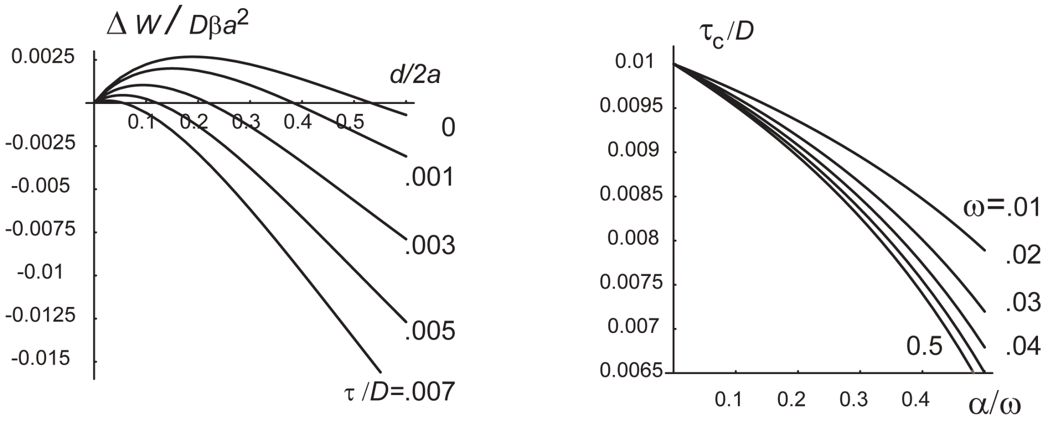


Figure 2. Generation of a misorientation band by splitting of the initial grain boundary disclination dipole $\pm\omega$ (a) into disclination dipoles $\pm\alpha$ and $\pm\beta$ (b).

To make possible the transition from the initial GBDD to the new split configuration, the total energy of the initial GBDD must be larger than that of the new split configuration. Thus, to find critical conditions for such a transition, one has to calculate and compare these energies. The total energy of the initial GBDD may be calculated as a work done to generate the GBDD in its proper elastic stress field [2]. As a result, we have the following expression for the energy per unit length of disclinations:

$$W_1 = D\omega^2 a^2 \left(2\ln\frac{R}{2a} + 1 \right), \tag{1}$$

where $D = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is Poisson ratio, and R is a characteristic parameter of screening of the disclination long-range elastic fields (e.g., the size of a sample).



(a) (b)

Figure 3. Energy difference ΔW and critical stress τ_c for split dipole configuration. Parameters for plots: $q = 10$, $b/2a = 10^{-3}$ and $\alpha = \pi/200$ (for (a)).

The total energy of the new split configuration (per unit length of disclinations) may be written as the following sum:

$$W_2 = W_\alpha + W_\beta + W_{\alpha-\beta} + 2\gamma d - A, \tag{2}$$

where W_α and W_β are the elastic energies of α- and β-dipoles (Fig.2b), respectively, $W_{\alpha-\beta}$ is the energy of their interaction, γ the effective surface energy of the two new misorientation boundaries, and A the work done by the external shear stress τ on the displacement d of the mobile β-dipole. The terms W_α and W_β are similar to those given by Eq.1 with the replacement of ω by α and β, respectively. The energy of dipole-dipole interaction $W_{\alpha-\beta}$ is calculated as the work done during the generation of one dipole in the stress field of another dipole, thus resulting in

$$W_{\alpha-\beta} = 2D\alpha\beta a^2 \left(\ln \frac{R^2}{4a^2 + d^2} - \frac{d^2}{4a^2} \ln \frac{4a^2 + d^2}{d^2} + 1 \right), \tag{3}$$

The work A is found in a similar way that gives $A = 2\tau\beta a d$.

To estimate γ, one can use the well-known approximation for the energy of a dislocation core [10] $W_c \approx Db^2/2$. Due to geometric reasons [10], the linear density of "geometrically-necessary" dislocations ρ_g within a misorientation boundary is equal to β/b. However, we have also to take into account the density of "statistically-stored" dislocations which have different orientations of their Burgers vectors and do not create any additional misorientation but give their income into the effective surface energy of the boundary. Let the total dislocation density within the misorientation boundaries ρ_t be equal to $q\rho_g$, where $q \geq 1$ is a dimensionless parameter, which accounts for the presence of "statistically-stored" dislocations. Hence, the number of dislocation cores, N, within a misorientation boundary is estimated as $N = \rho_t d = q\beta d/b$ and the total core energy of a misorientation boundary is $NW_c \approx qD\beta bd/2$. Than we have $\gamma \approx NW_c/d \approx qD\beta b/2$.

Consider now the energy difference:

$$\Delta W = W_2 - W_1 = D\beta a^2 \left\{ 4\tilde{d}\left(q\tilde{b} - \frac{\tau}{D} \right) - 2\alpha \left[(1+\tilde{d}^2)\ln(1+\tilde{d}^2) - \tilde{d}^2 \ln \tilde{d}^2 \right] \right\}, \quad (4)$$

where we have introduced dimensionless $\tilde{d} = d/2a$ and $\tilde{b} = b/2a$. The example for the dependence ΔW on the normalized displacement $d/2a$ is given in Fig.3a. Depending on τ (and also parameter q), the character of curves $\Delta W(\tilde{d})$ changes drastically from monotonous decreasing to non-monotonous one. For example, when $q = 1$ while τ and $\tilde{d}$ are small enough (here $0 \le \tau \le 0.007D$ and $\tilde{d} < 1$), $\Delta W < 0$ for $\tilde{d} > 0$. This means there is no energetic barrier for generating of the MB. In the other case, when $q = 10$ with the same values of τ and $\tilde{d}$, $\Delta W > 0$ for $\tilde{d} < \tilde{d}_c$ where $\tilde{d}_c$ is determined by the equation $\Delta W(\tilde{d} = \tilde{d}_c) = 0$ and $\Delta W < 0$ for $\tilde{d} > \tilde{d}_c$. This means there is an energetic barrier for generating of the MB for such a small τ. Let us introduce a characteristic critical value τ_c, which is determined by the equation $\tilde{d}_c = l/2a$, where l is the spacing between the "geometrically-necessary" dislocations creating the tilt misorientation angle β. If $\tau < \tau_c$, the generation of MB nucleus (an initial GBDD plus one dislocation dipole joined to the GBDD and localized at the distance l from it) is energetically unfavorable; if $\tau > \tau_c$, it is. For the case illustrated in Fig.3a, we assume $l/2a \approx 0.1$ and hence $\tau_c(q = 10) \approx 0.005D$. In a similar way, one can prove that $\tau_c(q = 5) \approx 0.001D$ and $\tau_c(q = 7) \approx 0.003D$. Using Eq.4, we can analytically estimate τ_c for the case $\tilde{d} << 1$ as follows

$$\tau_c \approx D\tilde{b}\left[q - \frac{\tilde{\alpha}}{1-\tilde{\alpha}} \left(\frac{1}{2} - \ln \frac{\tilde{b}/\omega}{1-\tilde{\alpha}} \right) \right], \quad (5)$$

where $\tilde{\alpha} = \alpha/\omega$. The plots $\tau_c(\tilde{\alpha})$ are shown in Fig. 3b for $q = 10$ and various values of the initial GBDD strength ω. One can conclude that τ_c decreases when both $\tilde{\alpha}$ and ω increase that is in accordance with physical intuition. When $q = 10$, the numerical estimate for τ_c gives the values of order $G/1000 - G/100$. The lower limit fits well with typical external stresses at the end of Stage II of deformation curves for BCC and FCC metals [1] while the upper limit corresponds to the level of deforming stress observed in nanocrystalline materials [3].

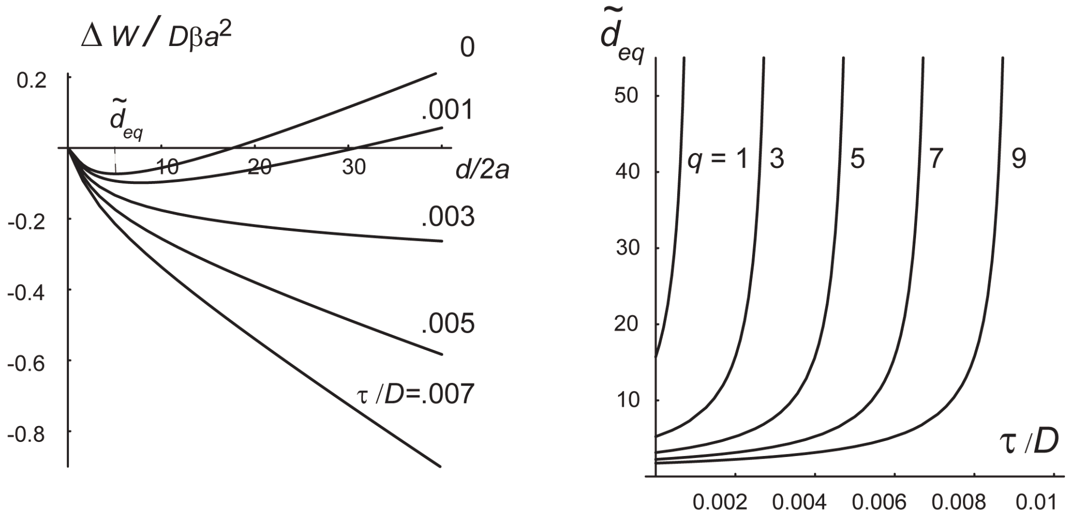
For MB generation at the vicinity of more realistic disclination quadrupole-like configurations, the interactions of mobile disclination dipole with all defects has to be taken into account. The results of these calculations will be presented elsewhere [9]. The results demonstrate that the value of the critical stress τ_c for MB generation in the framework of disclination mechanism remains in the same order of magnitude as it was obtained for the configuration presented in Fig.2, i.e., $\tau_c \approx G/1000 - G/100$.

REGIMES OF MISORIENTATION BAND PROPAGATION

In the previous section, we have analyzed the model for MB generation by using the expression for the energy of disclination dipole configuration given by Eqs.1 to 4, for the case $\tilde{d} << 1$. To study further propagation of MBs, one can use the same expressions but in the limit of $\tilde{d} \ge 1$. Consider again the model in Fig.2. The characteristic example of graphical representation of Eq.4 for the case $\tilde{d} \geq 1$ is given in Fig.4a. Depending on the value of τ, the curves $\Delta W(\tilde{d})$ behave in different ways. When τ is smaller than some limiting quantity τ_p (e.g., $\tau_p \approx 0.003D$ for $q = 3$), the curves $\Delta W(\tilde{d})$ are non-monotonous and show the minima,

(a) (b)

Figure 4. Energy difference ΔW and equilibrium length $\tilde{d}_{eq}$ for propagating dipole.



Parameters for plots: $b/2a = 10^{-3}$ and $\alpha = \pi/200$; $q = 3$ (for (a)).

which determine equilibrium values of the MB length $\tilde{d}_{eq}$. When $\tau > \tau_p$, the curves $\Delta W(\tilde{d})$ go with monotonous decrease, and $\tilde{d}_{eq}$ is absent. To find an analytical estimate for τ_p, one can solve the equation $\Delta W(\tau) = 0$ for the limiting case $\tilde{d} \to \infty$ that gives $\tau_p = Dq\tilde{b}$. Obviously this provides the linear relation between τ and q, where the last characterizes the effective surface energy of the misorientation boundaries. The equilibrium length $\tilde{d}_{eq}$ is found from the standard relation $\dfrac{\partial \Delta W}{\partial d} = 0$ with $\dfrac{\partial^2 \Delta W}{\partial d^2} > 0$ and $\tilde{d} > 1$. As a result, $\tilde{d}_{eq} \approx \dfrac{\alpha}{q\tilde{b} - \tau/D}$ if $\tau < \tau_p$. The dependence $\tilde{d}_{eq}(\tau)$ is illustrated in Fig.5b for different q. One can see that $\tilde{d}_{eq}$ increases with increasing τ and decreasing q.

It is thus shown that two main regimes of MB propagation are possible depending on the external shear stress τ: stable and unstable propagation. When $\tau < \tau_p$, the MB propagation is stable and may be characterized by the equilibrium length $\tilde{d}_{eq}$. When $\tau > \tau_p$ the MB propagation is unstable and there is no equilibrium length.

COMPUTER SIMULATION OF DISLOCATION-DISCLINATION INTERACTIONS

To check and refine the models of MB propagation through an ensemble of edge dislocations as well as to calculate some important parameters of dislocation-disclination interactions (e.g., the effective length of dislocation capturing by a disclination dipole), the technique of molecular dynamic simulation (dislocation dynamics) has been used (see [9] for details). The computer code objects are straight edge dislocations and straight wedge disclinations which can move within a two-dimensional rectangular box of the infinite elastically isotropic medium (Fig.5). The periodic boundary conditions are realized. The box sizes are chosen as 1 1 mm^2. All disclinations are arranged in dipole configurations, which are assumed to be immobile and considered as sources of elastic fields. The dislocations can move by gliding or climbing under the action of the total force due to external loading, elastic fields of other defects and dynamic friction. Giving initial coordinates and velocities to every defect, the system of motion equations is solved numerically and the dependences of coordinates x, y and velocity components v_x and v_y on time t are found.

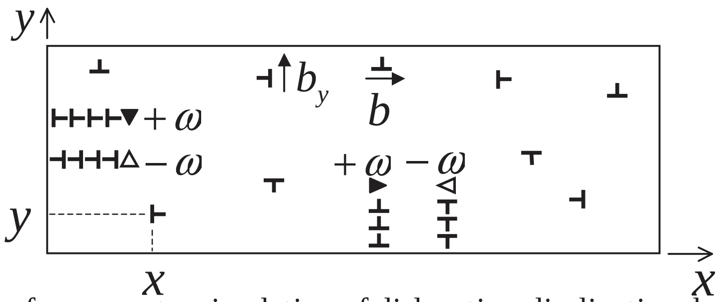


Figure 5. Box for computer simulation of dislocation-disclination dynamics.

The above approach has been used to consider the elastic interaction of a gliding edge dislocation with a two-axes wedge disclination dipole [9]. Some typical configurations have been studied for different orientations of the dipole arm, initial positions and velocities of the dislocation. It has been shown that the dislocation behavior may strongly vary depending on the problem parameters, but it is the elastic stress of the disclination dipole, which eventually dictates the result of interaction. For example, let the dislocation begin its motion under the influence of the horizontal-arm dipole (Fig.6a). The dislocation is accelerated within the region of relatively higher positive shear stresses of the dipole and stopped after at the zero-value stress contour outside the dipole (Fig.6b). The capturing of the dislocation by the dipole occurs at very small distances from the dipole only. The calculations show that the models of the disclination dipole motion have to be reconsidered to account for this observation.

The results described may be considered as an approval of the computation code readiness to model more complicated cases including more defects and varying conditions of external loading. Also the proposed approach permits to analyze the dynamics of dislocation-disclination interactions. Therefore it stimulates new interest to study the cooperative behavior of defects in materials under extreme deformation conditions.

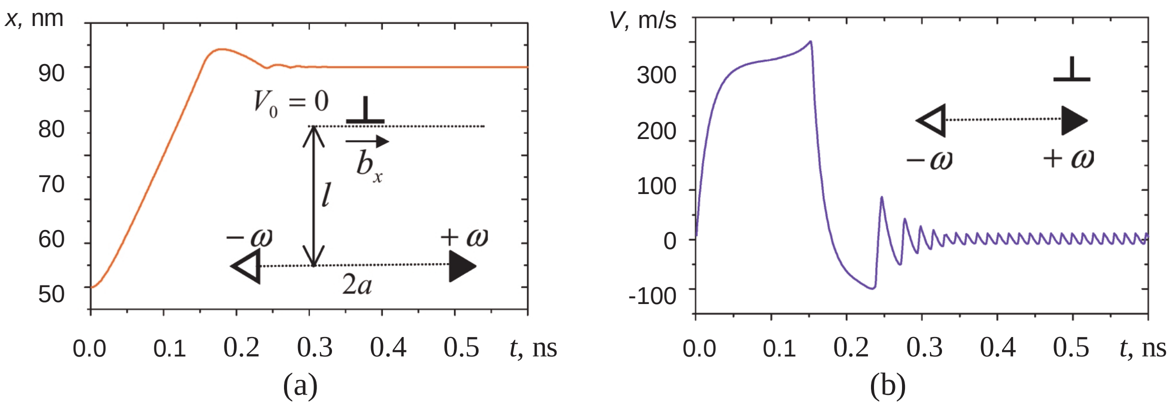


Figure 6. Capturing of a gliding edge dislocation by a wedge disclination dipole. The plots of dislocation position (a) and velocity (b) via time are shown for the following values of parameters: ω=.001, b_x=.256 nm, l=1nm, 2a=100 nm.

CONCLUSIONS

Disclination models of misorientation band (MB) generation at grain boundary faults predict the existence of a critical external shear stress τ_c for the MB nucleation events take place. The numerical estimates for the critical stress give the values of order $G/1000$ - $G/100$, which are in accordance with observed magnitudes for deforming stresses at the deformation Stage II to Stage III transition for monocrystalline and conventional polycrystalline metals or at the initial deformation stage for nanocrystalline materials. The critical stress depends on the geometry and strengths of initial grain boundary disclination configurations, on the misorientation angle as well as on the effective surface energy of arising misorientation boundaries. It increases when the initial disclination strength decreases and the misorientation angle increases. The critical stress is proportional to the effective surface energy of misorientation boundaries.

Disclination models of MB propagation predict the existence of a limiting external shear stress τ_p, which separates stable and unstable regimes of MB propagation. When the external stress is lower than the limiting stress, the MB propagation is stable and may be characterized by the equilibrium MB length which increases when the external stress increases and the effective surface energy of misorientation boundaries decreases. If the external stress is higher than the limiting stress, the MB propagation is unstable. The limiting external stress varies in direct proportion to the effective surface energy of misorientation boundaries, too.

Computer simulations by means of dislocation dynamics code have shown that the existing models for the disclination dipole motion must take into account that fact that the mobile dislocation capturing by a dipole occurs at very small distances only.

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