Nanoscale multiplane shear and twin deformation in nanowires and nanocrystalline solids

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A special physical micromechanism/mode of twin deformation in nanowires and nanocrystalline (NC) solids is suggested and theoretically described. This mode represents a nanoscale multiplane shear (NMS) defined as an ideal shear occurring within a nanometer-sized volume. We calculated the energy and stress characteristics of nanoscale twin deformation through NMS in Cu nanowires and NC Cu. It is shown that this deformation mode can occur in NC solids and defect-free nanowires at high stresses. © *2011 American Institute of Physics*. [doi:10.1063/1.3620934]

Nanoscale deformation processes in nanowires and nanocrystalline (NC) solids with superior strength represent the subject of rapidly growing research efforts.[1–14] Of special interest is the deformation nanotwinning (DNT) recognized as one of dominant deformation modes in NC metals[2,4,7,10,11,14,15] and nanowires.[16,17] DNT in NC metals occurs more easily than deformation twinning in coarse-grained metals.[10,15] This tendency is associated with specific DNT micromechanisms operating in NC metals.[4,7,10,11,15] In particular, since deformation nanotwins frequently grow from grain boundaries (GBs) in NC metals,[4,7,10,11,14,15] it was suggested that DNT occurs through consequent emission of twinning dislocations from GBs.[4,7] However, it is hardly possible for a partial dislocation to pre-exist at a GB on every slip plane to form a single twin.[10] In the case of ultrathin nanowires, simulations[16] and experiment[17] showed formation of nanoscale deformation twins in them, but DNT micromechanisms in ultrathin nanowires initially free from defects are unclear. The discussed uncertainty in DNT modes operating in defect-free nanowires and NC metals (poor in twinning dislocations) motivates large interest in both search for and identification of such DNT modes. The main aim of this paper is to suggest and theoretically describe DNT processes in NC metals and nanowires as those occurring through a special mode, the namely nanoscale multiplane shear (NMS) defined as an ideal shear within a nanometer-sized volume.

The notion of NMS is based on that of multiplane shear, an ideal shear occurring simultaneously along several neighboring crystal planes in crystals of *infinite sizes*. The latter has been introduced in paper[18] focusing on the ideal shear strength of defect-free solids under mechanical load. The multiplane shear is characterized by the shear magnitude s (which is identical at any time moment, for all the sheared planes) and the number n of the sheared planes.[18,19]

Here, we define NMS as a multiplane ideal shear occurring within a nanoscale region, a three-dimensional region having two or three nanoscopic sizes. For instance, NMS in nanowires (Figs. 1(a)–1(d)) occurs within a nanoscale region bounded by free surfaces and NMS-produced GBs separating it from the surrounding material (see a two-dimensional illustration in Figs. 1(b)–1(d)). Also, a NMS can occur within a nanoscale internal region of a deformed solid, in which case it is bounded by GBs. The interfaces (GBs and free surfaces) and nanoscopic sizes of nanoscale regions subjected to NMS cause dramatic effects on its behavior. Therefore, NMS has specific peculiarities differentiating it from previously described[18,19] conventional multiplane shear.

In a partial case where the nanoscale ideal shear occurs in one crystallographic plane ($n = 1$), NMS produces a nanodisturbance, a defect theoretically defined and experimentally observed in Gum metals.[20,21] In the case of nanowires, NMS with $n = 1$ results in formation of isolated stacking faults.[17,22,23]

Let us discuss features of the NMS as a special DNT mode in a nanowire (Figs. 1(a)–1(d)). For simplicity, we consider evolution of a two-dimensional rectangular section of a single crystalline Cu nanowire under tensile load (Figs. 1(a)–1(d)). The NMS occurs in n {111} neighboring planes that make 45° angle with the tension direction (Figs. 1(a)–1(d)). At the first stage of the nanotwin ABCD formation, the shear stress τ produces the NMS characterized by a tiny shear magnitude s (Fig. 1(b)). Then, s continuously increases (Fig. 1(c)). Finally, s reaches the Burgers vector magnitude b of Shockley partial dislocations, in which case the NMS results in formation of the nanotwin ABCD (Fig. 1(d)).

The nanotwin formation through NMS (Figs. 1(a)–1(d)) is characterized by the energy change ΔW dependent on s as well as the nanotwin sizes L and H. ΔW is given as

$$\Delta W(s, L, H) = W_{interior} + W_{AC-BD} - A + W_{step}. \quad (1)$$

Here $W_{interior}$ denotes the energy of the interior area of the plastically sheared nanocrystal ABCD; $W_{AC\text{-}BD}$ the energy of the interfaces AC and BD; A the work of the external shear stress τ, spent to the plastic shear within the region ABCD; and W_{step} the energy of free surface steps generated due to NMS.

In spirit of the approach,[18,19] the sum $W_{interior} + W_{AC\text{-}BD}$ can be represented as the product $= L\gamma_n(s)$, where $\gamma_n(s)$ is the energy density penalty due to multiplane shear occurring in

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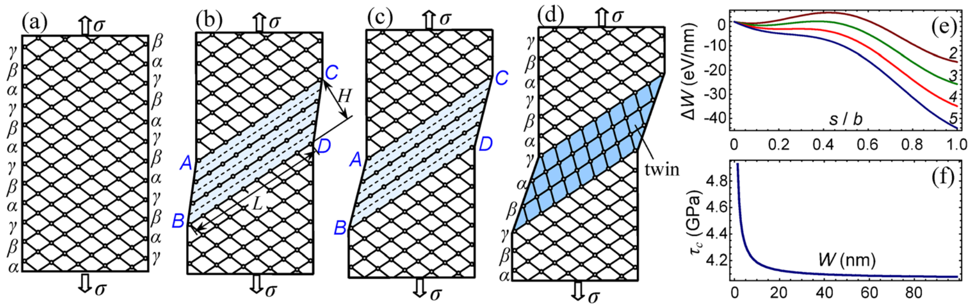

FIG. 1. (Color online) Nanoscale multiplane shear and its characteristics in a nanowire. (a)-(d) Evolution of a two-dimensional rectangular section of a single crystalline Cu nanowire under tensile load is schematically shown. The nanoscale multiplane shear occurs within the region ABCD in n {111} crystallographic planes making 45° angle with the tension direction (n = 3). (a) Initial state with the regular stacking sequence $\alpha\beta\gamma$ of {111} planes. (b) The shear stress τ produces the nanoscale multiplane shear characterized by a tiny shear magnitude s in n = 3 crystal planes. That is, each of these planes is sheared by s relative to its neighboring lower plane, and three generalized stacking faults (dashed lines) are formed between the sheared crystal planes. (c). The magnitude s continuously increases. (d) Finally, s reaches the Burgers vector magnitude b of twinning Shockley partials, the generalized stacking faults transform into conventional ones, and the nanotwin ABCD (with violations of the $\alpha\beta\gamma$ stacking sequence at twin boundaries AB and CD) is formed. (e) The dependences of the energy change ΔW on s, for τ = 2, 3, 4, and 5 GPa (see curves 2, 3, 4, and 5, respectively). (f) The dependence of the critical stress τ_c on the nanowire width W, for $H = 3$ nm.

n neighboring {111} planes of a solid of infinite sizes. In the case of ideal crystal of copper, the function $\gamma_n(s)$ and its derivatives $d\gamma_n(s)/ds$, for n = 1, 2, 3, and 15 and n = ∞, have been simulated by Boyer *et al.*[19] With the results of these simulations, the sum $W_{interior} + W_{AC\text{-}BD} = L\gamma_n(s)$ at finite n is effectively approximated by the following function:

$$W_{interior}(s) + W_{AC-BD}(s) = L\begin{cases} \dfrac{\gamma_0}{2}\left(1-\cos\dfrac{2\pi s}{b}\right), 0 \le s/b < 1/2, \\ \dfrac{\gamma_0+\gamma_{\min}}{2} - \dfrac{\gamma_0-\gamma_{\min}}{2}\cos\dfrac{2\pi s}{b}, 1/2 \le s/b < 1. \end{cases} \tag{2}$$

Here, $\gamma_0 = \gamma_n(b/2)$ is the maximum value of $\gamma_n\ (s)$ and $\gamma_{\min} = \gamma_n(b)$ is the minimum value of $\gamma_n(s)$.

The work A (per one shear plane) of the external shear stress τ is given in the standard way as: $A = \tau sL$. The energy W_{step} of n free surface steps (per one step, each having the height s) is evidently given as: $W_{step} = s\gamma_s$, where γ_s is the specific energy of the free surface (per its unit area).

With these expressions and formulas (1) and (2), we calculated dependences of ΔW on s in the case of Cu nanowire, for $H = 3$ nm ($n = 15$) and $L = 10$ nm, at various values of the applied stress. In doing so, we used the following typical values of parameters of Cu: $a = 0.36$ nm, $\gamma_s = 1.725$ J/m^2,[24] $\gamma_0 = 190$ mJ/m^2, and $\gamma_{\min} = 2.6$ mJ/m^2 (according to the simulations[19] in the case of n = 15). The dependences $\Delta W(s)$ are presented in Fig. 1(e). When the values of τ are high, ΔW always decreases with an increase in s (Fig. 1(e)), in which case the nanotwin forms in the non-barrier (athermal) way. The critical stress $\tau = \tau_c$ is defined as the minimum stress at which the non-barrier formation of the nanotwin occurs. In mathematical terms, τ_c is the minimum stress corresponding to the condition $\partial(\Delta W)/\partial s < 0$ in the range of s from 0 to b. With this condition, we calculated the dependence of τ_c on the nanowire width $W = L/2^{1/2}$ (Fig. 1(f)). This dependence corresponds to the experimentally documented "smaller is stronger" trend and ultrahigh flow stresses in ultrathin nanowires.[17,25] The recent experiment[26] shows the extensive deformation twinning and its suppression in Ti pillars with diameters in the ranges 1–8 and 0.25–0.7 μm, respectively. These data are explained in terms of the effects of pre-existent dislocations on twinning,[26] but they are not relevant to our case (Fig. 1) of ultrathin nanowires initially free from dislocations.

In the situation where a nanotwin is formed through NMS in a grain interior of a NC solid (Figs. 2(a)–2(e)), the formation process does need pre-existent dislocations at GBs. In this context, NMS can serve as a micromechanism for the experimentally observed[4,7,10,11,14,15] growth of nanotwins from GBs in NC metals.

Let us consider the DNT process in a NC Cu specimen (Figs. 2(a)–2(e)). In this case, a deformation twin is produced under the action of a shear stress τ through NMS or, in terms of the dislocation theory, through simultaneous nucleation of n dipoles of noncrystallographic dislocations with tiny Burgers vectors $\pm\mathbf{s}$ (Figs. 2(a)–2(e)). The noncrystallographic dislocations are formed at opposite GB fragments, AB and CD, on adjacent {111} planes. The Burgers vectors $\pm\mathbf{s}$ of all the dislocations are the same in magnitude and grow simultaneously from zero to the Burgers vectors $\pm\mathbf{b}$ of Shockley partials. The generated dipoles of Shockley partials form in adjacent slip planes {111} assumed to be normal to the GB fragments AB and CD. The region ABCD (a rectangle with sizes H and d) is subjected to NMS which results in the formation of a nanotwin within this region (Fig. 2(e)). In doing so, AC length = BD length = H; and AB length = CD length = d, where d is the grain size (Fig. 2). The distance p between the neighboring dislocations at GBs (Figs. 2(c)–2(e) equals to the distance between the {111} planes and is related to the lattice parameter a as $p = a/\sqrt{3}$. The Shockley dislocations are taken as edge dislocations with the Burgers vectors $\pm\mathbf{b}$ of the type $(a/6)\langle 11\bar{2}\rangle$, and $b = a/\sqrt{6}$ is the Burgers vector magnitude.

Let us calculate the energy change ΔW_N that characterizes DNT in a nanograin of NC Cu (Figs. 2(c)–2(e)). The difference between the energies ΔW (given by formula (1)) and ΔW_N is in two aspects. First, the term W_{step} is absent in ΔW_N, because free surface steps are not produced in the discussed case. Second, the dislocation dipoles (Figs. 2(c)–2(e)) at GB

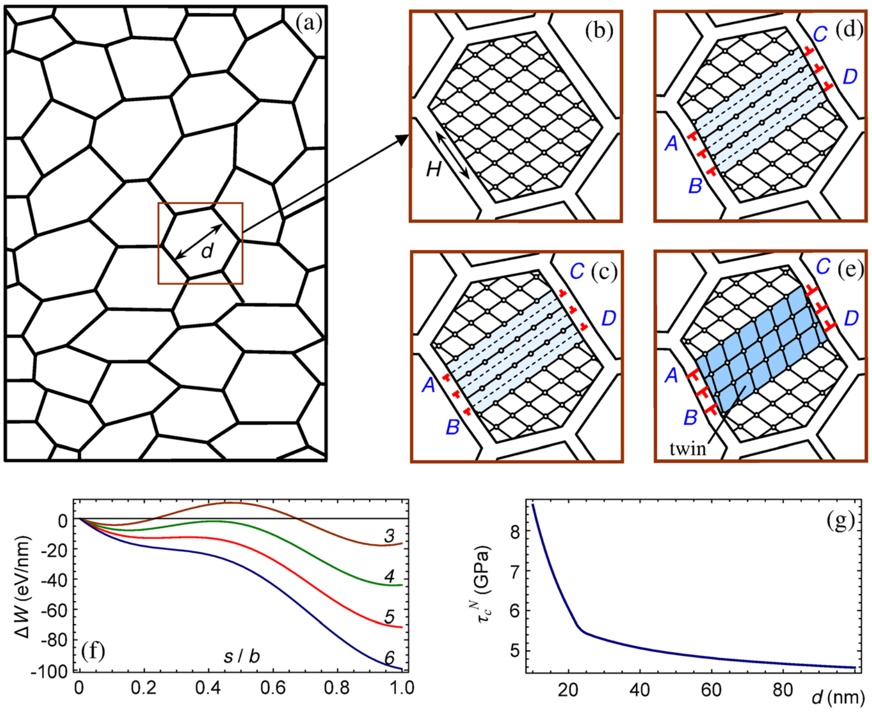

FIG. 2. (Color online) Deformation nanotwinning through nanoscale multiplane shear and its characteristics in a NC solid. (a) NC specimen (general view). (b)-(e) Evolution of a two-dimensional rectangular section of a grain where nanoscale multiplane shear occurs (schematically). (b) Initial state of a nanoscale grain. (c) Nanoscale multiplane shear occurs which is characterized by a tiny shear magnitude s. Two walls of dislocations with tiny Burgers vectors $\pm\mathbf{s}$ are formed at grain boundary fragments AB and CD. (d) The nanoscale shear and Burgers vector magnitude s gradually increases. (e) The noncrystallographic dislocations transform into twinning Shockley partials, and the nanowin is formed. (f) The dependences of the energy change ΔW_N on s, for $\tau = 3$, 4, 5, and 6 GPa (see curves 3, 4, 5, and 6, respectively). (g) The dependence of the critical stress τ_c^N on the grain size d, for $H = 3$ nm.

fragments, AB and CD, are generated due to NMS in a NC solid. The dislocations are specified by the elastic energy that crucially contributes to the energy $W_{AC\text{-}BD}$ of the interfaces AB and CD and thereby to ΔW_N. To summarize, the energy change ΔW_N (per one dislocation dipole and per unit dislocation length) due to NMS is given as

$$\Delta W_N = W_{interior}(s) + W_{AC-BD}(s) - A + W_{AB-CD}(s). \quad (3)$$

After some algebra based on the dislocation theory[24] and calculations like those in the previously considered case of nanowires, we find the following final expression for ΔW_N:

$$\Delta W_N = \frac{G}{2\pi(1-\nu)}\left\{s^2\left(\ln\frac{d}{s}+1\right) + \frac{1}{n}\sum_{k=1}^{n-1}\left[(n-k)\left(s^2\ln\frac{p^2k^2+d^2}{p^2k^2} - \frac{2s^2d^2}{p^2k^2+d^2}\right)\right]\right\} + d\gamma_n(s) - \tau ds. \quad (4)$$

Using formula (4), we calculated dependences of ΔW_N on s in the case of NC Cu, for $H = 3$ nm and $d = 30$ nm, at various values of the applied stress (Fig. 2(f)). As it follows from Fig. 2(f), when the values of τ are high, ΔW_N always decreases with an increase in s, in which case the nanotwin forms in the non-barrier way. The critical stress τ_c^N is defined as the minimum stress at which the nanotwin formation is non-barrier. We calculated the dependence of the critical stress τ_c^N on the grain size d (see Fig. 2(g)) and found that values of τ_c^N are very high. This stress level can be reached in NC solids at shock deformation and indenter load as well as in highly stressed local regions near blunt cracks of quasistatically loaded NC solids. The trend τ_c^N (d) (Fig. 2(g)) is consistent with the experiment[14] (showing also enhancement of ductility in NC Co deformed through DNT).

Thus, NMS effectively serves as a special mode of DNT experimentally observed in nanowires and NC metals (initially poor in twinning dislocations). The NMS can occur at only high stresses that can be reached in defect-free nanowires, dynamically loaded NC solids, and vicinities of blunt cracks in quasistatically loaded NC solids.

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