

Nanoscale rotational deformation in solids at high stresses

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A special physical mode of plastic flow and nanograin formation in nanocrystalline and polycrystalline solids deformed at high stresses is suggested and theoretically described. The mode represents the nanoscale rotational deformation (NRD) occurring through the collective events of ideal nanoscale shear in solids. We calculated its stress and energy characteristics. It is found that NRD can effectively occur in nanocrystalline and polycrystalline solids during dynamic loading. © 2011 American Institute of Physics. [doi:10.1063/1.3587637]

In recent years, plasticity and strength of nanocrystalline (NC) solids have attracted tremendous attention motivated by both fundamental interest to specific deformation mechanisms operating in these solids and their technological applications.^{1–14} Specific physical mechanisms of plastic deformation come into play in NC solids due to their specific structural features such as nanoscopic sizes of grains and large amounts of grain boundaries. These structural features significantly hamper or even suppress conventional lattice dislocation slip (dominating in coarse-grained polycrystals) and, at the same time, enhance grain boundary sliding, grain boundary diffusional creep, and twin and rotational deformation modes.^{1,2} Of particular interest is the rotational deformation mode—plastic deformation accompanied by crystal lattice rotations—which operates in NC solids characterized by superior strength.¹⁵ Experiments,^{7,8,13,16–19} computer simulations,²⁰ and theoretical models^{21–23} provided convincing evidence for the important role of rotational deformation mode in plastic flow processes in NC metals and ceramics. It has been found that rotational deformation strongly influences the unique mechanical characteristics of NC solids. Besides, similar to the discussed change in deformation mechanisms due to decrease in grain size down to the nanometer range, the physical mechanisms of plastic deformation can change in NC and polycrystalline solids when the external stress level increases from conventional up to very high values realized, in particular, at dynamic loading.²⁴ In the context discussed, there is large interest in the identification of deformation mechanisms operating in solids which have the NC structure and/or are deformed at extremely high stresses. The main aim of this letter is to suggest and theoretically describe a physical mode of rotational plastic deformation in NC and polycrystalline solids deformed at high stresses. The mode represents nanoscale rotational deformation (NRD) occurring through the collective events of nanoscale ideal shear in solids. This deformation mode (which is different from previously described^{21–23} rotational deformation modes) can also initiate formation of nanograins in solids.

Let us consider the geometry of NRD in a NC solid consisting of nanoscale grains divided by grain boundaries.

A two-dimensional section of the solid is schematically shown in Fig. 1(a). The solid is under a mechanical load producing the shear stress τ in the region ABCD presented in Fig. 1. We think that the generation of walls of dislocation dipoles by means of nanoscale ideal shears [Figs. 1(b)–1(e)] can serve as a mechanism of rotational deformation in NC solids. More precisely, nanoscale ideal shears simultaneously occur under the shear stress τ in several (n) parallel slip planes [Figs. 1(b)–1(e)]. Such shears are characterized by a tiny shear magnitude s and produce a wall of n generalized stacking faults having nanoscopic sizes [Fig. 1(c)]. [In the theory of crystals, a generalized stacking fault is defined as a planar defect resulting from a cut of a perfect crystal across a single plane into two parts which are then subjected to a relative displacement by an arbitrary vector s (lying in the cut plane) and rejoined.^{25–27}] The generalized stacking faults are bounded by “noncrystallographic” partial dislocations characterized by nonquantized (noncrystallographic) Burgers vectors $\pm s$ with quite a small magnitude $s < b$, where b is the magnitude of the Burgers vector of a perfect dislocation [Fig. 1(c)]. The noncrystallographic dislocation dipoles connected by generalized stacking faults are called nanodisturbances.^{28–30} (Nanodisturbances were defined and theoretically described as a kind of defects in Gum metals,²⁸ NC solids,²⁹ and nanowires.³⁰ Also, nanodisturbances were “*in situ*” observed by high resolution electron microscopy (HREM) in Gum metals during plastic deformation.³¹) At the following stage of deformation, the magnitude s continuously increases [Fig. 1(d)]. Finally, s reaches the magnitude b , and the nanodisturbances transform into conventional dipoles of perfect dislocations, in which case generalized stacking faults disappear [Fig. 1(e)].

The resultant finite walls of perfect dislocations bound a nanoscale region with the crystal lattice misoriented relative to that of the neighboring material [Fig. 1(e)]. That is, plastic deformation carried by the walls of nanodisturbances (Fig. 1) is accompanied by crystal lattice rotation and thereby can be treated as a special kind of rotational deformation.

Let us calculate the energy change ΔW that characterizes NRD occurring through the formation of a regular array of n nanodisturbances (dipoles of noncrystallographic dislocations with the Burgers vectors $\pm s$ and generalized stacking faults) (Fig. 1). We denote the interspacing between the neighboring nanodisturbances as p , and the nanodisturbance length as d [Fig. 1(c)]. We model the NC solid as an elasti-

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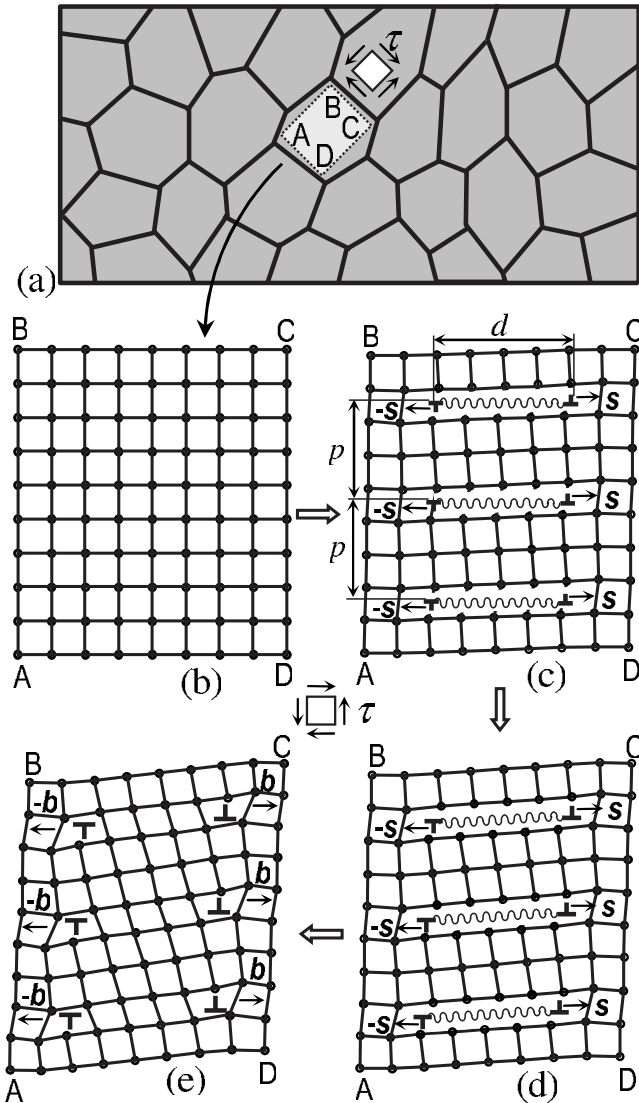


FIG. 1. NRD in NC solid. (a) Two-dimensional general view on NC specimen. [(b)–(e)] Two-dimensional view on NRD in a crystallographic plane of a grain with a cubic crystalline lattice. (b) Initial state of a nanoscale grain. (c) A wall of nanodisturbances is generated. Each nanodisturbance consists of a dipole of noncrystallographic dislocations with tiny Burgers vectors $\pm s$. Generalized stacking faults (wavy lines) are formed between the dislocations composing the nanodisturbances. (d) The Burgers vector magnitude s (characterizing the nanodisturbances) gradually increases, and generalized stacking faults evolve in parallel with growth of s . (e) The noncrystallographic dislocations transform into conventional perfect dislocations (when s reaches the Burgers vector magnitude b of a perfect dislocation), and generalized stacking faults disappear.

cally isotropic medium with the shear modulus G and the Poisson ratio ν . After some algebra, we find the following expression for the energy change ΔW (per unit dislocation line and per one dipole):

$$\Delta W(s) = \frac{Gs^2}{2\pi(1-\nu)} \left\{ \ln \frac{d}{s} + 1 + (1/n) \sum_{k=1}^{n-1} (n-k) \times \left[\ln \frac{p^2 k^2 + d^2}{p^2 k^2} - \frac{2d^2}{p^2 k^2 + d^2} \right] \right\} - \tau s d + \gamma(s) d, \quad (1)$$

where $\gamma(s)$ is the specific energy of a generalized stacking fault. The first term on the right hand side of formula (1) describes the total energy of the dislocation dipole, including its proper energy (the first two terms in braces) and the total

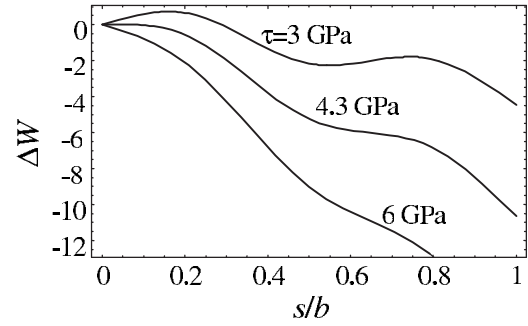


FIG. 2. Dependences of the energy change ΔW [in units of $Gb^2/[2\pi(1-\nu)]$] characterizing the nucleation of n nanodisturbances in NC Ni on the normalized dislocation Burgers vector magnitude s/b of nanodisturbances, for $d=20$ nm, $p=2$ nm, $n=10$, and various values of the applied shear stress τ .

energy of the dipole–dipole interaction per one dipole (the last term in braces); the second term ($-\tau s d$) is the work of the external stress, spent to dislocation formation; and the third term $[\gamma(s)d]$ characterizes the energy of a generalized stacking fault associated with a nanodisturbance [Fig. 1(c)]. The energy density $\gamma(s)$ is effectively approximated by the “two-humped” dependence as follows:²⁹

$$\gamma(s) = \begin{cases} \gamma_m \sin 2\pi u, & 0 \leq u < 1/4 \\ \frac{\gamma_m + \gamma_0}{2} - \frac{\gamma_m - \gamma_0}{2} \cos 4\pi u, & 1/4 \leq u \leq 3/4 \\ -\gamma_m \sin 2\pi u, & 3/4 < u \leq 1 \end{cases}, \quad (2)$$

where $u=s/b$, γ_m , and γ_0 are the maximum and minimum values of $\gamma(s)$, respectively.

Let us consider the case of NC nickel characterized by the following typical values of parameters: $\gamma_m \approx 0.17$ J m⁻² (Ref. 27), $\gamma_0 \approx 0.12$ J m⁻² (Ref. 27), the Burgers vector magnitude $b=a/\sqrt{2}$ of perfect dislocations (where $a=0.352$ nm is the Ni lattice parameter), $G=73$ GPa, and $\nu=0.34$. In this case, with formulas (1) and (2), we calculated the dependences of the energy change ΔW on s/b (Fig. 2), for $d=20$ nm, $p=2$ nm, $n=10$, and various values of τ . As it follows from Fig. 2, when the values of τ are not very high, ΔW increases at small s , in which case there is an energy barrier for NRD (see the upper curve in Fig. 2). When the values of τ are very high, ΔW always decreases with an increase in s . That is, the nonbarrier NRD takes place. The critical stress $\tau=\tau_c$ —the minimum stress at which NRD occurs in the nonbarrier way—corresponds to the condition $\partial\Delta W/\partial s=0$ at $s=0$ and $\tau=\tau_c$ (see the intermediate curve in Fig. 2). This condition yields the following:

$$\tau_c = 2\pi\gamma_m/b. \quad (3)$$

With formula (3), we found the value $\tau_c \approx 4.3$ GPa (or, in other terms, $\approx G/17$) of the critical shear stress in Ni. It is very high. Also, according to our estimates [based on computer simulations^{25–27,32} of the maximum value γ_m of the energy density function $\gamma(s)$], the values of the critical stress $\tau_c=2\pi\gamma_m/b$ for NRD are very high ($\tau_c > G/20$) in many other materials, such as Pd, Al, Ir, Pt, Cu, Au, SiC, Pb, Ag, and Fe. In these circumstances, NRD hardly occurs in crack-free solids at conventional conditions of quasistatic loading. Other deformation modes specified by comparatively low yield stresses operate at conventional conditions. At the same

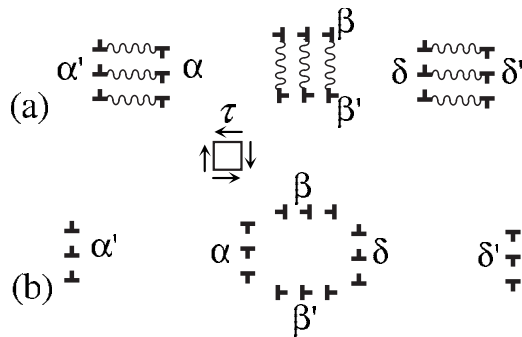


FIG. 3. NRD produces a nanograin. (a) Finite walls of nanodisturbances, $\alpha\alpha'$, $\beta\beta'$, and $\delta\delta'$, with different shear orientations are generated. (b) Nanodisturbances transform into dipoles of perfect dislocations, and dislocation motion results in formation of a nanograin $\alpha\beta\delta\beta'$.

time, NRD can come into play at extreme conditions characterized by very high values of both the applied stress and (at least, local) plastic strain rate. At the extreme conditions, conventional deformation modes—first of all, glide of pre-existent lattice dislocations and generation of individual dislocations by conventional mechanisms like dislocation cross-slip and Frank–Read sources—cannot provide high plastic strain rates. The extreme conditions are realized, in particular, at shock loading and ball milling, and it is natural to expect that NRD can occur at these deformation regimes. High plastic strain rates at extreme conditions are effectively provided by NRD involving intensive collective generation of dislocation groups (Fig. 1), but not dislocation motion and generation of individual dislocations. In particular, NRD can play a significant role in formation of high-density ensembles of dislocations experimentally observed²⁴ in shock-loaded polycrystals. Also, NRD can occur near internal stress sources/concentrators in materials with low γ_m , such as Ni, under ball mill treatment [producing impact stresses up to 5 GPa (Ref. 33)].

NRD leads to the formation of nanograins when the neighboring walls of nanodisturbances with different shear orientations are generated [Figs. 3(a) and 3(b)]. In doing so, in order to minimize the elastic energy of the dislocation structure under stress, dislocations belonging to neighboring walls form closed dislocation walls, as it is schematically shown in Figs. 3(a) and 3(b). As a result, nanoscale grains are generated which have NRD-produced low-angle boundaries. This scenario [Figs. 3(a) and 3(b)] naturally explains numerous experimental data³⁴ on the formation of the NC structure in metallic materials under ball milling.

In parallel with the extreme conditions, the NC structure of solids enhances NRD. This is because grain boundaries in NC solids stop glide of lattice dislocations, and high-density ensembles of dislocations should be generated and evolve to cause high-strain-rate deformation. This view is supported by the experimental observation (Ref. 4) of high-density ensembles of lattice dislocations generated in NC nickel at ultrahigh strain rates (10^7 s⁻¹) and shock pressures (20–70 GPa). Besides, high local shear stresses appear near crack tips in solids even in the situation with quasistatic loading, and, following our calculations (not presented here), such stresses can cause NRD.

Thus, the suggested deformation mode—NRD through formation and evolution of finite walls of nanodisturbances (Fig. 1)—effectively provides high plastic strains in NC and polycrystalline solids at high stresses. Besides, NRD can

cause nucleation of nanograins in solids (Fig. 3). With the results of our calculations of its energy characteristics and the critical stress for its onset, NRD can intensively occur both in dynamically loaded solids and near the crack tips of quasistatically loaded solids. The presented theoretical results are in good agreement with experimental observations of nanograin rotations^{7,8,13,16} and nanograin formation³⁴ in NC and polycrystalline solids deformed at high stresses.

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