Special mechanism for dislocation nucleation in nanomaterials

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A special mechanism of dislocation nucleation in deformed nanocrystalline materials (NCMs) is suggested and theoretically described. The mechanism represents nonlocal homogeneous nucleation of a nanoscale loop of "noncrystallographic" partial dislocation whose Burgers vector magnitude continuously grows during the nucleation process. It is shown that the special mechanism can effectively produce nanoscale loops of lattice and grain boundary dislocations in NCMs deformed at high mechanical stresses. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2206095]

Single-phase and composite nanocrystalline materials (NCMs) with outstanding mechanical properties represent the subject of rapidly growing research motivated by their diverse technological applications and interest in fundamentals of deformation phenomena at the nanoscale level.[1–19] Ultrahigh strength and other unusual mechanical characteristics of NCMs are associated with the specific deformation mechanisms operating in these materials; see reviews[16–18] and book.[19] In particular, the action of standard dislocation sources (such as Frank-Read ones) is suppressed by nanoscale and grain boundary (GB) effects in NCMs. In this situation, GBs are viewed to serve as alternative sources of lattice dislocations in deformed NCMs.[4–11,18–22] However, mechanisms for dislocation nucleation at GBs (or other alternative dislocation sources) in NCMs are not fully understood. At the same time, knowledge on dislocation nucleation mechanisms is of crucial importance for development of both fundamental theory and applications of the outstanding mechanical properties of NCMs. The main aim of this letter is to suggest and theoretically describe a special mechanism for dislocation nucleation in GBs and grain interiors of deformed NCMs. The special mechanism represents the nonlocal homogeneous nucleation of a nanoscale loop of "noncrystallographic" partial dislocation whose Burgers vector magnitude continuously grows during the nucleation process.

The standard mechanism for homogeneous nucleation of lattice dislocations in perfect crystals is realized through the nucleation of a loop of either perfect or partial dislocation with a Burgers vector of constant magnitude and its further expansion. In Figs. 1(a)–1(d) the nucleation process is illustrated in the case of a perfect dislocation loop with the Burgers vector $\boldsymbol{B}$. This mechanism is characterized by a high energy barrier for the dislocation loop nucleation[23,24] and thereby hardly operates in real solids. We think that there exists an alternative mechanism for dislocation loop nucleation that can operate in NCMs deformed at high mechanical stresses. This mechanism is the nonlocal homogeneous nucleation of a noncrystallographic partial dislocation loop characterized by the Burgers vector magnitude $\boldsymbol{s}$ growing from zero to the Burgers vector magnitude of a partial lattice dislocation (b) and further to that of a perfect lattice dislocation ($B \approx 2b$) as is schematically shown in Figs. 1(e)–1(h). A similar process is also possible for the generation of a perfect GB dislocation.

The special mechanism for dislocation loop nucleation is supposed to pass through two key stages in a mechanically loaded NCM [Figs. 1(e)–1(h)]. At the initial stage, an applied shear stress causes a "momentary" ideal (rigid-body) shear to occur along the nanoscale rectangular plane fragment of crystal lattice in a grain [Figs. 1(e) and 1(f)]. Such a shear is characterized by a small shear magnitude $\boldsymbol{s}$ and produces a planar stacking fault of finite nanoscopic area [Fig. 1(f)]. The stacking fault is bounded by the loop of a noncrystallographic partial dislocation characterized by a nonquantized (noncrystallographic) Burgers vector $\boldsymbol{s}$ with quite a small magnitude $s \ll b$ [Fig. 1(f)]. At the following stage, the magnitude s of the dislocation Burgers vector continuously increases until it reaches the magnitude b of the Burgers vector of a partial lattice dislocation [Fig. 1(g)]. Then s continuously grows further and finally reaches the magnitude B of the Burgers vector of a perfect lattice dislocation [Fig. 1(h)]. The final state [Fig. 1(h)] resulting from the special

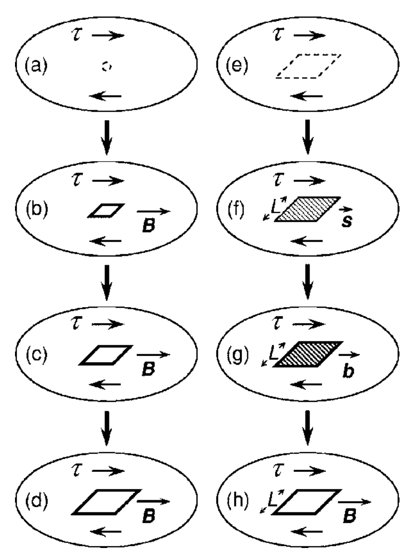

FIG. 1. Schematic representation of [(a)–(d)] standard homogeneous generation and extension of a gliding loop of perfect lattice dislocation with Burgers vector $\boldsymbol{B}$ and [(e)–(h)] nonlocal homogeneous generation of a gliding loop of "noncrystallographic" partial dislocation with a finite size L and small Burgers vector $\boldsymbol{s}$ ($0<s<b$) under an external shear stress τ. When s increases and achieves the magnitude b, the latter loop is transformed into a "normal" loop of partial lattice dislocation with Burgers vector $\boldsymbol{b}$; with further increase of s, it transforms into a normal loop of perfect lattice dislocation with Burgers vector $\boldsymbol{B} \approx 2\boldsymbol{b}$.

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mechanism is identical to that for the perfect lattice dislocation loop nucleated by the standard mechanism [Fig. 1(d)]. The difference between the mechanisms cannot be identified by conventional "postmortem" experiments.

Let us consider the energy characteristics of the nonlocal homogeneous nucleation of a glide loop of noncrystallographic partial dislocation [Figs. 1(e)–1(h)] in an infinite elastically isotropic solid under the action of an external shear stress τ. In our model, the loop has the shape of a planar square of size L and is characterized by the Burgers vector $\boldsymbol{s}$, whose magnitude continuously grows from 0 to B ($\approx 2b$) during the nucleation process. When such a model dislocation loop is generated under the external shear stress τ, the total energy of the system is changed by the value ΔW:

$$\Delta W = W_e + W_\gamma - A, \tag{1}$$

where W_e is the strain energy of the dislocation loop, W_γ is the energy of the stacking fault bounded by the loop, and A is the work spent by the shear stress τ to generate the loop.

In the case of a square loop with the size L, W_e can be adapted from Ref. 25 as follows:

$$W_e \approx Ds^3(2-\nu)\frac{L}{s}\left(\ln\frac{L}{s} - 0.78\right), \tag{2}$$

where $D = G/[2\pi(1-\nu)]$, G is the shear modulus, and ν is the Poisson ratio.

In the situation under discussion, the stacking fault energy W_γ is supposed to consist of two terms. The first term corresponds to the energy of the stacking fault within the area $(L-2s)^2$, while the second term describes the energy of the dislocation loop core. In the framework of the model suggested, the first term is approximated by a periodic function of s in the range from 0 to B ($\approx 2b$), and the result reads

$$W_\gamma = \gamma(L-2s)^2 \sin\frac{\pi s}{2b} + Ds^2 2L(2-\nu). \tag{3}$$

Here γ is the specific energy of the stacking fault. The work A is given by

$$A = L^2 s\tau. \tag{4}$$

With formulas (1)–(4), the energy change ΔW reads

$$\Delta W = Db^3\left[xp^2(2-\nu)\left(\ln\frac{x}{p} + 1.22\right) + (x - 2p)^2\kappa\frac{B}{b}\sin\frac{\pi p}{2} - x^2 p\frac{\tau}{D}\right], \tag{5}$$

where $x = L/b$ and $p = \boldsymbol{s}/b$ are the dimensionless parameters. The function $\Delta W(p)$ is shown in Fig. 2(a) for the case of pure Ni with the following parameters:[22,23] $G = 73$ GPa, $\nu = 0.34$, $b \approx 0.125$ nm, $\gamma = 183$ mJ/m^2 (the solid curves), and different combinations of the applied shear stress τ and normalized loop size L. Here the stacking fault energy value of 183 mJ/m^2 is taken from the estimate $\gamma \approx$ GB/100 suggested in Ref. 22. It is rather close to the mean value of 187.5 mJ/m^2 among those (from 125 to 250 mJ/m^2) found in experiments and cited in the recent literature.[23,26,27] We also used the lowest value of 125 mJ/m^2 taken from Ref. 23 for a comparison (the dashed curve).

These plots demonstrate rather different behaviors of $\Delta W(p)$ depending on the pairs (L, τ). The most interesting case is illustrated by the lowest curves (solid and dashed ones) describing the nucleation of a lattice dislocation loop with $L = 20$ nm and Burgers vector magnitude $s_{\mathrm{eq}} = 2b$ at the shear stress $\tau = 3$ GPa. It is the lattice dislocation loop nucleation characterized by the absence of any energy barrier (because the derivative $\partial\Delta W/\partial p < 0$, when p grows from 0 to $2b$). Thus, the nonlocal homogeneous nucleation of lattice dislocation loops can occur in the nonbarrier way in NCMs deformed at high mechanical stresses ($\tau = 3$ GPa or more) realized, in particular, under shock loading conditions.[28] It seems rather natural that the lower stacking fault energy (the dashed curve) is much more favorable for the process.

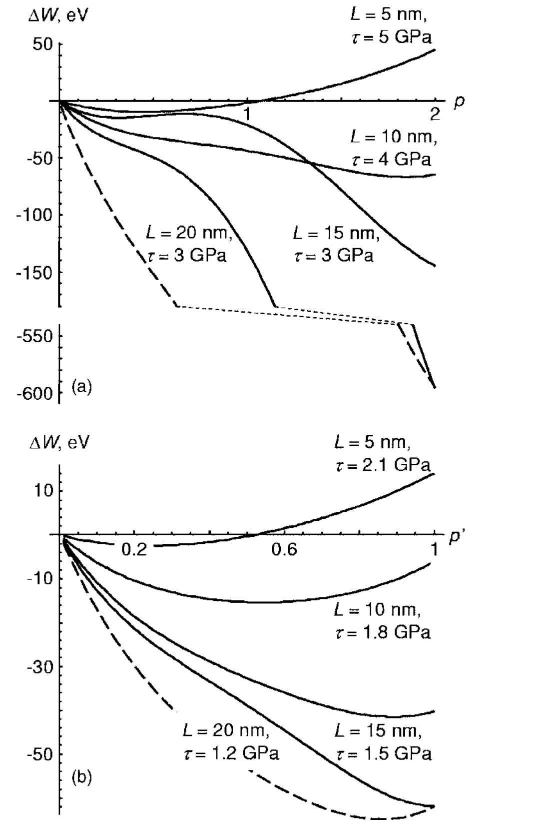

FIG. 2. The plots of the energy differences (a) $\Delta W(p)$ for the generation of a lattice dislocation loop and (b) $\Delta W(p')$ for the generation of a grain boundary dislocation loop. The pairs (L, τ) denote the loop size and the applied shear stress value. The solid curves are calculated for the stacking fault energy value of 183 mJ/m^2 (Ref. 22), while the dashed curves for that of 125 mJ/m^2 (Ref. 23).

Other curves in Fig. 2(a) describe the situations with nonbarrier nucleation of the partial noncrystallographic dislocation loops characterized by equilibrium Burgers vector magnitudes ($s_{\mathrm{eq}} \approx 0.45b$, $0.32b$, and $1.84b$) corresponding to minima of the $\Delta W(p)$ dependences. Further nonbarrier evolution of the dislocation loops can occur by their expansion. This evolution will be described in detail elsewhere.

Now let us consider the special mechanism for nucleation of GB dislocation loops in NCMs where the volume fraction occupied by the GB phase is very large (up to 10% or even more). Perfect GB dislocations serve as carriers of GB sliding[29] that can effectively contribute to plastic flow of NCMs.[19,30] Perfect GB dislocations in a GB are characterized by Burgers vectors being lattice vectors of the dense-shift-complete lattice that describes the GB symmetry.[29] Typical values of the GB Burgers vector magnitude b_{GB} characterizing a perfect GB dislocation are around 0.06–0.10 nm.[29] Nucleation of a perfect GB dislocation loop by the special mechanism occurs through nonlocal nucleation of a nonperfect GB dislocation loop of nanoscale area in the way similar to that shown in Figs. 1(e)–1(h). The main difference between nucleation events for lattice and GB dislocation loops is in their Burgers vector magnitude. During the nucleation of a GB dislocation loop, its characteristic Burgers vector magnitude s continuously grows from 0 to b_{GB}. As with the dislocation loop shown in [Figs. 1(e)–1(h)], we consider a nonperfect GB dislocation loop having the shape of a planar square of size L. The strength of the GB dislocation loop is characterized by the dimensionless parameter $p'=s/b_{GB}$ continuously growing from 0 to 1 during the nucleation process. The case of $p'=1$ corresponds to a perfect GB dislocation loop.

The nonperfect GB dislocation loop bounds a stacking fault in the GB plane [Figs. 1(e)–1(h)]. The stacking fault is not well defined in the GB phase whose structure is more disordered than the perfect crystal structure.[29,31] In any event, the energy density (per unit area) of the stacking fault in an initially disordered GB structure is much lower than that of the "true" stacking fault in a perfect crystal. In particular, the energy density of the stacking fault in the GB phase in nanocrystalline materials fabricated by highly nonequilibrium methods (such as severe plastic deformation or ball milling) is infinitesimally small because the GB structures are very disordered in these materials.[31] In this case, the stacking fault formation [Figs. 1(e)–1(h)] just slightly influences the GB structure and thereby energy characteristics. To take this into account, we diminish the stacking fault energy by factor $\lambda<1$ in our estimates of the GB dislocation loop nucleation.

To describe the energy characteristics of the nucleation of a GB dislocation loop [Fig. 1(e)–1(h)], we use the same analytical procedure as with lattice dislocation loop [see formulas (1)–(5)], with the replacements of γ by $\lambda\gamma$, b by b_{GB}, x by $x'(=L/b_{GB})$, p by p', and $\sin(\pi p/2)$ by $\sin(\pi p')$. The results of numerical calculations in the case of pure Ni with $\lambda=0.1$ and $b_{GB}=0.1$ nm are presented in Fig. 2(b). The curves $\Delta W(p)$ are rather similar to those in Fig. 2(a) plotted for a lattice dislocation loop. The main difference is related to the needed levels of τ which are much smaller in the situation with the GB dislocation loop. In particular, the nonbarrier nucleation of a GB dislocation loop with $L=20$ nm and Burgers vector magnitude $b_{GB}=0.1$ nm occurs at the shear stress $\tau=1.2$ GPa. This value can be reached in shock-loaded nanocrystalline Ni or near local stress concentrators during its quasistatic deformation.

Thus, in this letter a special mechanism for dislocation nucleation in deformed NCMs—the nucleation of noncrystallographic dislocation loops with continuously growing Burgers vector magnitude [Figs. 1(e)–1(h)]—has been suggested. According to our analysis of the energy characteristics of this mechanism, it can effectively operate in a barrierless regime and produce loops of lattice and GB dislocations in NCMs deformed at high mechanical stresses. In this context, plastic flow processes associated with lattice and GB dislocation activity in NCMs should be experimentally examined and theoretically described in the future, with the features of the special dislocation nucleation mechanism [Figs. 1(e)–1(h)] taken into account. Of particular importance would be experimental "*in situ*" observation of the dislocation loop nucleation events in deformed NCMs with various compositions and geometric parameters. This potentially allows one to identify the conditions at which the special dislocation nucleation mechanism is dominant. Finally, the discussed mechanism for dislocation nucleation is of large fundamental interest, because it can effectively contribute to relaxation processes in various solid structures such as shock-loaded crystals,[28] Gum Metal structures,[32] nanoscale continuous, and island films.

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