Grain boundary migration as rotational deformation mode in nanocrystalline materials

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Stress-induced grain boundary migration is theoretically described as a new mode of rotational plastic deformation in nanocrystalline materials. We have calculated the strain energy change due to migration of a grain boundary that carries rotational plastic flow. It is shown that, depending on the stress level, the grain boundary can either be immobile or mobile, and in the latter case it can migrate in either a stable or unstable regime. The critical stress values, which correspond to the transitions between these migration regimes, are estimated and discussed. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2147721]

Nanocrystalline materials (NCMs) exhibit outstanding mechanical properties due to their unique deformation mechanisms controlled by grain boundary (GB) processes.[1–14] For example, in NCMs with the finest grains, GBs serve as sources of partial lattice dislocations and twins[3–9] and effectively conduct such deformation modes as GB sliding,[14–18] Coble creep,[19,20] triple junction diffusional creep,[21] and rotational deformation.[22–26] Also, recent experimental observations[17,27,28] and computer simulations[29] indicate that GB migration and grain growth processes intensively occur in NCMs at plastic and superplastic deformation regimes. However, the nature of these processes and their role in plastic flow of NCMs are not understood. The main aim of this letter is to suggest a theoretical model describing stress-induced GB migration as a new mode of rotational plastic deformation in NCMs. In doing so, we theoretically investigate the conditions and regimes of the GB migration conducting plastic flow associated with crystal lattice rotations in nanoscale grains.

Let us consider a model arrangement of rectangular grains with low-angle tilt boundaries GB1–GB5, where GB3 is a finite wall of periodically spaced perfect lattice dislocations, as shown in Fig. 1(a). Under an external shear stress τ, the GB3 migrates from initial position AB to a new position $A'B'$. In this case, both plastic deformation carried by glide of the perfect lattice dislocations (belonging to the GB3) and associated change of crystal lattice orientation occur in the area $ABB'A'$ swept by the migrating GB3 [Fig. 1(b)]. Thus, stress-induced migration of the low-angle tilt GB3 leads to rotational deformation, with plastic deformation accompanied by crystal lattice rotation.

In the initial state [Fig. 1(a)], the grain boundaries GB1–GB5 form two triple junctions, A and B, which are supposed to be geometrically compensated. There are no angle gaps at these triple junctions; in other words, the sum of GB misorientation angles at each of these junctions is equal to zero. When the GB3—a finite wall of lattice dislocations—characterized by the tilt misorientation parameter ω migrates from the position AB to a position $A'B'$ [Fig. 1(a)], the angle gaps $-\omega$ and $+\omega$ appear at the GB junctions A and B [Fig. 1(b)], respectively, and two new triple junctions A' and B' are formed. These triple junctions A' and B' are characterized by the angle gaps $+\omega$ and $-\omega$, respectively, carried by the GB3. In the theory of defects in solids, straight-line defects (junctions) A, B, B', and A' characterized by the angle gaps $\pm\omega$ are defined as partial wedge disclinations (rotational defects) that serve as powerful stress sources characterized by the disclination strength $\pm\omega$ (Ref. 30). The motion of the disclinations produces rotational plastic deformation.[30] Thus, stress-induced migration of the low-angle tilt GB3 carries rotational deformation and results in the formation of a quadrupole of wedge disclinations A, B, B', and A' characterized by strength values $\pm\omega$ as shown in Fig. 1(b). The same processes occur when GB1–GB5 are high-angle tilt boundaries and the GB3 migrates [Figs. 1(c) and 1(d)], in which case ω is the tilt misorientation parameter of the high-angle GB3.

Let us analyze the energy of the system during its evolution (Fig. 1) under discussion. When the disclination structure appears as a result of the GB3 migration [Figs. 1(b) and 1(d)] the total energy of the system drastically changes. Fol-

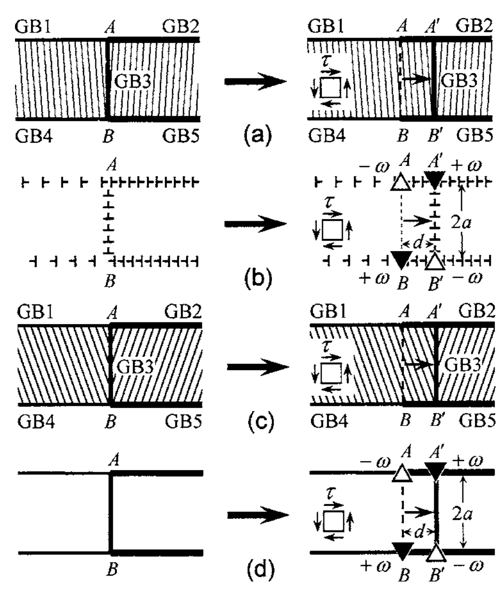

FIG. 1. Stress-induced migration of a low-angle (a, b) or high-angle (c, d) grain boundary (GB3) as a mechanism of rotational deformation realized through the glide of a wall of lattice dislocations (b) or motion of a dipole of wedge disclinations (d), respectively.

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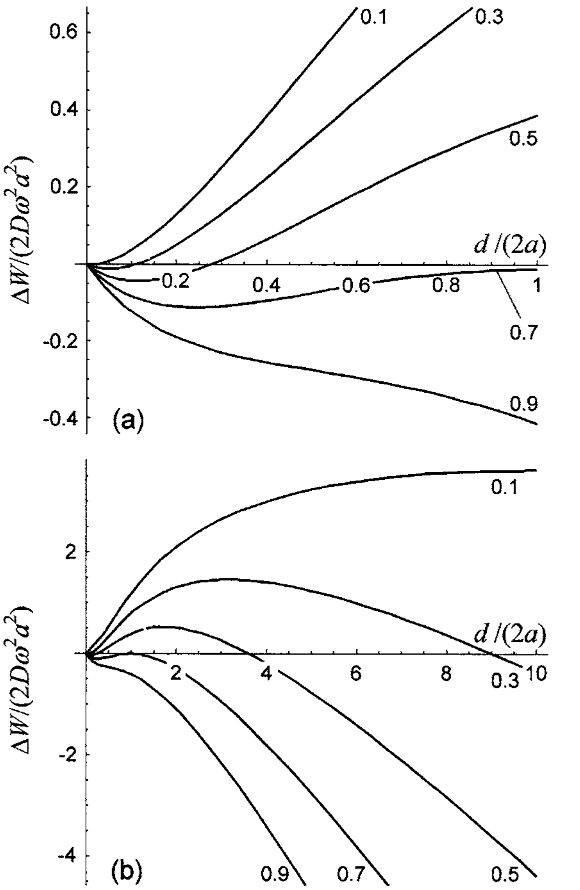

FIG. 2. The dependence of the energy gain ΔW on the migration distance d for different values of the external shear stress τ shown at the curves in units of $D\omega$. The case of (a) relatively small d ($d \leq 2a$) and (b) relatively large d.

lowing the approach,[31] the energy change ΔW can be written as follows:

$$\Delta W = 2D\omega^2 a^2 \left\{ (1+x^2)\ln(1+x^2) - x^2 \ln x^2 - \frac{2\tau}{D\omega} x \right\}, \tag{1}$$

where $D=G/[2\pi(1-\nu)]$, G denotes the shear modulus, ν the Poisson ratio, $2a$ the arm of a disclination dipole (AB or $A'B'$), τ the external shear stress, $x=d/(2a)$, and d is the distance between the dipoles AB and $A'B'$ (in other words, the distance of the GB3 migration). In the brackets, first two terms represent the sum of self-strain energies of disclination dipoles AB and $A'B'$, and the energy of their elastic interaction, while the third term is the work spent by the external shear stress τ to produce the disclination configuration under discussion (in other words, to produce plastic deformation in the process of the GB3 migration). All of these terms are calculated per unit of the disclination length. The dependence of the energy change ΔW on the normalized distance x for different levels of the stress τ is shown in Fig. 2. As follows from Fig. 2, the function $\Delta W(x)$ may behave in rather different ways depending on the stress τ level.

If τ is small enough (here at $\tau=0.1D\omega$), the function $\Delta W(x)$ is always positive and grows monotonously with rising x. In this case the generation of the disclination configuration AB-$A'B'$ (the GB3 migration) is energetically unfavorable and therefore impossible.

When τ becomes higher, the function $\Delta W(x)$ can change its sign and becomes nonmonotonous. With rising x from 0, first $\Delta W(x)$ is negative, it decreases and achieves its minimum, then it increases and achieves its maximum; after that $\Delta W(x)$ finally drops [here for $\tau=(0.3\ldots0.7)D\omega$]. In this case the generation of the disclination configuration AB-$A'B'$ (the GB3 migration) is energetically favorable. Moreover, the mobile dipole $A'B'$ must move until the point of minimum which determines the stable equilibrium position x_{eq} (in other words, the equilibrium migration distance d_{eq}) corresponding to the given value of τ. The point of maximum determines the energy barrier for further movement of the disclination dipole $A'B'$ (migration of the GB3) under the stress τ.

Finally, when τ is high enough (here at $\tau=0.9D\omega$), the function $\Delta W(x)$ is always negative and drops monotonously with increasing x. In this case, both the generation and unstable extension of the disclination configuration AB-$A'B'$ (unstable migration of the GB3) are energetically favorable. There exist no stable equilibrium positions or energy barriers for such a high level of τ.

Let the first critical shear stress $\tau=\tau_{c1}$ be the lowest stress at which generation of the disclination configuration AB-$A'B'$ becomes energetically favorable or, in other words, stable migration of the GB3 starts to occur. As follows from Fig. 2(a), the energy change ΔW must be negative just at the beginning of the curve $\Delta W(x)$, when $x \ll 1$ (or $d \ll 2a$). In this limiting case, formula (1) is simplified and gives

$$\Delta W(x \ll 1) \approx 4D\omega^2 a^2 x \left\{ -x \ln x - \frac{\tau}{D\omega} \right\}. \tag{2}$$

Elementary migration of the GB3 by interatomic distance b is possible, if $\Delta W(x=b/2a)<0$. Therefore, the equation $\Delta W(x=b/2a)=0$ determines the critical shear stress τ_{c1} as follows:

$$\tau_{c1} \approx \frac{D\omega b}{2a} \ln \frac{2a}{b}. \tag{3}$$

It is seen that τ_{c1} strongly depends on the grain size S (here $S \sim 2a$), following the law $\tau_{c1} \sim S^{-1} \ln S$.

Let us estimate the characteristic values of τ_{c1} for the exemplary case of pure nanocrystalline Al with the elastic moduli $G=27$ GPa and $\nu=0.31$, and $b \approx 0.25$ nm. We take two characteristic values for the disclination strength $\omega = 0.085(\approx 5°)$ and 0.52 $(\approx 30°)$. Then for the grain size values $2a=10$, 30, and 100 nm, formula (3) gives $\tau_{c1} \approx 47$, 23.5, and 7.6 MPa at $\omega=0.085(\approx 5°)$, and $\tau_{c1} \approx 288$, 144, and 46.5 MPa at $\omega=0.52(\approx 30°)$, respectively. These stress values are easily available in real experiments with nanocrystalline Al. Therefore, the GB migration may give a notable contribution to plastic deformation of NCMs where usual dislocation activity is suppressed by small grain size.

Figure 2(a) clearly demonstrates that stable equilibrium positions for the mobile dipole $A'B'$ (the GB3) appear in the region $x<1$. The mathematical conditions are $\partial \Delta W/\partial x=0$ and $\partial^2 \Delta W/\partial x^2>0$. The first formula gives the relationship $\tau = D\omega x_{eq} \ln(1+1/x_{eq}^2)$, while the second one results in the following inequality: $\ln(1+1/x_{eq}^2) > 2/(1+x_{eq}^2)$. To deal with these formulas, it is convenient to introduce an additional function $\tau' = D\omega 2x_{eq}/(1+x_{eq}^2)$. This allows us to resolve the system graphically, by plotting the curves $\tau(x_{eq})$ and $\tau'(x_{eq})$ together and choosing that part of the dependence $\tau(x_{eq})$,

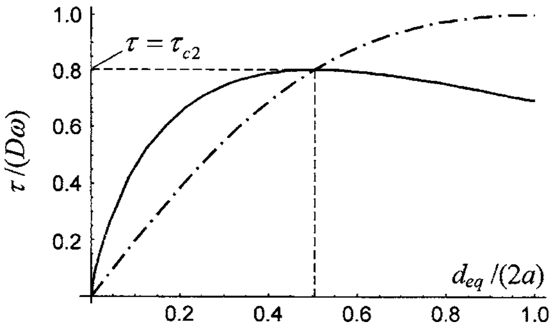

FIG. 3. Correspondence between the equilibrium position d_{eq} of the migrating grain boundary and the external shear stress τ (solid curve on the left side from the intersection point $(\approx 0.5, \approx 0.8)$). The pointed-and-dashed curve is used to show the area ($d_{eq} \leq a$, $\tau \leq 0.8 D\omega$) where the correspondence between d_{eq} and τ is correct. The stress value $\tau = \tau_{c2}$ is the highest stress level at which the grain boundary migration can be stable.

which lies above the curve $\tau'(x_{eq})$ (see Fig. 3). As follows from Fig. 3, $\tau > \tau'$ until x_{eq} is smaller than ≈ 0.5. In this region formula $\tau = D\omega x_{eq} \ln(1+1/x_{eq}^2)$ gives a correct relationship between τ and x_{eq}.

We conclude that the stable equilibrium path of the moving dipole $A'B'$ (the migrating GB3) increases with growing τ when τ is smaller than the second critical stress value $\tau_{c2} \approx 0.8 D\omega$ (Fig. 3). If τ is higher than τ_{c2}, the dipole motion (the GB3 migration) becomes unstable. Thus, the second critical stress τ_{c2} controls the transition from stable to unstable GB migration. The numerical estimates, done for the same set of parameters which are characteristic for the nanocrystalline Al, give $\tau_{c2} \approx 0.4$ GPa at $\omega = 0.085 (\approx 5°)$ and 2.5 GPa at $\omega = 0.52 (\approx 30°)$.

In summary, we have theoretically described stress-driven GB migration as a special mode of rotational plastic deformation in NCMs. Based on the disclination representation of uncompensated GB junctions, which appear during migration, we have investigated the conditions and regimes of the migration process. It has been shown that there are three main ranges in the value of the external shear stress τ acting on a GB in a NCM. When $\tau < \tau_{c1}$, the GB migration is not possible. If $\tau_{c1} \leq \tau < \tau_{c2}$, the GB can migrate in a stable regime when its propagation is determined by the level of τ. If $\tau > \tau_{c2}$, the GB migration becomes unstable when the GB propagation does not depend on the level of τ. The numerical values of these two critical stresses, τ_{c1} and τ_{c2}, strongly depend on the elastic modules of the material, as well as on the strength of disclinationlike defects appearing at the GB junctions in the process of migration. The first critical value τ_{c1} also depends on the grain size S and varies as $\tau_{c1} \sim S^{-1} \ln S$. Our estimates have shown that stress-induced GB migration can substantially contribute to plastic deformation of NCMs.

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