

STRESS-DRIVEN FORMATION OF NANOGRAIN CHAINS IN NANOCRYSTALLINE AND ULTRAFINE-GRAINED MATERIALS

N.F. Morozov^{1,2}, I.A. Ovid'ko^{1,2} and N.V. Skiba^{1,2}

¹Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vasilievskii Ostrov, St. Petersburg 199178, Russia

² Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198504, Russia

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Abstract. Stress-driven formation of nanograin chains - groups of two or more elongated nanograins - in nanocrystalline (NC) and ultrafine-grained (UFG) materials is theoretically described. Within the suggested theoretical description, stress-driven formation of new nanograins is enhanced at previously generated nanograins with disclinations at their grain boundary junctions. The formation process occurs through splitting transformations of grain boundaries (containing disclination dipoles) into immobile and mobile grain boundaries. Stress-driven migration of mobile grain boundaries serves as a plastic flow mode at the nanograin level and results in formation of nanograin chains. It is shown that the transformations under consideration are energetically favorable in mechanically loaded nanoceramics α -Al₂O₃ (sapphire) and NC/UFG Al (aluminum) in certain ranges of their parameters.

1. INTRODUCTION

The outstanding mechanical properties of NC and UFG materials represent the subject of intensive studies motivated by their high technological potential; see, e.g., [1-18]. From a microscopic viewpoint, the mechanical properties of NC and UFG materials are dramatically influenced by specific deformation mechanisms which effectively operate in these materials. The fact is that the lattice slip is hampered by large amounts of grain boundaries existing in NC and UFG structures. In these circumstances, in parallel with the lattice dislocation slip, grain boundary deformation mechanisms - grain boundary sliding, grain boundary diffusional creep (Coble creep), rotational deformation (carried by grain boundary defects) and stress-driven grain boundary migration - effectively come into play in NC and UFG materials [1-10]. Of particular interest

is the stress-driven grain boundary migration which by definition represents a plastic deformation mode carried by migrating grain boundaries [3,19-24]. It is conventionally treated that the stress-driven grain boundary migration carries both nanoscale plastic flow and grain growth [3,19-24]. In particular, this role of the stress-driven grain boundary migration is indirectly supported by experimental observations [25,26] of the athermal grain growth in the vicinities of cracks in NC materials. Recently, it has been suggested that the stress-driven grain boundary migration plays an alternative role as a process carrying nucleation of new grains in NC and UFG materials [27-30]. In doing so, the grain nucleation is considered as a process occurring through splitting and migration of grain boundaries, in parallel with splitting and movement of grain boundary disclinations (rotational defects) [27-30]. In papers [27-30], the two types of the initial grain boundary

Corresponding author: I.A. Ovid'ko, email: ovidko@nano.ipme.ru

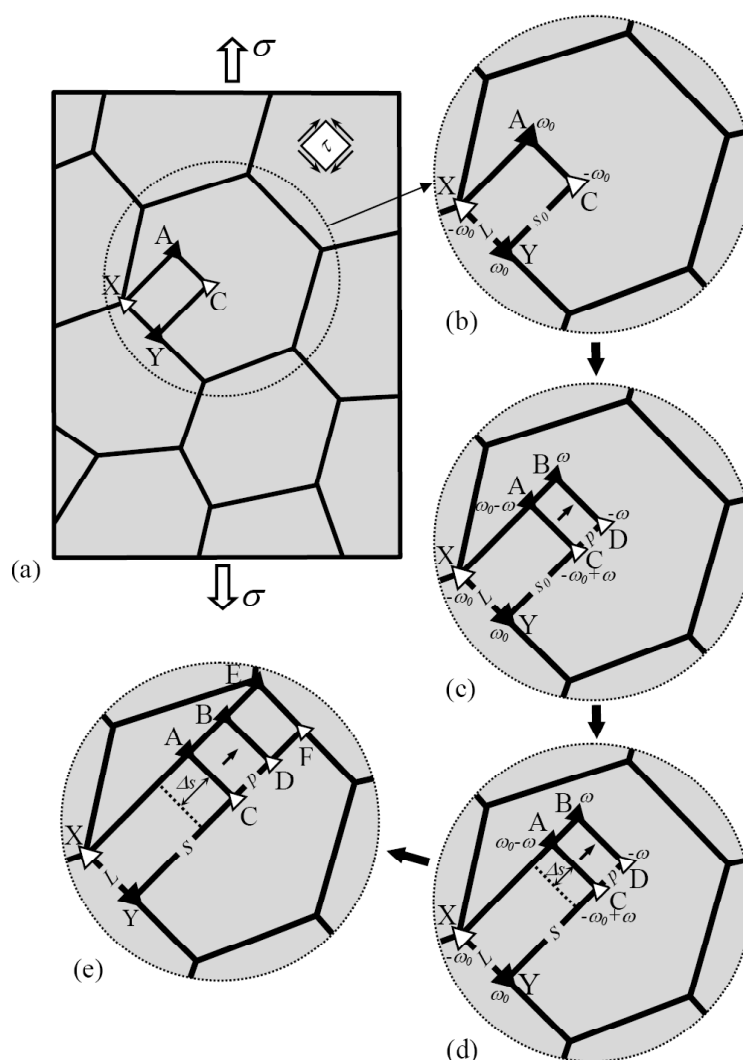


Fig. 1. Structural transformations in an ultrafine-grained specimen under mechanical load. (a) A mechanically loaded specimen with the ultrafine-grained structure. General view. (b) - (e) Magnified insets show evolution of a specimen fragment, resulting in formation of a nanograin at a previously formed nanograin. (b) Initial state with previously formed nanograin $ACYX$ containing quadrupole of wedge $\pm\omega_0$ -disclinations (triangles) located at its junctions. (c) The grain boundary AC splits into the immobile grain boundary (also called AC) and the mobile grain boundary BD that migrates over the distance p . The migration is accompanied by formation of new grain boundaries AB and CD . The junction points B and D of the mobile grain boundary contain the disclinations with strengths $\pm\omega$. These disclinations are resulted from splitting of the initial disclinations with strengths $\pm\omega_0$, and they form a mobile dipole configuration. As a result of the splitting transformations of the grain boundary AC and disclinations, a new nanograin $ABDC$ is formed. (d) Further growth (elongation) of grains $ACYX$ and $ABDC$ occurs. As a result, a nanograin chain configuration (consisting of two elongated grains) is formed. (e) A new splitting process for the grain boundary BD may result in both formation of new nanograin $BDEF$ and development of nanograin chain.

structure (before the grain nucleation) were considered: a highly stressed, disclination-free region near a crack tip of a NC solid [29], and a grain boundary structure containing a disclination dipole in the vicinity of a triple junction of grain boundaries [27,28,30]. The main aim of this paper is to theoretically describe the stress-driven grain nucleation

(occurring through transformations of grain boundary disclinations and serving as a plastic flow mode at the nanograin level) in a previously unconsidered, but rather typical situation. In this situation, the initial grain boundary structure contains a quadrupole of disclinations located at grain boundary junctions of a previously formed nanograin in a NC or UFG

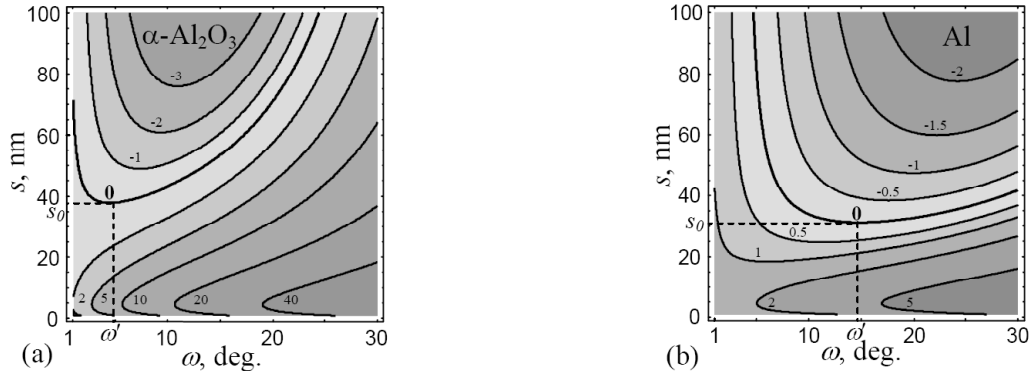


Fig. 2. The map of the characteristic energy change ΔW in the coordinate plane of ω (the strength magnitude that characterizes the mobile dipole BD of $\pm\omega_0$ -disclinations) and s (the arm of the $\pm\omega_0$ -disclination quadrupole) at the external stress value $\tau = 1$ GPa, for (a) nanocrystalline ceramics $\alpha\text{-Al}_2\text{O}_3$ (sapphire) and (b) nanocrystalline Al.

in its initial state with the $\pm\omega_0$ -disclination quadrupole (Fig. 1b), and W_2 is the energy of the defect configuration in its final state (Fig. 1d). The transformation is energetically favorable, if $\Delta W < 0$. In terms of the theory of defects in solids, the energy change ΔW is written as follows:

$$\Delta W = E_s^{\omega_0} + E_s^{\omega} + E_s^{\omega_0-\omega} + E_{\text{int}}^{\omega_0-\omega} + E_{\text{int}}^{\omega_0-(\omega_0-\omega)} + E_{\text{int}}^{\omega-(\omega_0-\omega)} + E_\gamma - E_\tau - E_s^q \quad (1)$$

Here $E_s^{\omega_0}$, E_s^{ω} , $E_s^{\omega_0-\omega}$ and E_s^q are the proper elastic energies of the dipole XY of $\pm\omega_0$ -disclinations, the dipole BD of $\pm\omega$ -disclinations, the dipole AC of $\pm(\omega_0-\omega)$ -disclinations and the initial quadrupole $XACY$ of $\pm\omega_0$ -disclinations, respectively; $E_{\text{int}}^{\omega_0-\omega}$ is the energy that characterizes the elastic interaction between the dipole XY of $\pm\omega_0$ -disclinations and the dipole BD of $\pm\omega$ -disclinations; $E_{\text{int}}^{\omega_0-(\omega_0-\omega)}$ is the energy that characterizes the elastic interaction between the dipole XY of $\pm\omega_0$ -disclinations and the dipole AC of $\pm(\omega_0-\omega)$ -disclinations; $E_{\text{int}}^{\omega-(\omega_0-\omega)}$ is the energy that characterizes the elastic interaction between the dipole BD of $\pm\omega$ -disclinations and the dipole AC of $\pm(\omega_0-\omega)$ -disclinations; E_γ denotes the sum of the specific energies (per unit area) of the new grain boundaries AB , CD , and BD ; and E_τ is the work spent by the external shear stress τ to displacements of the disclination dipoles AC and BD (Fig. 1d).

The proper elastic energies $E_s^{\omega_0-\omega}$, $E_{\text{int}}^{\omega_0-(\omega_0-\omega)}$ and $E_{\text{int}}^{\omega-(\omega_0-\omega)}$ are given by the following formulas [34]:

$$E_s^{\omega_0} = \frac{D\omega_0^2 L^2}{2} \left(\ln \frac{R}{L} + \frac{1}{2} \right), \quad (2)$$

$$E_s^{\omega} = \frac{D\omega^2 L^2}{2} \left(\ln \frac{R}{L} + \frac{1}{2} \right), \quad (3)$$

$$E_s^{\omega_0-\omega} = \frac{D(\omega_0 - \omega)^2 L^2}{2} \left(\ln \frac{R}{L} + \frac{1}{2} \right), \quad (4)$$

$$E_s^q = \frac{D\omega_0^2}{2} \left(L^2 \ln \frac{L^2 + s^2}{L^2} + s^2 \ln \frac{L^2 + s^2}{s^2} \right), \quad (5)$$

where $D = G/[2\pi(1 - \nu)]$, and R is the screening length for the disclination stress fields. With results [27,28], the expressions for the interaction energies $E_{\text{int}}^{\omega_0-\omega}$, $E_{\text{int}}^{\omega_0-(\omega_0-\omega)}$ and $E_{\text{int}}^{\omega-(\omega_0-\omega)}$ are as follows:

$$E_{\text{int}}^{\omega_0-\omega} = -\frac{D\omega_0\omega}{2} \left(L^2 + L^2 \ln \frac{R^2}{L^2 + (s+p)^2} - (s+p)^2 \ln \frac{L^2 + (s+p)^2}{(s+p)^2} \right), \quad (6)$$

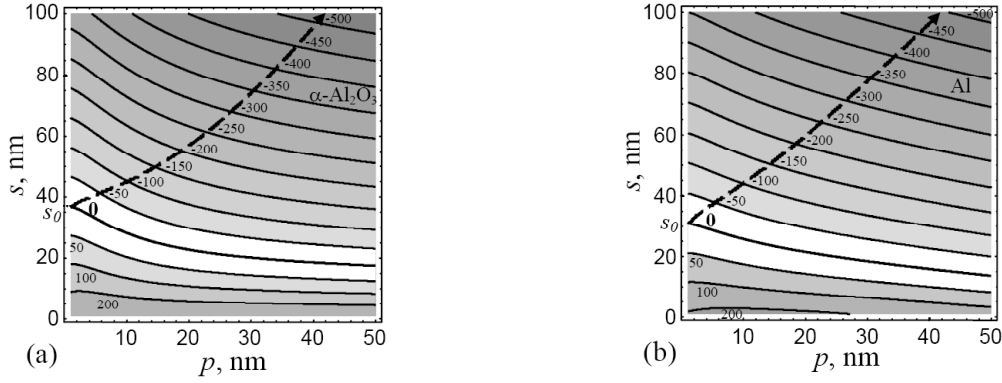


Fig. 3. The map of the characteristic energy change ΔW in the coordinates p and s , for (a) nanocrystalline $\alpha\text{-Al}_2\text{O}_3$ (sapphire) at $\omega = 5^\circ$, and (b) nanocrystalline Al at $\omega = 14^\circ$.

$$E_{\text{int}}^{\omega_0 - (\omega_0 - \omega)} = -\frac{D\omega_0(\omega_0 - \omega)}{2} \left(L^2 + L^2 \ln \frac{R^2}{L^2 + s^2} - s^2 \ln \frac{L^2 + s^2}{s^2} \right), \quad (7)$$

$$E_{\text{int}}^{\omega - (\omega_0 - \omega)} = -\frac{D\omega_0(\omega_0 - \omega)}{2} \left(L^2 + L^2 \ln \frac{R^2}{L^2 + p^2} - p^2 \ln \frac{L^2 + p^2}{p^2} \right), \quad (8)$$

The sum E_γ of the specific energies (per unit area) of grain boundaries AB , CD , and BD is evidently given as:

$$E_\gamma = (2(p + \Delta s) + L) \gamma_{gb}, \quad (9)$$

where $\Delta s = s - s_0$.

In spirit of the approach [27-30], the work E_τ (spent by the external shear stress τ to displacements of the disclination dipoles AC and BD over the distances Δs and $p + \Delta s$, respectively; see Fig. 1d) can be written as follows:

$$E_\tau = (\omega_0 \Delta s + \omega p) L \tau. \quad (10)$$

With formulas (1)-(10), we find the following expression for the energy change ΔW :

$$\begin{aligned} \Delta W = & \frac{D\omega^2}{2} \left(L^2 \ln \frac{L^2 + p^2}{L^2} + p^2 \ln \frac{L^2 + p^2}{p^2} \right) + \frac{D\omega_0\omega}{2} \left(L^2 \ln \frac{L^2}{L^2 + s^2} + L^2 \ln \frac{L^2 + (s+p)^2}{L^2 + p^2} + \right. \\ & \left. (s+p)^2 \ln \frac{L^2 + (s+p)^2}{(s+p)^2} - s^2 \ln \frac{L^2 + s^2}{s^2} - p^2 \ln \frac{L^2 + p^2}{p^2} \right) - \\ & (\omega_0 \Delta s + \omega p) L \tau + (2(p + \Delta s) + L) \gamma_{gb}. \end{aligned} \quad (11)$$

Let us analyze the energy change ΔW (given by formula (11)). To do so, in the exemplary cases of nanocrystalline ceramics $\alpha\text{-Al}_2\text{O}_3$ (sapphire) and nanocrystalline Al (aluminum), we calculated the maps ΔW in coordinates of the arm s of the initial $\pm\omega_0$ -disclination quadrupole and the disclination strength ω of the mobile $\pm\omega$ -disclination dipole (Fig. 2). In our calculations, we used the following typical values of parameters [38,39]: $G=169$ GPa and $\nu=0.23$, for $\alpha\text{-Al}_2\text{O}_3$; and $G=26.5$ GPa and $\nu=0.34$, for Al. The values γ_{gb} of the energy of special grain boundaries in $\alpha\text{-Al}_2\text{O}_3$ and Al are as follows: $\gamma_{gb}^{\text{Al}_2\text{O}_3} = 0.05$ J/m² [40] and $\gamma_{gb}^{\text{Al}} = 0.1$ J/m² [41,42]. The arm and strength of the initial $\pm\omega_0$ -disclination dipole AC (Fig. 1b) are taken as $L = 10$ nm and $\omega_0 = 30^\circ$, respectively. The calculated maps $\Delta W(\omega, s)$ are presented (in units of [eV/nm²]) in Fig. 2, for the external stress values $\tau = 1$ GPa and the distance $p = 1$ nm corresponding to the start of the splitting process for the grain boundary AC (Figs. 1b and 1c).

(Note that the shear stress value $\tau = 1$ GPa is typically reached during quasistatic plastic deformation in high-strength ceramics α -Al₂O₃, but hardly in crack-free specimens of Al. At the same time, this value ($\tau = 1$ GPa) can come into play in either shock-loaded Al or near crack tips in quasistatically loaded Al.)

As it follows from Fig. 2, the splitting process is energetically favorable when the initial distance between the grain boundaries XY and AC has value of $s_0 \approx 37$ nm at the disclination strength $\omega' \approx 5^\circ$, for α -Al₂O₃ (Fig. 2a); and $s_0 \approx 31$ nm at $\omega' \approx 14^\circ$, for Al (Fig. 2b). In both the cases under examination, when the distance s (with the proviso that $s > s_0$) increases, so does the interval of disclination strength values ω at which the splitting process is energetically favorable (Fig. 2).

Also, with formula (11), we calculated the energy change maps $\Delta W(p, s)$ in the coordinates p and s , for $\omega \approx 5^\circ$ and $s = s_0 = 37$ nm in the case of α -Al₂O₃ (Fig. 3a), and $\omega \approx 14^\circ$ and $s = s_0 = 31$ nm in the case of Al (Fig. 3b). Other values of the parameters involved in our calculations are taken as those in the previous situation illustrated in Fig. 2. The dashed curves in Fig. 3a and 3b show the most energetically favorable evolutions in the space (s, p) , corresponding to the structural transformation under our examination (Figs. 1b-1d), in nanocrystalline α -Al₂O₃ and Al, respectively. As it follows from Fig. 3, growth in the size s of the initial grain induces growth in the size p of the new grain.

4. DISCUSSION. CONCLUDING REMARKS

Thus, the splitting transformations of grain boundaries containing disclination dipoles effectively transfer plastic flow at the nanograin level in deformed nanocrystalline materials. In particular, such processes are energetically favorable and can initiate nucleation of new nanograins at previously formed nanograins with disclination quadrupoles at their junctions (Figs. 1b-1d) in nanocrystalline α -Al₂O₃ and Al in wide ranges of their parameters. Nanograin chains (Figs. 1d and 1e) are resulted from the transformations under our examination. Such chains may serve as nuclei for experimentally observed [31-33] nanograin agglomerates (groups of nanograins with low-angle and/or special boundaries within comparatively large grains having high-angle boundaries) in NC and UFG materials.

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