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ScienceDirect

Scripta Materialia 78–79 (2014) 5–8

Scripta MATERIALIA

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On nanograin rotation by dislocation climb in nanocrystalline materials

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Received 20 November 2013; revised 27 December 2013; accepted 27 December 2013
Available online 4 January 2014

A theoretical model has been developed for nanograin rotation that could be achieved through dislocation climb. The results obtained show that the occurrence of nanograin rotation and the coalescence of grains depend on the external stress level, structure of grain boundary and grain size. Moreover, a critical misorientation parameter that represents the crossover between nanograin rotation and shear-coupled migration of grain boundaries has also been found, based on which a coupling mechanism between nanograin rotation and shear-coupled migration was proposed.

Keywords: Nanograin rotation; Dislocation climb; Shear-coupled migration of grain boundaries; Nanograin growth; Strength and ductility

Nanocrystalline (NC) materials are usually strong but brittle compared to their coarse-grained counterparts due to the suppression of conventional dislocation slip in nanograins [1]. Many researchers have made great efforts in the past decades to address the strength–ductility paradox, and numerous NC samples possessing extraordinary strain hardening and ductility have been successfully fabricated [2,3]; their outstanding mechanical behaviors have been attributed to a number of grain boundary (GB)-mediated deformation mechanisms, such as stress-driven nanograin growth [2–5].

Of all the GB-mediated deformation mechanisms, nanograin growth behavior has attracted the greatest scientific interest because of its close correlation with the exceptional ductility of many NC metals/alloys [2,3]. However, the specific mechanism by which nanograin growth enhances the mechanical behavior of NC materials remains unclear. Experimental studies and molecular dynamics (MD) simulations carried out by researchers have shown that there are two main modes of nanograin growth, i.e. shear-coupled migration (SCM) of grain boundaries [4,6–10] and nanograin rotation (NGR) [5,11–13]. The SCM mode has been identified as a generic mode of plastic deformation [14], as well as an effective toughening mechanism in NC materials [15], and it can enhance the intrinsic ductility of NC materials considerably [16]. It has also been found in some experiments and mesoscale simulations that the dominant mode of operation depends on grain size, and that these two modes are usually coupled [4]. Nevertheless, the specific mechanism that leads to the above phenomenon remains unclear. Therefore, the main aim of this letter is to develop a theoretical model for studying stress-driven NGR to address the above-mentioned issues. Recent studies have shown that, in the SCM process, a high-angle boundary moves in a similar way to a low-angle boundary, where the displacement shift complete (DSC) dislocations [17], disconnections [18] or structural units [19] composing the former could play the role of lattice dislocations forming the latter. Therefore, it is reasonable for us to postulate that, in the process of NGR, the structural units, DSC dislocations and disconnections in high-angle boundaries could act like the dislocations in low-angle boundaries. As a result, we postulate that NGR could be achieved by dislocation climb for both low- and

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http://dx.doi.org/10.1016/j.scriptamat.2013.12.021
1359-6462/

high-angle GBs according to the existing experimental and MD observations [12,13]. To simplify the calculation, only a symmetrical tilt boundary that consists of one set of discrete dislocations is considered in the present model.

Consider the rotation of two grains, G1 and G2, that are divided by GB "AB" in a deformed elastically isotropic NC specimen, which is subjected to a remote tensile stress σ (Fig. 1a). The GB "AB" is modeled as a finite wall of dislocations with identical Burgers vector **b** for both high- and low-angle boundaries (Fig. 1b and c). Under external shear stress τ, the leading GB dislocation climbs to the triple junction A [12,20] and dissociates into two Shockley partials, i.e. $\mathbf{b_1}$ and $\mathbf{b_2}$, which glide along GBs "AC" and "AD", respectively. The two gliding partials meet partials of opposite sign generated by other GBs adjacent to GB "AB" through similar rotating process or extrinsic GB dislocations, which are the lattice dislocations trapped by the GBs "AC" and "AD", and then annihilate. The GB dislocations remaining in the GB "AB" are assumed to climb following the dissociation of the leading GB dislocation, and finally distribute uniformly along the GB "AB" [20]. Therefore, the spacing between any two GB dislocations is increased from D_0 to D_1 (Fig. 1c and d) due to the dissociation of the leading GB dislocation. With the repetition of the above processes, the original two grains, G1 and G2, would ultimately coalesce into one elongated grain, G1–G2 (Fig. 1f).

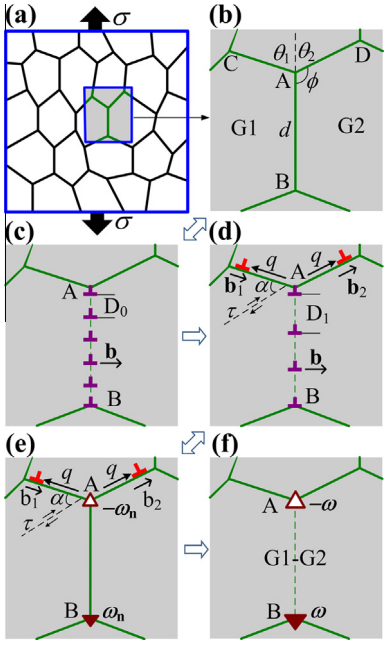

Figure 1. Climb-induced grain rotation process in a nanocrystalline specimen: (a) general two-dimensional microstructure; (b) initial configuration of two grains, i.e. G1 and G2, divided by GB "AB"; (c) equivalent configuration of (b), in which the GB "AB" is modeled as a finite array of discrete dislocations with identical Burgers vector **b**; (d) under external shear stress τ, n leading GB dislocations climb one by one to the triple junction A and dissociate into two partials, i.e. $\mathbf{b_1}$ and $\mathbf{b_2}$, which then glide along the GBs "AC" and "AD", respectively, and annihilate at some points along the said GBs; (e) equivalent configuration of (d), where a disclination dipole (small triangles) is formed due to the loss of GB dislocations; (f) repetition of processes (c) and (d) leads to ultimate coalescence of grains G1 and G2 into one grain, i.e. G1–G2.

In the initial stage, there are two triple junctions between the two grains (G1 and G2) formed by the GB "AB", which is characterized by a tilt misorientation parameter θ_0, corresponding to n_0 GB dislocations. There exist no angle gaps at these two junctions due to the compensation of GB misorientation angles with each other. However, when n leading GB dislocations have climbed, dissociated and disappeared, the misorientation parameter is reduced from θ_0 to θ_n, and the resulting angle gaps at the two triple junctions A and B are $-\omega_n$ and $+\omega_n$, respectively, due to the GB dislocation loss. Therefore, a disclination dipole of arm d and strength $\pm\omega_n$ occurs at GB "AB", as observed in experiments [13]. Once all the GB dislocations have climbed and dissociated, the strength of the disclination dipole is increased up to $\pm\omega$ (Fig. 1f).

Consider the energy change ΔW produced by the nanograin rotation process in which n GB dislocations climbed to the triple junction A and dissociated (from Fig. 1b to e). The rotation process is energetically favorable if $\Delta W < 0$. The energy change ΔW (per unit length along the axis perpendicular to the plane of Fig. 1e) can be expressed as follows:

$$\Delta W = W + \Delta E_d + E_{\text{int}}^{b_1 b_2} + E_{\text{int}}^{\omega - b_1 b_2} - A_c - A_g \tag{1}$$

where W, ΔE_d, $E_{\text{int}}^{b_1 b_2}$ and $E_{\text{int}}^{\omega - b_1 b_2}$ are the self-energy of the disclination dipole "AB", the energy loss due to the dissociation process, the energy resulting from the interaction between the two partials, and the energy that characterizes the interaction between the two partials and the disclination dipole, respectively; A_c and A_g are the work done by the external shear stress τ for climbing of the GB dislocations along the GB "AB" and gliding of the partials along the GBs "AC" and "AD", respectively.

The above energy terms for a NC specimen with shear modulus G and Poisson ratio υ can be calculated as follows: $W = D\omega_n^2 d^2(\ln(R/d) + 1/2)/2$ [21], where $D = G/[2\pi(1-\upsilon)]$, $\omega_n = \theta_0 - \theta_n = nb/d$, $b = a/\sqrt{2}$, a is the lattice parameter and R is the screening parameter for the stress fields induced by the disclination dipole; $\Delta E_d = -(3n-2)Da^2(\ln(R_1/r_0) + 1)/12$, where r_0 is the dislocation core radius and is assumed to be the same for all the dislocations, i.e. $r_0 \approx b_1$, and R_1 is the screening length for the long-range stress field of partial dislocation. The energy resulting from the interaction between the two partials can be calculated in the standard way as the work done in generating one partial in the stress field created by another, i.e.

$$\begin{aligned} E_{\text{int}}^{b_1 b_2} = D b_1 b_2 \Bigg[& \frac{\cos\Psi}{2} \ln A - \frac{qI}{2\sin^2\Psi}(2+\cos 2\Psi)\cos^2\Psi \\ & - \frac{q}{2A\sin^2\Psi}[x(2+\cos\Psi\cos 3\Psi) \\ & + q(2+\cos 2\Psi)\cos\Psi] \Bigg]_{x=q}^{x=R_1} \end{aligned} \tag{2}$$

where $b_1 = b_2 = a/\sqrt{6}$, $A = x^2 + 2xq\cos\Psi + q^2$, $\Psi = \pi - \theta_1 - \theta_2$, $I = \arctan[(x + q\cos\Psi)/(q\sin\Psi)]/(q\sin\Psi)$. Similarly,