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Athermal grain growth through cooperative migration of grain boundaries in deformed nanomaterials

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A special mode of both athermal grain growth and associated plastic deformation in nanocrystalline metals and ceramics is theoretically described. The mode represents the stress-induced cooperative migration of grain boundaries when the migration involves two or more neighboring boundaries. We calculated two critical external stress levels attributed to the start of migration of two neighboring boundaries and their meeting, respectively. After their convergence, grain boundaries can annihilate, stop, move together or move in opposite directions, depending on their characteristics.

Keywords: Grain growth; Grain-boundary migration; Plastic deformation; Nanocrystalline materials; Disclinations

The extraordinary mechanical properties of nanocrystalline (nc) materials are strongly influenced by specific grain-boundary-mediated mechanisms of plasticity [1–5]. In recent years, special attention has been paid to one of these mechanisms, namely stress-induced grain growth. Many experiments have demonstrated that it occurs during plastic deformation in ultrafine-grained (ufg) and nc metals and alloys at room [6–16] and cryogenic [9,10] temperatures. Stress-induced grain growth and elongation have been observed in superplastic ufg [17–19] and nc [20] ceramics at high temperatures. Although the basic micromechanisms of low-temperature stress-induced grain growth in nc/ufg metals and high-temperature strain-induced grain elongation in nc/ufg ceramics may be different, one expects some common features in these phenomena.

Recent computer simulations [21–27] have shown that low-temperature stress-induced grain growth in nc metals is athermal. Its basic mechanisms are found to be stress-induced migration of grain boundaries (GBs) and their triple junctions, GB sliding, grain rotation and coalescence. Also, stress-induced GB migration and athermal grain growth have been described theoretically with the aid of two-dimensional (2-D) dislocation–disclination models [28–31]. These models predict the existence of critical stresses for migration of low- and high-angle GBs. However, the models [28–31] are focused on only sole GBs. At the same time, stress-induced migration often involves two or more neighboring GBs that may converge, and this cooperative migration is significantly different from migration of a sole GB. The main aim of this paper is to theoretically describe collective migration of two interacting GBs as a special mode of both athermal grain growth and associated plastic deformation in nc materials.

Consider a model 2-D arrangement of rectangular grains G1–G3, with G1/G2 and G2/G3 being two low-angle tilt GBs, finite walls of perfect lattice dislocations characterized by the tilt misorientation parameters Ω and ω (Fig. 1a and b). In the initial state, these GBs form four triple junctions which are supposed to be geometrically balanced (the sum of GB misorientation angles at each of these junctions is equal to zero). Under an external shear stress τ, athermal migration of GBs from their initial positions A and D to new positions B and C occurs. As a result, the angle gaps $\pm\Omega$ and $\pm\omega$ appear at the double junctions at A and D, and four new triple junctions with the angle gaps $\pm\Omega$ and $\pm\omega$ are formed at B and C, respectively. Straight line defects (double junctions at A and D, and triple junctions at B and C) characterized by the angle gaps $\pm\Omega$ and $\pm\omega$ are partial wedge disclinations whose motion produces rotational plastic deformation [32]. Thus, stress-induced migration of the low-angle tilt GBs G1/G2 and G2/G3 carries plastic deformation and results in the formation

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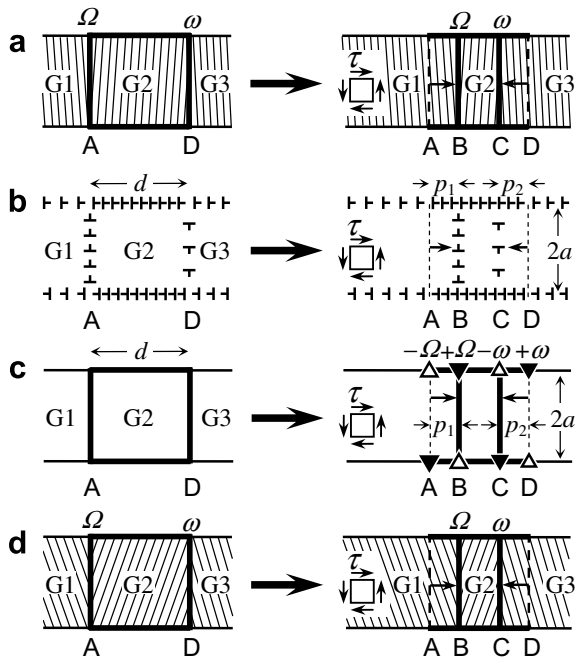

Figure 1. Geometric (a, d), dislocation (b) and disclination (c) models for stress-induced cooperative migration of two low-angle (a, b) or high-angle (c, d) grain boundaries under an external shear stress τ.

of four two-axis dipoles of partial wedge disclinations (Fig. 1c): two Ω-dipoles (A and B) and two ω-dipoles (C and D). The same is true for migration of two high-angle tilt GBs with large Ω and ω (Fig. 1c and d).

Our 2-D model does not include factors relevant to real nc materials, such as the general type and finite size of GBs, their distribution in size and misorientation, or the strong influence of impurities [7,8,16,33] and applied stress gradient [6–10,12,33] on dislocation glide and GB migration. Nevertheless, it allows us to discern new essential features in collective GB migration.

Let us analyze the energy of the system during its evolution. When the disclination structure appears as a result of the GB migration (Fig. 1c), the total energy of the system drastically changes. Following Refs. [32,34], we find the energy change ΔW (per unit of the disclination length) as

$$\begin{aligned}\Delta W = 2Da^2\Omega^2\{&(x^2+1)\ln(x^2+1) - x^2\ln x^2\\ &+\lambda^2[(y^2+1)\ln(y^2+1) - y^2\ln y^2]\\ &+\lambda\{(z^2+1)\ln(z^2+1) - z^2\ln z^2\\ &+[(z-x-y)^2+1]\ln[(z-x-y)^2+1]\\ &-(z-x-y)^2\ln(z-x-y)^2\\ &-[(z-x)^2+1]\ln[(z-x)^2+1]\\ &+(z-x)^2\ln(z-x)^2\\ &-[(z-y)^2+1]\ln[(z-y)^2+1]\\ &+(z-y)^2\ln(z-y)^2\} - \frac{2\tau}{D\Omega}(x+\lambda y)\},\end{aligned} \tag{1}$$

where $D = G/[2\pi(1-\nu)]$, G is the shear modulus, ν is the Poisson ratio, $2a$ is the arm of a disclination dipole (A, B, C or D), $x = p_1/2a, y = p_2/2a, z = d/2a$ and $\lambda = \omega/\Omega$. Here p_1 and p_2 are the distances passed by the migrated GBs G1/G2 and G2/G3, respectively, and d is the initial size (length) of grain G2.

Since ΔW depends upon two variables, x and y, it is convenient to study its behavior with contour maps $\Delta W(x,y) = \text{const}$ (due to the restrictions of space, we do not show them here). They enable one to examine some characteristic features of the system's evolution. In particular, we analyzed local minima of the function $\Delta W(x,y)$ (Fig. 2a and c) and the most probable trajectories along the maximum gradient of ΔW (Fig. 2b and d) of the system's development in the space (x,y). Let us first consider the case of an initially equiaxed ($z = 1$) grain G2 with $\lambda = 1$. If the external stress τ is small (here $\tau < 0.3D\Omega$), ΔW is always positive and the GB migration is impossible. When τ becomes larger than some critical level τ_c, ΔW is negative at small x and y, reaching a minimum, with coordinates x and y determining the stable equilibrium positions of migrating GBs B (G1/G2) and C (G2/G3). These equilibrium positions are marked by open circles in Figure 2a, where the dashed arrow shows the general direction of the system's evolution from one equilibrium state to another. The insets schematically demonstrate the stable equilibrium states of the GB arrangement under a given value of τ. Due to the anti-symmetry of the disclination model in the case where $\lambda = 1$, the equilibrium points lie at the bisectrix 1–4. In other words, GBs B and C synchronously migrate to each other (see insets 1–4) under increasing τ.

Using Eq. (1), one can estimate τ_c as follows. Let $x = y$, $z = 1$, $\lambda = 1$ and $x \ll 1$. Then Eq. (1) results in $\Delta W \approx -2Dd^2\Omega^2 x(x + x\ln x + \tau/D\Omega)$. Elementary migration of a GB by an interatomic distance b is possible if $\Delta W(x = b/d) < 0$. Therefore, the equation $\Delta W(x = b/d) = 0$ gives the critical stress τ_c:

$$\tau_c \approx \frac{D\Omega b}{d}\left(\ln\frac{d}{b} - 1\right) \tag{2}$$

If we omit the unit in the brackets, we obtain formula (3) in Ref. [31], which estimates the critical stress τ_{c1} for the migration of a sole GB. More careful examination of the model from Ref. [31] gives $\tau_{c1} \approx D\Omega(b/d)[\ln(d/b) + 1]$, and hence the difference $\Delta\tau_c = \tau_{c1} - \tau_c \approx 3D\Omega b/(2d)$ reflects the effect of elastic interaction of migrating GBs on the critical stress. It is evident that $\Delta\tau_c \sim d^{-1}$. Let us estimate τ_c and $\Delta\tau_c$ for nc metal (Al) and ceramic (β-Si_3N_4) with typical values $\Omega = 0.085(\approx 5°)$ and $d = 100$ nm. For Al with $G = 27$ GPa, $\nu = 0.31$ and $b \approx 0.25$ nm, we get $\tau_c \approx 7$ MPa and $\Delta\tau_c \approx 2$ MPa. For β-Si_3N_4, we use the elastic moduli measured at 1375° C [35]: $G \approx 128$ GPa and $\nu = 0.32$. The hexagonal lattice parameters are $a \approx 0.76$ nm and $c \approx 0.29$ nm [35]. Therefore, we take $b = a$ for GB migration in the a-direction (the a-case) and $b = c$ for GB migration in the c-direction (the c-case). As a result, in the a-case, $\tau_c \approx 75$ MPa and $\Delta\tau_c \approx 29$ MPa. In the c-case, $\tau_c \approx 36$ MPa and $\Delta\tau_c \approx 11$ MPa. These values of τ_c are easily achievable in real experiments on tension of nc Al [14,15] and compression [20] and tension [35] of β-Si_3N_4. When the external stress τ achieves another characteristic value τ_m, GBs B and C meet and can annihilate or pass through each other. This stress value is determined from