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GENERATION OF NANOSCALE DEFORMATION TWINS AT FREE SURFACES IN NANOCRYSTALLINE AND ULTRAFINE-GRAINED BULK MATERIALS, THIN FILMS AND MICROPILLARS

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Abstract. Mechanisms for generation of nanoscale twins at free surfaces in nanomaterials during their plastic deformation are theoretically described. The three mechanisms are examined which represent (i) successive events of partial dislocation generation at free surfaces and their further glide in adjacent grain; (ii) cooperative generation of partial dislocations at free surfaces and their further cooperative glide in adjacent grain; and (iii) nanoscale multiplane shear initiated at free surfaces. The energy and stress characteristics of the nanoscale twin formation through these mechanisms in nanocrystalline copper (Cu) are calculated. Competition between the twin generation mechanisms in nanomaterials is discussed in the exemplary case of copper.

1. INTRODUCTION

In parallel with conventional dislocation slip, specific deformation mechanisms/modes effectively operate in nanocrystalline and ultrafine-grained materials (hereinafter called nanomaterials) and strongly affect their excellent mechanical properties; see, e.g., [1-11]. In particular, following experimental data, computer simulations and theoretical models [6,12-25], one of such specific mechanisms is the deformation twinning carried by nanoscale twins generated at grain boundaries. This mechanism comes into play in interior regions of nanomaterials at high mechanical stresses. At the same time, there are several classes of nanomaterials – nanocrystalline and ultrafine-grained films of nanoscale thickness, nanowires, micropillars, etc. – where free surfaces play important roles in plastic deformation processes. In the context discussed, it is highly interesting to understand and describe the effects of free surfaces on deformation twinning. The main aim of this paper is to suggest and theoretically describe special mechanisms for formation of nanoscale deformation twins at free surfaces in nanomaterials. Within the suggested approach, the twin formation mechanisms represent (i) successive events of partial dislocation generation at free surfaces and their further glide in adjacent grain; (ii) cooperative generation of partial dislocations at free surfaces and their further cooperative glide in adjacent grain; and (iii) nanoscale multiplane shear initiated at free surfaces.

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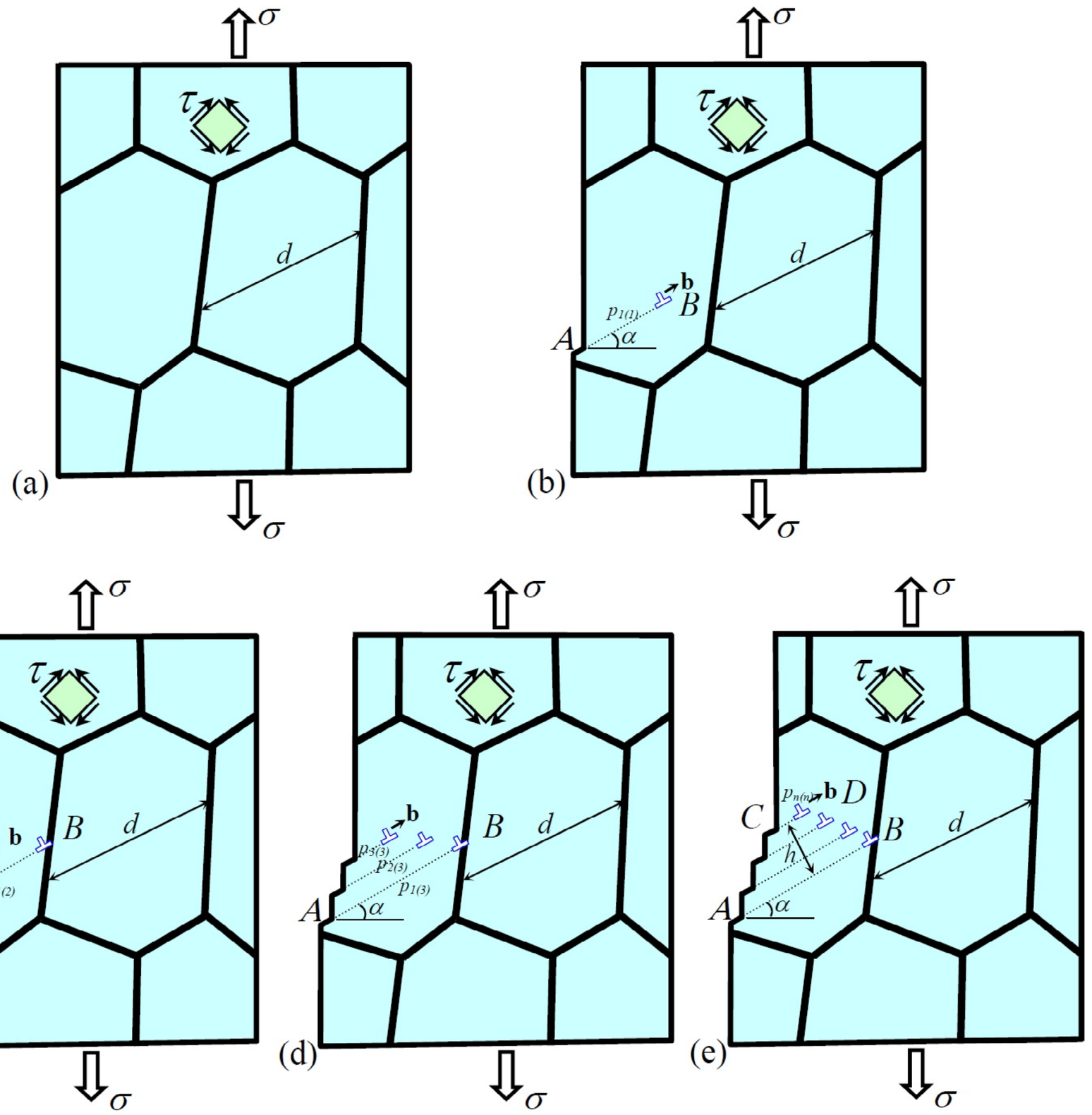

Fig. 1. (Color online) Nanotwin generation occurs through successive events of partial dislocation generation at free surface and their further glide in adjacent grain (schematically). (a) Nanocrystalline specimen under tensile load in its initial state is shown (a two-dimensional view). Figures (b-e) highlight successive events of partial dislocation generation at free surfaces and their further glide in adjacent grain. As a result, a nanoscale twin *ABCD* is formed (for details, see text).

2. MECHANISMS FOR FORMATION OF NANOSCALE DEFORMATION TWINS AT FREE SURFACES IN NANOMATERIALS: GEOMETRIC FEATURES

Let us consider a nanocrystalline specimen having an average grain size d and being under external mechanical load σ (see a 2-dimensional illustration in Fig. 1a). We examine the situation where the specimen has face-centered cubic (FCC) crystal lattice, and nanoscale twins are generated under the external shear stress τ at the specimen free surface. Within the suggested approach, we focus our theoretical analysis on the three following mechanisms for generation of nanoscale deformation twins, the namely twin generation through (i) successive events of partial dislocation generation at free surfaces and their further glide in adjacent grain; (ii) cooperative generation of partial dislocations at free surfaces and their further cooperative glide in adjacent grain; and (iii) nanoscale multiplane shear initiated at free surfaces. This section addresses the specific geometric features of the mechanisms in question.

2.1. Generation of nanoscale deformation twins through successive events of partial dislocation generation at free surfaces

Deformation twins in FCC crystals are typically formed through slip of Shockley partial dislocations along several neighbouring crystallographic {111} planes in the same direction [6]. In the framework

of our model, the Shockley dislocations are edge dislocations of the (a/6)<11 $\bar{2}$> type. They are characterized by the Burgers vector having the magnitude of $b = a/\sqrt{6}$, where a is the crystal lattice parameter. The distance δ between their neighboring slip planes {111} is in the following relationship with the parameter a: $\delta = a/\sqrt{3}$. The slip planes {111} of the partial b-dislocations make an angle α with the specimen free surface.

Formation of a nanoscale deformation twin through the successive events of partial dislocation generation at the free surface and their subsequent slip (Figs. 1b-1e) occurs under the shear stress τ. In doing so, generation of each partial b-dislocation leads to formation of a step at the free surface (Figs. 1b-1e). The step size (b) is equal by magnitude to the dislocation Burgers vector. The first partial dislocation is emitted from the free surface and moves across the adjacent grain interior towards its grain boundary (Fig. 1b) when the shear stress τ reaches its critical value of $\tau_{c(1)}$. This dislocation moves over some distance $p_{1(1)}$ in the grain interior or is stopped by the opposite GB (it depends from the level of the shear stress τ) (Fig. 1b) and creates the stress fields hampering generation of a new dislocation. As a corollary, the critical stress $\tau_{c(2)}$ for emission of the second partial dislocation from the free surface is larger than that for emission of the first dislocation: $\tau_{c(2)} > \tau_{c(1)}$. Since $\tau_{c(2)} > \tau_{c(1)}$, the first dislocation at the stress level $\tau_{c(2)}$ can move by the distance $p_{1(2)}$ (Fig. 1c) which is larger than the distance $p_{1(1)}$ moved by this dislocation at the stress $\tau_{c(1)}$ (Fig. 1b). (Hereinafter $p_{k(n)}$ denotes the distance moved by the kth partial dislocation (emitted from the free surface) at the critical stress $\tau_{c(n)}$ needed to generate the nth partial dislocation at the free surface ($n \geq k$)). At the same time, the second dislocation under the critical shear stress $\tau_{c(2)}$ moves over some distance $p_{2(2)}$ which is typically shorter than the distance $p_{1(2)}$ moved by the first dislocation (Fig. 1c). It is because the stress field created by the first dislocation hampers slip of the second partial dislocation.

When the first dislocation moves in the grain interior, a stacking fault is formed behind it (Fig. 1b). The stacking fault is characterized by the specific energy (per its unit area) γ_{sf}. When the second partial dislocation moves over the distance $p_{2(2)}$, a nanoscale twin nucleus of thickness δ and length $p_{2(2)}$ is generated (Fig. 1c). Its energy includes the specific energies γ_{TB} (per unit area) of twin boundaries. The twin nucleus co-exists with a segment (of the length $p_{1(2)}$-$p_{2(2)}$) of the stacking fault formed behind the first partial dislocation (Fig. 1c).

Further events of the successive dislocation emission from the free surface lead to both widening of the nanoscale twin and movement of its front (Figs. 1d and 1e). The discussed mechanism (Fig. 1) provides generation of the nanoscale twin *ABCD*.

2.2. Generation of nanoscale deformation twins through cooperative emission of partial dislocations from free surfaces

Another mechanism represents formation of nanoscale twins through cooperative emission of partial dislocations from free surfaces (Fig. 2). In doing so, n partial b-dislocations are simultaneously generated at the specimen free surface (Fig. 2b) and then cooperatively move in the adjacent grain interior (Figs. 2c and 2d). The process under consideration is accompanied by formation of n free surface steps each having the size of b (Figs. 2b-2d). The mechanism for twin generation (Fig. 2) operates when the shear stress τ reaches its critical value of $\tau'_{c(n)}$. In the case of $\tau \geq \tau'_{c(n)}$, a group of partial b-dislocations can move from the free surface to its opposite grain boundary. As a result, the nanoscale twin *ABCD* is formed (Fig. 2d).

2.3. Formation of nanoscale deformation twins through nanoscale multiplane shear initiated at free surfaces

We now consider the third mechanism for formation of nanoscale twins, the namely nanoscale multiplane shear initiated at free surfaces in nanomaterials (Fig. 3). The nanoscale multiplane shear is defined [25] as a multiplane ideal shear occurring within a nanoscale region, a three-dimensional region having two or three nanoscopic sizes. (This notion is based on that of multiplane ideal shear in infinite crystals [26,27] The nanoscale multiplane shear is characterized by the shear magnitude s (which is identical at any time moment, for all the planes where the shear occurs), sizes of the sheared region, and the number n of the planes involved in the shear process [25].

In terms of dislocations, the nanoscale multiplane shear represents simultaneous generation of n non-crystallographic dislocations specified by tiny Burgers vector magnitudes s in a subsurface region/grain (Fig. 3b) and their further evolution through growth of s (Fig. 3c and 3d). Non-crystallographic dislocations are generated at a grain boundary of a

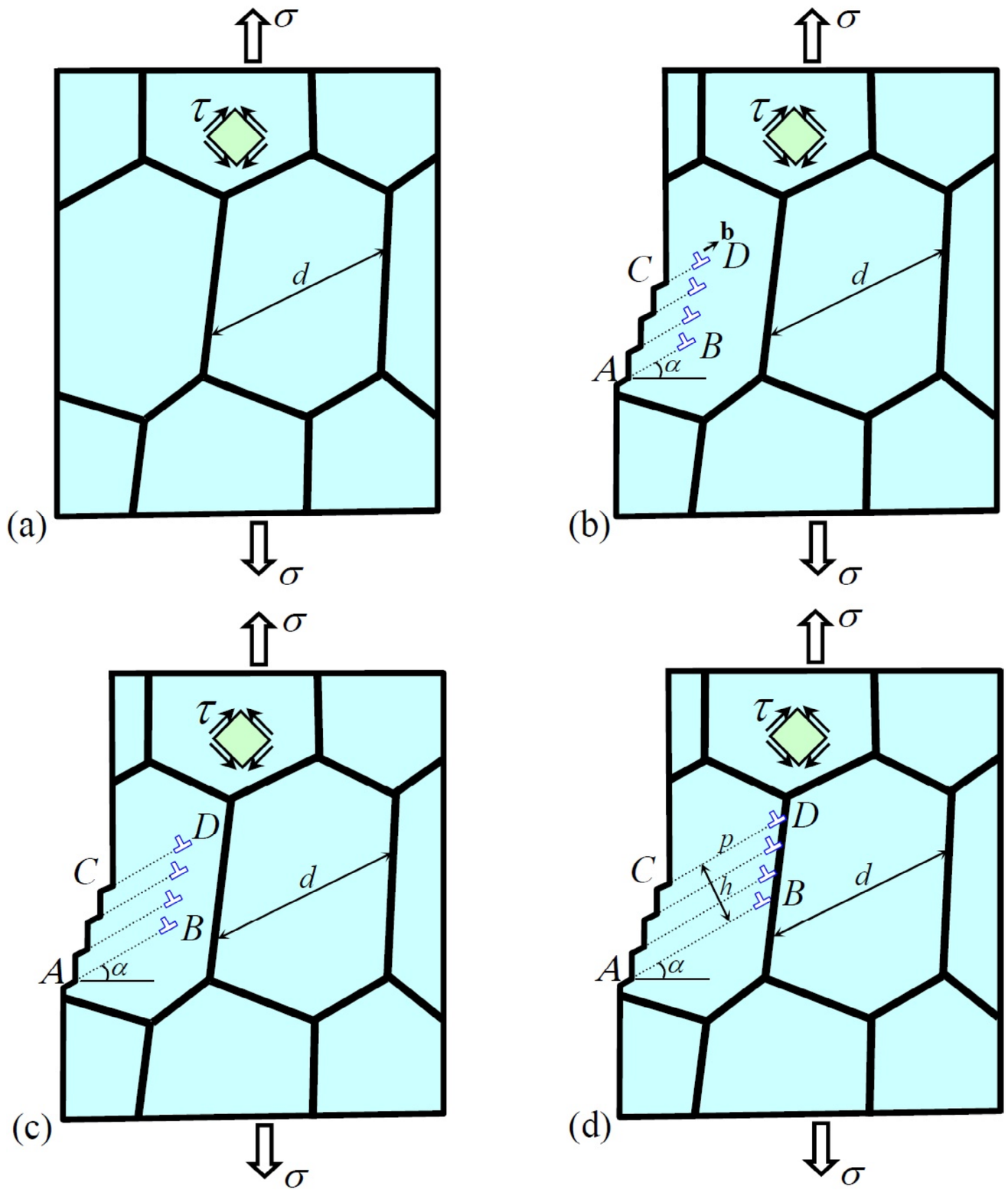

Fig. 2. (Color online) Nanotwin generation occurs through cooperative generation of partial dislocations at free surface and their further cooperative glide in adjacent grain. (a) Nanocrystalline specimen under tensile load in its initial state is shown (a two-dimensional view). Figures (b-d) highlight cooperative generation of partial dislocations at free surfaces and their further cooperative glide in adjacent grain. As a result, a nanoscale twin *ABCD* is formed (for details, see text).

grain adjacent to the free surface and result in formation of *n* free surface steps each having size of *s* (Fig. 3b). Also, the non-crystallographic dislocations are joined by generalized stacking faults in slip planes {111} with the free surface (Figs. 3b and 3c). Growth of *s* from 0 to the Burgers vector magnitude *b* of Shockley dislocations (Fig. 3c) leads to growth of surface steps and evolution of generalized stacking faults. Finally, these processes at some critical shear stress τ_c result in formation of the nanoscale twin *ABCD* (Fig. 3d) (for more details of the nanoscale multiplane shear, see [25]).

Thus, from a geometric viewpoint the three mechanisms (Figs. 1-3) under discussion can result in formation of nanoscale twins at free surfaces in nanomaterials. In order to reveal the most preferred mechanism in nanomaterials, in next section, we consider energy and stress characteristics of these mechanisms.

3. ENERGY AND STRESS CHARACTERISTICS THAT SPECIFY FORMATION OF NANOSCALE DEFORMATION TWINS AT FREE SURFACES OF NANOMATERIALS

3.1. Energy and stress characteristics that specify formation of nanoscale deformation twins through successive events of partial dislocation generation at free surfaces

First, let us consider the energy characteristics of the nanotwin formation through successive events of partial dislocation emission from free surfaces (Fig. 1) Generation of the *n*th *b*-dislocation at the

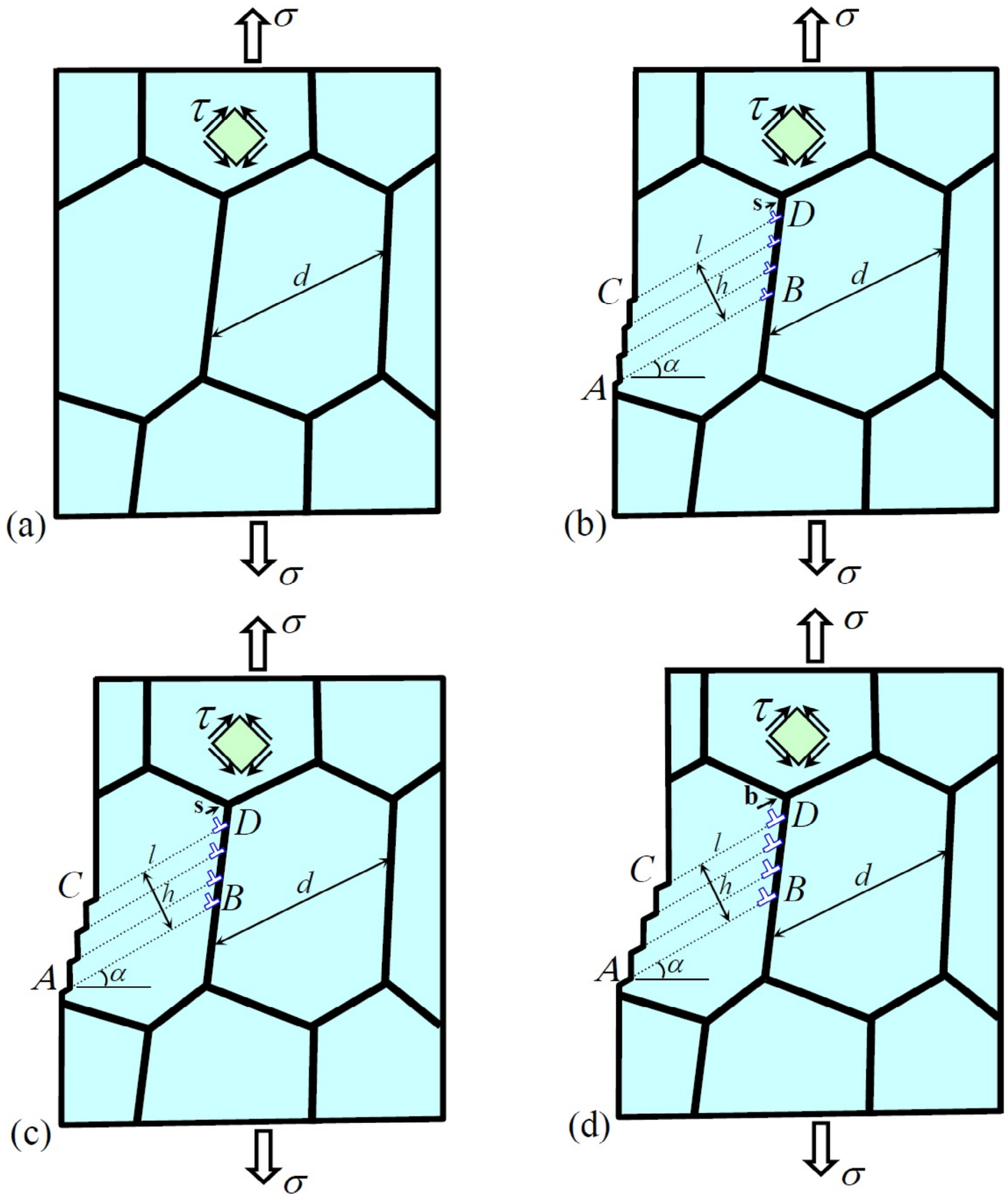

Fig. 3. (Color online) Nanotwin generation occurs through nanoscale multiplane shear initiated at free surface. (a) Nanocrystalline specimen under tensile load in its initial state is shown (a two-dimensional view). Figures (b-d) highlight nanoscale multiplane shear initiated at free surface. As a result, a nanoscale twin *ABCD* is formed (for details, see text).

specimen free surface (Figs. 1b-1e) is specified by the energy change $\Delta W_n = W_{n-1} - W_n$, where W_n and W_{n-1} are the energies of the system in the (n-1)th and nth states, respectively (in which cases (n-1) and n partial b-dislocations are generated at the free surface, respectively). Formation of a nanoscale twin through generation of n partial b-dislocations is energetically favourable, if $\Delta W_n < 0$. The energy change ΔW_n is given as follows:

$$\Delta W_n = E^{b}_{\Sigma n} - E^{b}_{\Sigma(n-1)} + E^{b-b}_{\Sigma n} - E^{b-b}_{\Sigma(n-1)} + E^{\gamma}_{n} - E^{\gamma}_{n-1} + E^{\gamma_s}_{n} - E^{\gamma_s}_{n-1} + E^{\tau}_{\Sigma n} - E^{\tau}_{\Sigma(n-1)}, \quad (1)$$

where $E^{b}_{\Sigma(n-1)}$ and $E^{b}_{\Sigma(n)}$ are the sums of proper energies of (n-1) and n partial b-dislocations, respectively; $E^{b-b}_{\Sigma(n-1)}$ and $E^{b-b}_{\Sigma(n)}$ are the sums of energies that characterize interactions between all the partial b-dislocations in the situations with (n-1) and n dislocations, respectively; E^{γ}_{n-1} is the energy of twin boundaries and adjacent stacking faults having lengths ($p_{1(n-1)}$-$p_{2(n-1)}$) in the situation with (n-1) dislocations; E^{γ}_{n} denotes the energy of twin boundaries and adjacent stacking faults having lengths ($p_{1(n)}$-$p_{2(n}$) in the situation with n dislocations; $E^{\gamma_s}_{n-1}$ and $E^{\gamma_s}_{n}$ are the sums of energies that characterize free surface steps in the situations with (n-1) and n dislocations, respectively; $E^{\tau}_{\Sigma(n-1)}$ and $E^{\tau}_{\Sigma(n)}$ are the sums of energies that characterize interactions of the external shear stress t with (n-1)th and nth partial b-dislocations, respectively.

The sum $E^{b}_{\Sigma(n-1)}$ of proper energies of (n-1) partial b-dislocations located near the free surface is given by the following formula [28-30]:

$$E^{b}_{\Sigma(n-1)} = \sum_{i=1}^{n-1} \frac{Db^2}{2}\left(\ln\frac{p'_{i(n-1)}}{b} + 1\right), \quad (2)$$

where $D = G/[2\pi(1 - \nu)]$, G is the shear modulus, ν is the Poisson ratio, and $p'_{i(n-1)} = p_{i(n-1)}\cos\alpha$ is dis-

tance between the *i*th partial *b*-dislocation and the free surface.

The energy that specifies interaction between the *i*th and *j*th partial *b*-dislocations is calculated as the work spent to generation of the *i*th dislocation in the stress field created by the *j*th dislocation. The energy $E^{b-b}_{\Sigma(n-1)}$ is the sum of such energies characterizing dislocation pair interactions in the situation with (*n*-1) partial *b*-dislocations. This energy can be represented as a double sum over indexes *i* and *j* as follows [29,30]:

$$E^{b-b}_{\Sigma(n-1)} = \frac{Db^2}{2} \times$$

$$\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\left\{\frac{4x_{ij}^2\left(-4x_{ij}^2+y_{ij}^2\right)}{\left(4x_{ij}^2+y_{ij}^2\right)^2}+\ln\left[1+\frac{4x_{ij}^2}{y_{ij}^2}\right]\right\}, \quad (3)$$

where $x_{ij} = (p_{j(n\text{-}1)} - p_{i(n\text{-}1)})\cos\alpha$, and $y_{ij} = (p_{j(n\text{-}1)} - p_{i(n\text{-}1)})\sin\alpha$.

The energies E^{γ}_{n-1}, $E^{\gamma_s}_{n-1}$, and $E^{\tau}_{\Sigma(n-1)}$ are given by the following formulas (see, e.g., [24,28]:

$$E^{\gamma}_{n-1}=\begin{cases}\gamma_{sf}p_{1(n-1)}, & n-1<2,\\ \gamma_{sf}\left(p_{1(n-1)}-p_{2(n-1)}\right)+2\gamma_{TB}p_{2(n-1)}, & n-1\geq 2,\end{cases} \quad (4)$$

$$E^{\gamma_s}_{n-1} = n\gamma_s b, \quad (5)$$

$$E^{\tau}_{\Sigma(n-1)} = -b\tau\cos 2\alpha\sum_{i=1}^{n-1}p_{i(n-1)}, \quad (6)$$

where γ_{sf} is the specific (per unit area) energy of a stacking fault, and γ_s is the specific (per unit area) energy of the specimen free surface.

The expressions for the energies $E^{b}_{\Sigma(n)}$, $E^{b-b}_{\Sigma(n)}$, E^{γ}_{n}, $E^{\gamma_s}_{n}$, and $E^{\tau}_{\Sigma n}$ are formulas (2), (3), (4), (5), and (6), respectively, where (n-1) is replaced by *n*, and new positions $p_{i(n)}$ of previously generated dislocations are utilized.

Formulas (1)-(6) and their modified versions (see previous paragraph) allow one to calculate the energy change ΔW_n. The critical stress $\tau_{c(n)}$ is defined as the minimum shear stress at which generation of the *n*th *b*-dislocation is energetically favourable. The stress $\tau_{c(n)}$ can be derived from the condition that $\Delta W_n(p_{n(n)} = 1\text{ nm}) = 0$ (for details, see discussions of similar subjects in Refs. [21,22,24]).

The stable positions $p_{i(i)}$ of partial *b*-dislocations correspond to minimums of the dependences $\Delta W_n(p_{i(i)})$ and can be found from equations $\partial\Delta W_n/\partial p_{i(i)} = 0$. Calculation details for such stable positions are presented in Refs. [21,22,24].

3.2. Energy and stress characteristics that specify formation of nanoscale deformation twins through cooperative emission of partial dislocations from free surfaces

We now consider energy and stress characteristics that specify formation of nanoscale deformation twins through cooperative emission of partial dislocations from free surfaces (Fig. 2). Simultaneous generation and cooperative movement of *n* partial *b*-dislocations (Figs. 2b-2d) are characterized by the energy change $\Delta W'_n = W'_n - W'$, where W'_n and W' are the energies of the final and initial states of the system, respectively (see Figs. 2d and 2a, respectively). Formation of the nanoscale twin *ABCD* (Fig. 2) is energetically favourable, if $\Delta W'_n < 0$. In the discussed case, the energy change $\Delta W'_n$ has the five terms:

$$\Delta W'_n = E'^{b}_{\Sigma n} + E'^{b-b}_{\Sigma n} + E'^{\gamma}_{n} + E'^{\gamma_s}_{n} + E'^{\tau}_{\Sigma n}, \quad (7)$$

where $E'^{b}_{\Sigma(n)}$ is the sum of proper energies of *n* partial *b*-dislocations; $E'^{b-b}_{\Sigma(n)}$ is the sum of energies that characterize interactions between all the partial *b*-dislocations; E'^{γ}_{n} is the energy of twin boundaries for the nanoscale twin *ABCD*; $E'^{\gamma_s}_{n}$ is the sum of the energies that specify free energy steps; and $E'^{\tau}_{\Sigma n}$ denotes the sum of the energies that specify interactions between the external shear stress t and *n* partial *b*-dislocations.

The sum $E'^{b}_{\Sigma(n)}$ of proper energies of *n* partial *b*-dislocations near the free surface is as follows [28-30]:

$$E'^{b}_{\Sigma(n)} = \frac{nDb^2}{2}\left(\ln\frac{p'}{b}+1\right), \quad (8)$$

where *p* is the path moved by each of the dislocations, and $p' = p\cos\alpha$ is the distance between the free surface and each of the dislocations.

The interaction energy $E'^{b-b}_{\Sigma(n)}$ is calculated in the same way, as with formula (3). As a result, we find:

$$E'^{b-b}_{\Sigma(n)} = \frac{Db^2}{2} \times$$

$$\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\left\{\frac{4p'^2\left(-4p'^2+(j-i)^2\delta^2\cos^2\alpha\right)}{\left(4p'^2+(j-i)^2\delta^2\cos^2\alpha\right)}+\right.$$

$$\left.\ln\left[1+\frac{4p'^2}{(j-i)^2\delta^2\cos^2\alpha}\right]\right\}, \quad (9)$$

The energies $E_n'^{\gamma}$, $E_n'^{\gamma_s}$, and $E_{\Sigma n}'^{\tau}$ are given by the following formulas [24,28]:

$$E_n'^{\gamma} = 2\gamma_{TB}p, \quad n \geq 2 \tag{10}$$

$$E_n'^{\gamma_s} = n\gamma_s b, \tag{11}$$

$$E_{\Sigma(n)}'^{\tau} = -npb\tau\cos 2\alpha, \tag{12}$$

Formulas (7)-(12) allow us to calculate the energy change $\Delta W_n'$. With the energy change $\Delta W_n'$, we also calculate the critical stress $\tau_{c(n)}'$ for generation of nanoscale twins through cooperative emission of partial dislocations from free surfaces (Fig. 2). The critical stress $\tau_{c(n)}'$ is defined as the minimum shear stress at which generation of a nanoscale twin (Fig. 2) is energetically favorable. This stress can be calculated from the following conditions: $\Delta W_n'(p = \tilde{p}) = 0$ (where $\tilde{p}$ = 1nm), $\Delta W_n'\big|_{p>\tilde{p}} < 0$ and $\partial\Delta W_n' / \partial p\big|_{p>\tilde{p}} \leq 0$. Note that, if inequalities $\Delta W_n'\big|_{p>\tilde{p}} < 0$ and $\partial\Delta W_n' / \partial p\big|_{p>\tilde{p}} < 0$ are valid, the dependences $\Delta W_n'(p)$ are negatively valued and monotonously decrease with rising the path p cooperatively moved by the b-dislocations. In the discussed case, the b-dislocations at the nanoscale twin front BD athermally move towards the nearest grain boundary (Fig. 2).

3.3. Energy and stress characteristics that specify formation of nanoscale deformation twins through nanoscale multiplane shear initiated at free surfaces.

Let us examine energy and stress characteristics that specify the third mechanism, that is, formation of nanoscale deformation twins through nanoscale multiplane shear initiated at free surfaces (Fig. 3). This process is characterized by the energy change $\Delta W_n''$ which is given as follows:

$$\Delta W_n'' = E_{\Sigma n}^{s} + E_{\Sigma n}^{s-s} + W_{\text{int}}(s) + W_{AB-CD}(s) + E_n^{\tau} + E_n^{\gamma_s}, \tag{13}$$

where $E_{\Sigma n}^{s}$ is the sum of proper energies of n non-crystallographic dislocations characterized by Burgers vector magnitude s (s-dislocations); $E_{\Sigma n}^{s-s}$ is the sum of the energies that specify pair interactions between all the s-dislocations; $W_{\text{int}}(s)$ is the energy of the region $ABCD$ where the nanoscale multiplane shear occurs; $W_{AB\text{-}CD}(s)$ is the energy of interfaces AB and CD between the nanoscale region $ABCD$ (subjected to the shear) and the surrounding non-deformed material; E_n^{τ} is the work spent by the external shear stress τ to plastic flow within the nanoscale region $ABCD$; $E_n^{\gamma_s}$ is the sum of energies that characterize of n free surface steps.

The proper energy $E_{\Sigma n}^{s}$ and the interaction energy $E_{\Sigma n}^{s-s}$ are given by the expressions being analogues of formulas (8) and (9), respectively, in which case we have [28-30]:

$$E_{\Sigma n}^{s} = \frac{nDs^2}{2}\left(\ln\frac{l'}{s} + 1\right), \tag{14}$$

$$E_{\Sigma n}^{s-s} = \frac{Ds^2}{2} \times \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\left\{\frac{4l'^2\left(-4l^2 + (j-i)^2\delta^2\cos^2\alpha\right)}{\left(4l'^2 + (j-i)^2\delta^2\cos^2\alpha\right)^2} + \ln\left[1 + \frac{4l'^2}{(j-i)^2\delta^2\cos^2\alpha}\right]\right\}, \tag{15}$$

where $l' = l\cos\alpha$ is the distance between the free surface and each of the s-dislocations, and $l \approx d - s$.

In spirit of the approach [26,27], the sum $W_{\text{int}} + W_{AB\text{-}CD}$ (figuring in formula (13)) 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 n neighboring {111} crystallographic 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 = 1,2,3,15, and n = ∞, have been simulated by [27]. With the results of these simulations, the sum $W_{\text{int}}(s) + W_{AB\text{-}CD}(s) = l\gamma_n(s)$ at finite n is effectively approximated by the following function of s [25-27]:

$$W_{\text{int}}(s) + W_{AB-CD}(s) = l\begin{cases}\dfrac{\gamma_0}{2}\left(1 - \cos\dfrac{2\pi s}{b}\right), & 0 \leq s/b < 1/2, \\ \dfrac{\gamma_0 + \gamma_{\min}}{2} - \dfrac{\gamma_0 - \gamma_{\min}}{2}\cos\dfrac{2\pi s}{b}, & 1/2 \leq s/b < 1.\end{cases} \tag{16}$$

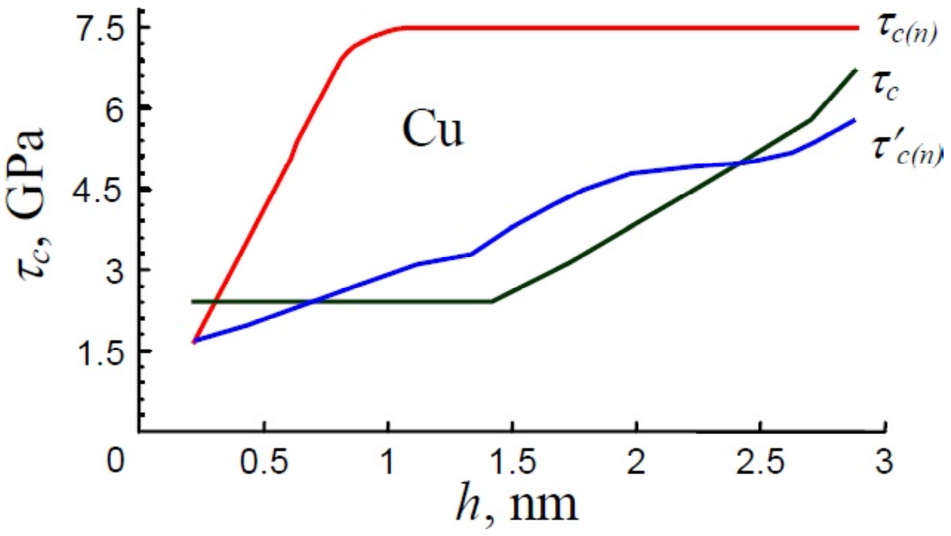

Fig. 4. (Color online) Dependences of critical stresses $\tau_{c(n)}$, $\tau'_{c(n)}$, and τ_c (specifying various mechanisms for nanotwin generation at free surfaces) on nanotwin thickness h, for nanocrystalline Cu (for details, see text).

where $\gamma_0 = \gamma_n(b/2)$ is the maximum value of function $\gamma_n(s)$, and $\gamma_{\min} = \gamma_n(b)$ is the value of function $\gamma_n(s)$ at its minimum corresponding to $s = b$.

The work E_n^{τ} spent by the external shear stress τ to plastic flow within the nanoscale region *ABCD* is evidently given as:

$$E_n^{\tau} = -nls\tau\cos 2\alpha. \qquad (17)$$

The sum of energies $E_n^{\gamma_s}$ that characterize free surface steps is given by the following formula:

$$E_n^{\gamma_s} = ns\gamma_s. \qquad (18)$$

With formulas (13)-(17), one can calculate the energy change $\Delta W_n''(s)$. In the discussed case, the critical stress τ_c is defined as the minimum shear stress at which the Burgers vector magnitudes s of non-crystallographic dislocations (Figs. 3b and 3c) reach value of b characterizing partial Shokley dislocations (Fig. 3d) in the athermal, non-barrier way. In doing so, the dependences $\Delta W_n''(s)$ are negatively valued and monotonously decrease when s grows from 0 to b.

4. COMPARISON OF STRESS CHARACTERISTICS FOR VARIOUS MECHANISMS OF NANOTWIN GENERATION AT FREE SURFACES IN NANOMATERIALS

Let us compare critical stresses for the examined mechanisms of nanotwin generation at free surfaces in nanomaterials. To do so, we calculated dependences of the critical stresses $\tau_{c(n)}$, $\tau'_{c(n)}$, and τ_c on the twin thickness h in the exemplary case of copper (Cu). These dependences are presented in Fig. 4, for the following values of material parameters specifying Cu: G=44 GPa, n=0.3, a=0.358 nm [30], γ_{sf} = 45 mJ/m^2 [31], γ_0 = 190 mJ/m^2, $\gamma_{\min}$ = 2.6 mJ/m^2 [27], and γ_s = 1.725 J/m^2 [32]. The twin thickness h depends on the number n of dislocations contributing to twin formation as follows: $h = (n - 1)\delta$. In our calculations, the grain size d and the angle α are taken as d = 30 nm and α = 45°, respectively.

As it follows from Fig. 4, the critical stresses $\tau_{c(n)}(h)$, $\tau'_{c(n)}(h)$, and $\tau_c(h)$ increase with rising the twin thickness h. Also, the generation of ultrathin nanotwins with thickness h<0.7 nm through cooperative emission of partial dislocations from locally deformation-distorted GBs (Fig. 2) occurs at the lowest stress level (Fig. 4). At the same time, for Cu, in the range of h from 0.7 to 2.5 nm, the generation of nanotwins through nanoscale multiplane shear (Fig. 3) is more favorable; it occurs at the lowest stress level (Fig. 4). In the case of h>2.5 nm, again, the cooperative emission of partial dislocations from GBs (Fig. 2) in copper is the most favorable process characterized by the lowest critical stress (Fig. 4).

5. CONCLUDING REMARKS

Thus, special physical mechanisms for formation of nanoscale deformation twins at free surfaces can effectively operate in nanocrystalline and ultrafine-grained bulk materials, thin films and micropillars. The mechanisms under discussion represent (i) successive events of partial dislocation generation at free surfaces and their further glide in adjacent grain (Fig. 1); (ii) cooperative generation of partial dislocations at free surfaces and their further cooperative glide in adjacent grain (Fig. 2); and (iii) nanoscale multiplane shear initiated at free surfaces (Fig. 3). We calculated the energy and stress characteristics of the nanoscale twin formation through these special mechanisms in the exemplary case of nanocrystalline copper.

In general, the deformation twinning mechanisms are in competition specified by their critical stress levels. In our description, for each mechanism, the critical shear stress is defined as the minimum shear stress at which the energetically favorable formation of a nanotwin occurs. As it follows from Fig. 4, the generation of ultrathin nanotwins with thickness h>0.7 nm through cooperative emission of partial dislocations from locally deformation-distorted GBs (Fig. 2) occurs at the lowest stress level (Fig. 4). At the same time, for Cu, in the range of h from 0.7 to 2.5 nm, the generation of nanotwins through nanoscale multiplane shear (Fig. 3) is more favorable; it occurs at the lowest stress level (Fig. 4). In the case of h>2.5 nm, again, the cooperative emis-

sion of partial dislocations from GBs (Fig. 2) in copper is the most favorable process characterized by the lowest critical stress (Fig. 4).

Also, note that values of the critical shear stresses are very high (Fig. 4). Such values (> 1.5 GPa) cannot be achieved in quasistatic deformation regimes for copper. At the same time, ultrahigh values of stresses are typical for extreme conditions of mechanical loading, say, at high-strain-rate deformation, diamond anvil cell tests and nanoindentation. Thus, the deformation twinning mechanisms (Figs. 1-3) can operate in subsurface areas of nanocrystalline and ultrafine-grained bulk materials, thin films and micropillars at very high, but realistic stress levels realized at extreme conditions of mechanical testing.

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REFERENCES

[1] R.Z. Valiev and T.G. Langdon // *Progr. Mater. Sci.* **51** (2006) 881.
[2] M. Kawasaki and T.G. Langdon // *J. Mater. Sci.* **42** (2007) 1782.
[3] M. Dao, L. Lu, R.J. Asaro, J.T.M. De Hosson and E. Ma // *Acta Mater*. **55** (2007) 4041.
[4] C.S. Pande and K.P. Cooper // *Progr. Mater. Sci*. **54** (2009) 689.
[5] R.Z. Valiev, I. Sabirov, A.P. Zhilyaev and T.G. Langdon // *JOM* **64** (2012) 1134.
[6] Y.T. Zhu, X.Z. Liao and X.L. Wu // *Prog. Mater. Sci.* **57** (2012) 1.
[7] I.A. Ovid'ko and E.C. Aifantis // *Rev. Adv. Mater. Sci.* **35** (2013) 1.
[8] A.P. Zhilyaev, S.N. Sergeev, V.A. Popov and A.V. Orlov // *Rev. Adv. Mater. Sci.* **39** (2014) 15.
[9] A.A. Samigullina, A.A. Nazarov, R.R. Mulyukov, Yu.V. Tsarenko and V.V. Rubanik // *Rev. Adv. Mater. Sci.* **39** (2014) 48.
[10] R.K. Islamgaliev, V.D. Sitdikov, K.M. Nesterov and D.L. Pankratov // *Rev. Adv. Mater. Sci.* **39** (2014) 61.
[11] I.A. Ovid'ko and A.G. Sheinerman // *Rev. Adv. Mater. Sci.* **39** (2014) 99.
[12] X.-L. Wu, Y.T. Zhu and E. Ma // *Appl. Phys. Lett*. **88** (2006) 121905.
[13] X.-L. Wu and E. Ma // *Mater. Sci. Eng. A* **483-484** (2008) 84.
[14] Y.T. Zhu, J. Narayan, J.P. Hirth, S. Mahajan, X.-L. Wu and X.Z. Liao // *Acta Mater*. **57** (2009) 3763.
[15] Y.T. Zhu, X.Z. Liao and X.-L. Wu // *JOM* **60** (2008) 60.
[16] X.Z. Liao, F. Zhou, E.J. Lavernia, D.W. He and Y.T. Zhu // *Appl. Phys. Lett.* 83 (2003) 5062.
[17] X.Z. Liao, F. Zhou, S.G. Srinivasan, Y.T. Zhu, R.Z. Valiev and D.V. Gunderov // *Appl. Phys. Lett.* **84** (2004) 592.
[18] S.V. Bobylev, M.Yu Gutkin and I.A. Ovid'ko // *Phys. Rev. B* **73** (2006) 064102.
[19] Y.T. Zhu, X.L. Wu, X.Z. Liao, J. Narayan, S.N. Mathaudhu and L.J. Kecskes // *Appl. Phys. Lett.* **95** (2009) 031909.
[20] M.Yu Gutkin, I.A. Ovid'ko and N.V. Skiba // *Phys. Rev. B* **74** (2006) 172107.
[21] M.Yu Gutkin, I.A. Ovid'ko and N.V. Skiba // *Phys. Sol. State.* **49** (2007) 874.
[22] I.A. Ovid'ko, N.V. Skiba // *Scripta Mater.* **71** (2014) 33.
[23] I.A. Ovid'ko and N.V. Skiba // *Mater. Phys. Mech.* **21** (2014) 288.
[24] I.A. Ovid'ko and N.V. Skiba // *Int. J. Plasticity* **62** (2014) 50.
[25] I.A. Ovid'ko // *Appl. Phys. Lett.* **99** (2011) 061907.
[26] S. Ogata, J. Li and S. Yip // *Science* **298** (2002) 807-811.
[27] R. D. Boyer, J. Li, S. Ogata and S. Yip // *Modell. Simul. Mater. Sci. Eng.* **12** (2004) 1017.
[28] S.V. Bobylev and I.A. Ovid'ko // *Phys. Rev. Lett.* **103** (2009) 135501.
[29] T. Mura, *Micromechanics of Defects in Solids*, (Dordrecht: Martinus Nijhoff Publishers,1987).
[30] J.P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982).
[31] S. Kibey, J.B. Liu, D.D. Johnson and H. Sehitoglu // *Acta Mater.* **55** (2007) 6843.
[32] I. A. Ovid'ko and A. G. Sheinerman // *Phys. Rev. B* **66** (2002) 245309.