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GENERATION OF DEFORMATION TWIN PAIRS AT GRAIN BOUNDARIES IN NANOMATERIALS

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Abstract. A special micromechanism for generation of nanoscale deformation twins – the generation of nanotwin pairs at grain boundary (GB) dislocation pile-ups - in nanocrystalline and ultrafine-grained materials is suggested and theoretically described. In doing so, the generation of a pair of nanotwins at a grain boundary is realized through simultaneously occurring events of stress-driven splitting of a gliding GB dislocation into two partial lattice dislocations (emitted to adjacent grains) and a sessile GB dislocation. The energy and stress characteristics of the generation process in question are calculated.

1. INTRODUCTION

Plastic deformation and fracture processes in nanocrystalline and ultrafine-grained materials (hereinafter called nanomaterials) are crucially influenced by grain boundaries (GBs); see, e.g., [1–10]. In particular, GB-mediated deformation mechanisms (GB sliding, GB diffusional creep, etc.) intensively operate, and cracks are often generated at GBs in nanomaterials. Among with "pure" GB-mediated deformation mechanisms, deformation modes come into play that are carried by dislocations and twins generated at GBs (and emitted to adjacent grains) in nanomaterials; see, e.g., [1–10]. In the context discussed, there is a large interest in understanding micromechanisms for generation of dislocations and twins at GBs in nanomaterials under mechanical load. In most cases, theoretical models in this area describe emission of dislocations and twins generated at a GB to one of its adjacent grains; for a review, see [10]. Recently, a theoretical model has been suggested describing emission of two dislocations from a GB to its two neighboring grains [11]. The main aim of this paper is to generalize the approach [11] to the situation where a pair of deformation nanotwins is generated at a GB, and these nanotwins are emitted to two grains adjacent to the GB.

2. GENERATION OF NANOTWIN PAIRS AT GRAIN BOUNDARIES IN NANOMATERIALS: GEOMETRIC ASPECTS

Let us consider behaviour of a nanocrystalline specimen (Fig. 1a) under shear stresses rapidly growing from 0 to very high values >10 GPa. At the first stage of plastic deformation with shear stresses being in the range of ~1–2 GPa, GB dislocations are intensively generated at GBs whose volume fractions in nanomaterials are extremely high [1-9]. For higher shear stresses ~3–5 GPa (or more), as it has been demonstrated in the theoretical work [11], generation of lattice dislocations occurs at such GB dislo-

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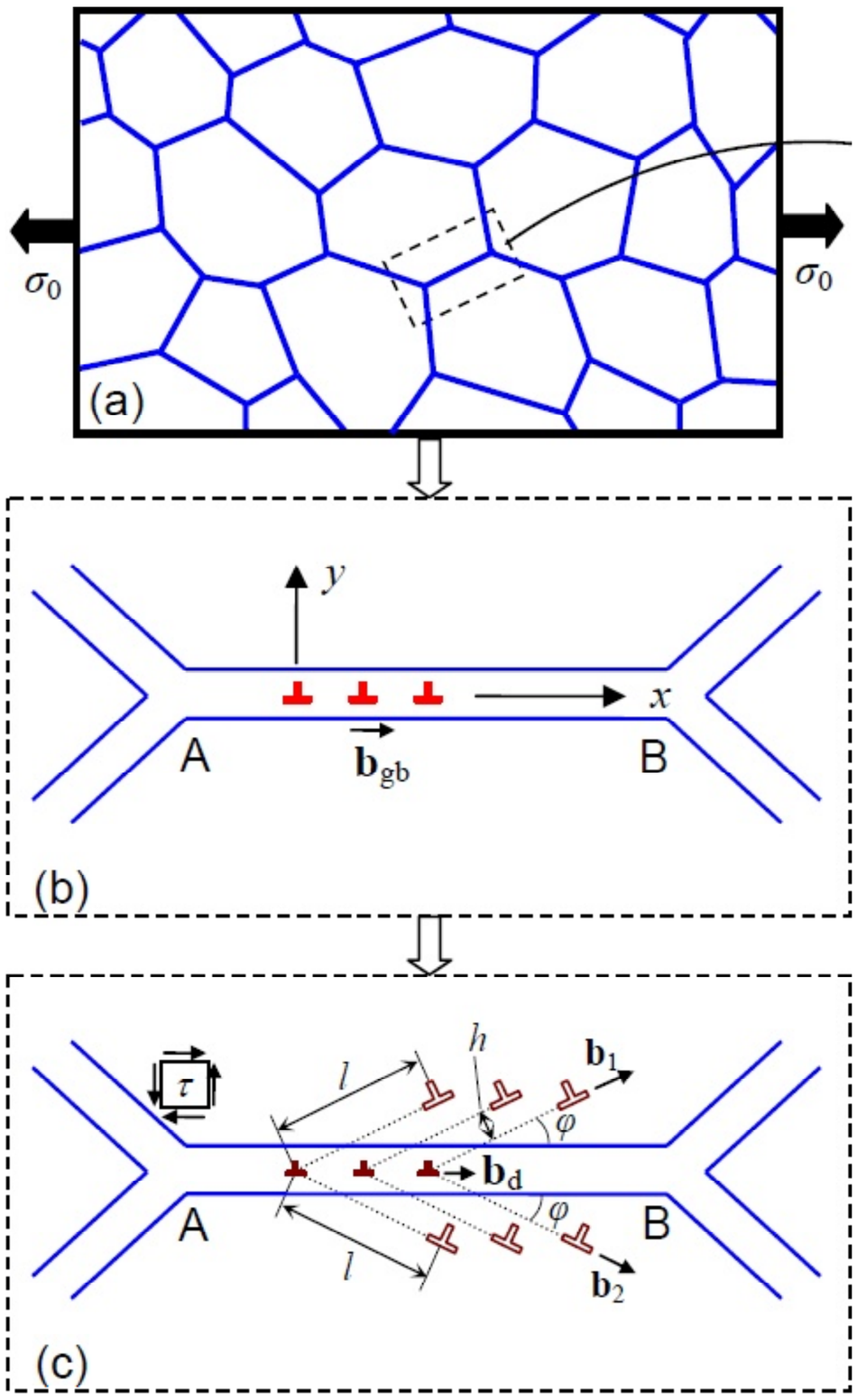

Fig. 1. (Colour online) Generation of nanotwin pairs at grain boundaries in a nanocrystalline specimen (schematically). (a) Nanocrystalline specimen under mechanical load. A general view. (b) Initial state with a pile-up of gliding grain boundary dislocations (characterized by Burgers vector $\mathbf{b}_{gb}$) at the grain boundary AB. For definiteness, three grain boundary dislocations are shown. (c) Grain boundary dislocations split emitting partial lattice dislocations to adjacent grains. The partial dislocations specified by Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are connected by stacking faults of length l with residual grain boundary dislocations characterized by Burgers vectors $\mathbf{b}_d$ and located at sites of the initial grain boundary dislocations. Glide of the partial dislocations in each of the adjacent grains occurs along neighbouring crystallographic planes. As a corollary, glide of such dislocations result in formation of a nanoscale twin in each of the adjacent grains.

cations that undergo splitting transformations. In general, in addition to the considered generation of lattice dislocations at GB dislocations, nanotwins can be generated in a similar way. In this section, we examine geometric aspects concerning generation of deformation nanotwin pairs at GBs in nanomaterials in spirit of the previously formulated [11] model of dislocation pair generation at GBs.

Let us consider heterogeneous generation and growth of nanotwin pairs at GB dislocation pile-ups that can be intensively formed at GBs under high shear stresses. Let us suppose that the GB AB initially contains a pile-up of N GB edge dislocations specified by the Burgers vector $\mathbf{b}_{gb}$ (Fig. 1b). (For definiteness, three ($N = 3$) GB dislocations are shown in this Figure). Such pile-ups are typically formed at structural obstacles (GB steps, GB inclusions) for glide of GB dislocations along GBs. Within our model, we make the following assumptions (that will simplify our theoretical analysis and, at the same time, allow us to catch the key aspects of the problem): (i) GB dislocations are regularly arranged (that is, the distances between neighbouring GB dislocations are identical). (ii) The shear stress τ acts in the GB plane. This stress forces each GB dislocation to split into three dislocations: two mobile partial lattice dislocations and one sessile GB dislocations (Fig. 1c). The partial dislocations have Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ with the same modulus $b_1=b_2=b$ and simultaneously glide in adjacent grains over the same distance l in planes making the angle φ with the GB plane, in which case stacking faults (dashed lines in Fig. 1c) are formed behind the dislocations. The sessile GB dislocation is located at the site of the pre-existent GB dislocation and is characterized by Burgers vector $\mathbf{b}_d$ (Fig. 1c). (iii) The pre-existent GB dislocations are arranged in such a way as to emit partial dislocations along neighbouring crystallographic planes (Fig. 1c). In doing so, the distance between the neighbouring crystallographic planes is h, and the distance between the neighbouring GB dislocations in the pile-up is $h/\sin\varphi$. The assumption (iii) is dictated by geometry of deformation twinning. More precisely, following the theory of dislocations in crystals [12], glide of partial dislocations along neighbouring crystallographic planes (in fcc crystals) and associated formation of stacking faults result in generation of twins. As a corollary, in the case shown in Fig. 1c, a pair of deformation nanotwins is generated at the GB.

The assumption (ii) is also dictated by geometry of deformation twinning. The fact is that formation of deformation twin as a group of moving partial dislocations needs the distance between slip planes to be constant (which is associated with crystallography of a material) and identical in both the grains adjacent to the GB. Since the distance in question is strictly related to the period of the initial GB dislocation pile-up (see our previous discussion) and

the dislocation emission angles, these emission angles for the adjacent grains should be identical. In this context, the GB AB should be symmetric (Fig. 1b). In the situation with an asymmetric GB, one twin can be generated in a grain adjacent to the GB. (Such a situation is beyond the examination of this paper).

3. GENERATION OF NANOTWIN PAIRS AT GRAIN BOUNDARIES IN NANOMATERIALS: ENERGY AND STRESS CHARACTERISTICS

Let us calculate the change ΔW of the energy of the defect configuration due to generation of deformation nanotwins at a GB (Fig. 1). The energy change ΔW is as follows:

$$\Delta W = W_1 - W_0 - A, \tag{1}$$

where W_0 and W_1 are the energies of the defect configuration in its initial and final states, respectively (Figs. 1b and 1c, respectively), and A is the work spent by the external shear stress τ to glide of partial dislocations. The energies W_0 and W_1 are given by the following expressions:

$$W_0 = NW_s(b_{gb}), \tag{2}$$

$$\begin{aligned} W_1 = {} & 2NW_s(b) + NW_s(b_d) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} W_{\text{int}}\left(b_d, \varphi_d, \frac{(i-1)h}{\sin\varphi}, 0, b_d, \varphi_d, \frac{(j-1)h}{\sin\varphi}, 0\right) + \\ & 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} W_{\text{int}}\left(b, \varphi, \frac{(i-1)h}{\sin\varphi} + l\cos\varphi, l\sin\varphi, b, \varphi, \frac{(j-1)h}{\sin\varphi} + l\cos\varphi, l\sin\varphi\right) + \\ & \sum_{i=1}^{N}\sum_{j=1}^{N} W_{\text{int}}\left(b, \varphi, \frac{(i-1)h}{\sin\varphi} + l\cos\varphi, l\sin\varphi, b, -\varphi, \frac{(j-1)h}{\sin\varphi} + l\cos\varphi, -l\sin\varphi\right) + \\ & 2\sum_{i=1}^{N}\sum_{j=1}^{N} W_{\text{int}}\left(b_d, \varphi_d, \frac{(i-1)h}{\sin\varphi}, 0, b, \varphi, \frac{(j-1)h}{\sin\varphi} + l\cos\varphi, l\sin\varphi\right) + W_{tb}, \end{aligned} \tag{3}$$

Here $W_s(b)$ denotes the proper energy (including the dislocation core energy) of an edge dislocation with the Burgers vector magnitude b; b_d is the magnitude of the Burgers vector $\mathbf{b}_d$ that characterizes the residual GB dislocation; φ_d is the angle between the Burgers vector $\mathbf{b}_d$ and the axis x; W_{tb} denotes the energy of twin boundaries; and $W_{\text{int}}(b_1,\alpha_1,x_1,y_1,b_2,\alpha_2,x_2,y_2)$ is the energy that specifies the elastic interaction between two edge dislocations characterized by coordinates (x_1,y_1) and (x_2,y_2) (in the coordinate system shown in Fig. 1) as well as Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, Also, the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ have magnitudes b_1 and b_2, respectively, whereas α_1 and α_2 are the angles between the axis x and the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, respectively.

Formula (3) takes into account the facts that the Burgers vectors of the emitted dislocations make the angles φ and $-\varphi$ with axis x, and the dislocation coordinates (in the coordinate system shown in Fig. 1b) are given by the following expressions:

$$x_i^{gb} = \frac{(i-1)h}{\sin\varphi},\ y_i^{gb} = 0,\ i = 1,\ldots,N, \tag{4}$$

in the case of GB dislocations; and

$$x_i^{p} = \frac{(i-1)h}{\sin\varphi} + l\cos\varphi,\ y_i^{p} = l\sin\varphi,\ i = 1,\ldots,N, \tag{5}$$

in the case of the partial lattice dislocations emitted to the upper grain (Fig. 1c). For the partial lattice dislocations emitted to the bottom grain (Fig. 1c), the coordinates x_i^p are also specified by expression (5), whereas the coordinates y_i^p are replaced by those with their signs opposite to the corresponding signs exploited in formula (5).

The proper energy of an edge dislocation with Burgers vector modulus b is given by the following formula [12]:

$$W_s(b) = \frac{Db^2}{2}\left(\log\frac{R}{b} + 1\right), \tag{6}$$

where $D=G/[2\pi(1-\nu)]$, G is the shear modulus, ν is the Poisson ratio, and R denotes the screening length for dislocation stress fields. The energy $W_{int}(b_1,\alpha_1,x_1,y_1,b_2,\alpha_2,x_2,y_2)$ specifying the pair interaction between dislocations is calculated by the standard method [13] as the work spent to generation of one dislocation in the stress field created by another dislocation (see, for instance, such a calculation in Ref. [14]). In doing so, after some algebra, we find:

$$W_{int}(b_1,\alpha_1,x_1,y_1,b_2,\alpha_2,x_2,y_2) = Db_1b_2\left(\frac{\cos(\alpha_1-\alpha_2)}{2}\ln\frac{R^2}{(x_1-x_2)^2+(y_1-y_2)^2} - \right.$$

$$\left.\frac{(y_1-y_2)((y_1-y_2)\cos(\alpha_1+\alpha_2)-(x_1-x_2)\sin(\alpha_1+\alpha_2))}{(x_1-x_2)^2+(y_1-y_2)^2}\right). \tag{7}$$

The Burgers vector $\mathbf{b}_d$ of the residual dislocation represents the difference between the Burgers vectors of the initial GB dislocation and the emitted partial dislocation. From Fig. 1c it follows that the Burgers vector modulus b_d and the angle φ_d are given as:

$$b_d = \left|b_{gb} - 2b\cos\varphi\right|,\ \varphi_d = 0. \tag{8}$$

The sum energy of twin boundaries is as follows:

$$W_{tb} = 4\gamma_{tb}l, \tag{9}$$

with γ_{tb} being the specific (per unit area) energy of a twin boundary. The work A spent by the external shear stress τ to the glide of the partial dislocations (Fig. 1c) is given by the following formula:

$$A = 2\tau bl\cos 2\varphi. \tag{10}$$

With formulas (2), (3), and (6)–(10) substituted to the expression (1), one can find the total energy change ΔW that characterizes the generation of nanotwin pairs at a GB containing GB dislocations (Fig. 1). Final formula for the energy change ΔW is space-consuming, and thereby we do not present it in the text.

With formulas (1)–(10), we calculated the total energy change ΔW in the exemplary case of copper (Cu). In doing so, we used the following typical values of its parameters: G=48 GPa, ν=0.34 [12], and γ_{tb}=0.024 J/m^2 [15]. Also, we considered Shockley dislocations (specified by the Burgers vector magnitude b=1.47 Å in copper) as partial lattice dislocations. The distance between neighbouring slip planes (111) for such dislocations in FCC metals is equal to $h=a\sqrt{3}$, where a is the lattice parameter. In the case of copper, one has a=3.61 Å [12].

Fig. 2 presents typical dependences of the energy change ΔW on the distance l moved by the partial dislocations, for values of b_{gb}=1 Å and φ=15° as well as various levels of the applied shear stress τ=0.001G, 0.02G, 0.04G, 0.06G, and 0.1G (curves *1, 2, 3, 4,* and *5,* respectively). In Fig. 2, it is seen that the dependence $\Delta W(l)$ at relatively low values of the stress is monotonously growing (see curve *1* in Fig. 2), that is, $\Delta W>0$ in the whole range of other parameters. In this situation, generation of the partial dislocations at a GB is energetically unfavourable. When the stress level increases, the dependences $\Delta W(l)$ exhibit a variable character: first (at low values of l), the dependences are growing, then they become decreasing (see curves *2*, *3,* and *4* in Fig. 2). In this situation, generation of the partial dislocations at a GB is energetically favourable, but needs overcoming an energy barrier (W_b). In doing so, the energy barrier W_b decreases with rising the applied stress (see curves *2*, *3,* and *4* in Fig. 2). When the stress reaches its critical value τ_c, the energy barrier W_b = 0 (curve *5* in Fig. 2). In this situation, generation of nanotwin pairs at a GB (Fig. 1) is always energetically favourable and occurs in the athermal, non-barrier way. In the context discussed, the critical shear stress τ_c serves as an important characteristic for the generation of nanotwin pairs at a GB.

We calculated the dependences of the critical stress τ_c on the dislocation emission angle φ, for copper and nickel (Figs. 3a and 3b, respectively). In doing so, we exploited both the previously considered parameters for copper and the following typical values of parameters characterizing nickel: G=73 GPa, ν=0.34,

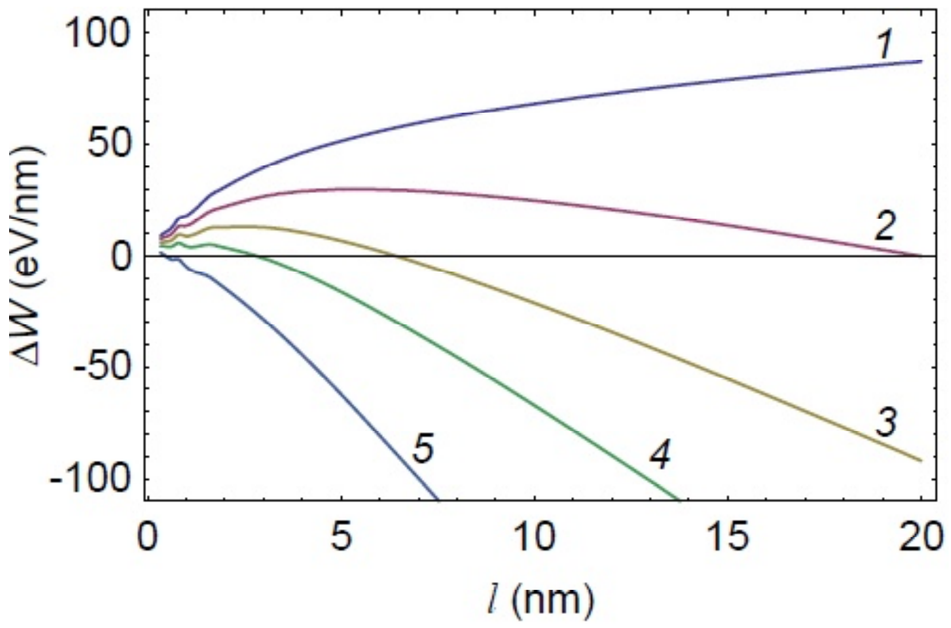

Fig. 2. (Colour online) Typical dependences of the total energy change ΔW on the distance l moved by the partial dislocations in copper. The dependences are calculated, for b_{gb}=1 Å, φ=15°, and τ=0.001G, 0.02G, 0.04G, 0.06G, and 0.1G (curves *1, 2, 3, 4,* and *5* , respectively).

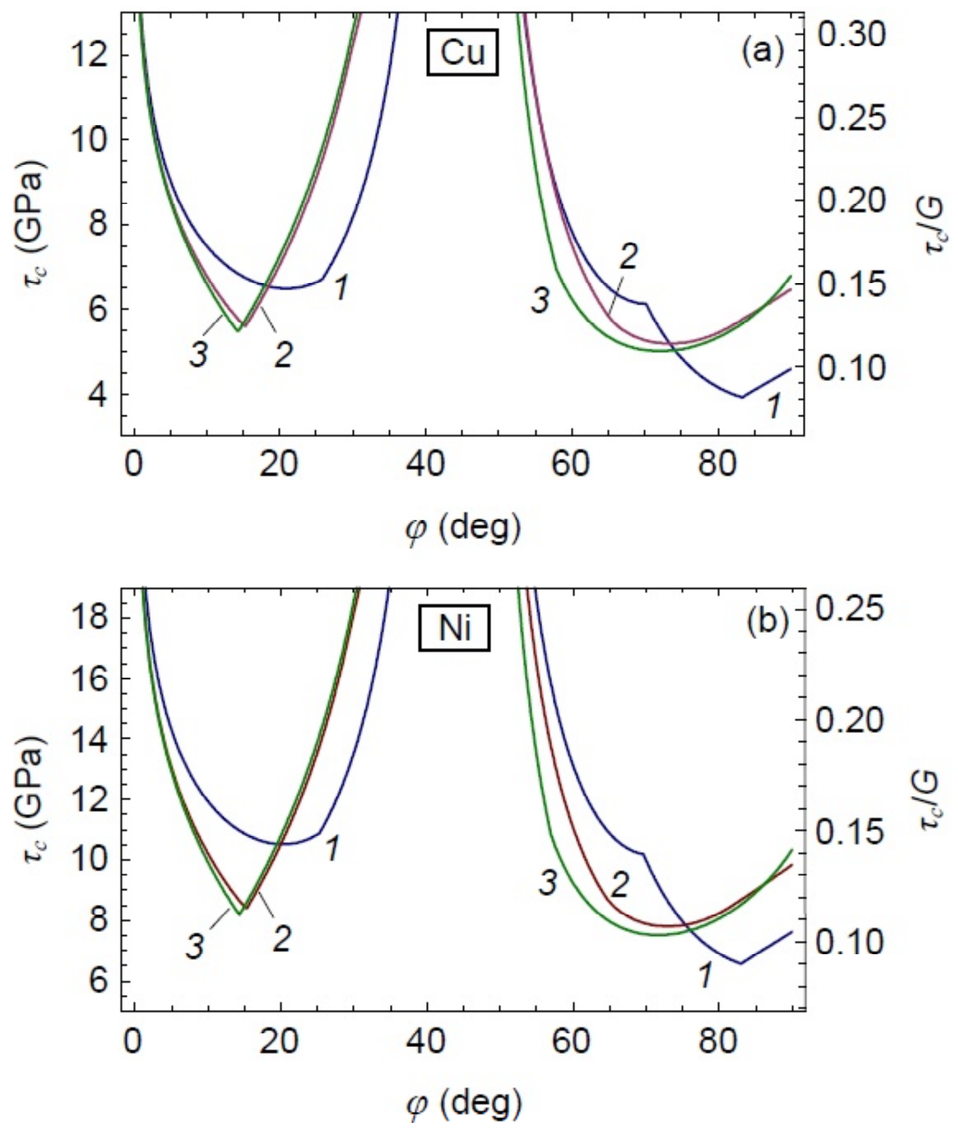

Fig. 3. (Colour online) Dependences of the critical shear stress τ_c on the dislocation emission angle φ in (a) Cu and (b) Ni. Curves *1*, *2,* and *3* correspond to the number N (1, 3, 5, respectively) of the emitted dislocations. Curves 2 and 3 specify emission of nanotwin pairs. Curve *1* is calculated for the situation where a sole dislocation is emitted to each of two grains neighbouring to the GB AB. Burgers vector magnitude for each of initial grain boundary dislocations is taken as b_{gb}=1 Å.

a=3.52 Å, b=1.44 Å [12], γ_{tb}=0.043 J/m^2 [15]. Curves *1*, *2,* and *3* in Fig. 3 correspond to the number N (1, 3, and 5, respectively) of the emitted dislocations. Curves *2* and *3* specify emission of nanotwin pairs. Curve *1* is calculated for the situation where a sole dislocation is emitted to each of two grains adjacent to the GB AB. Formulas presented in this manuscript can be effectively used for calculation of τ_c in the considered situation (N=1), with the following modification: the energy of twin boundaries (see formula (9)) should be replaced by the energy of sole stacking faults $W_\gamma=2\gamma l$, with γ being the specific (per unit area) energy of a stacking fault (γ=0.06 J/m^2, for copper; and γ=0.183 J/m^2, for nickel [12]). In Fig. 3, left branches (φ<45°) of the dependences $\tau_c(\varphi)$ correspond to positive values of the stress, whereas the right branches (φ>45°) of the dependences $\tau_c(\varphi)$ correspond to negative values of the stress.

From Fig. 3 it follows that the generation of nanotwin pairs is a non-barrier process at very high values of the stress (the critical stress τ_c>0.1G, that is, > 5 GPa in copper; and > 7 GPa in nickel). Such a stress level is hardly realized in conventional quasistatic deformation tests. At the same time, stresses > 5–7 GPa are typical for high-strain-rate deformation [16–20], indentation loads and diamond anvil tests [21]. In addition, nanowires and micropillars with nanocrystalline structures can serve as solids where the generation of nanotwin pairs at GBs effectively occurs (because ultrahigh stresses can operate in nanowires and micropillars due to the free-surface and nanoscale effects [22–25]).

Also, Fig. 3 shows that, within various ranges of the dislocation emission angle φ (caused by misorientation of grains adjacent to the GB AB), the most favourable process can be either the generation of sole dislocations (see, e.g., curve *1*) or the generation of nanotwin pairs (see, e.g., curves *2* and *3*). In particular, in the ranges of φ<20° and 45°<φ<75°, the critical stress τ_c for the generation of nanotwin pairs is lower than that for the generation of sole dislocations. In contrast, in the ranges of 20°<φ<45° and 75°<φ<90°, the generation of sole dislocations is most preferred. In doing so, the minimum absolute values of the critical stress τ_c~0.08-0.09G specify the generation of sole dislocations at $\varphi\approx$84°. In the case of nanotwin pairs emitted from GBs, the minimum values of the critical stress τ_c are slightly higher (~0.11-0.12G), and they come into play at $\varphi\approx$70-75°. In general, the generation of both sole dislocations and nanotwin pairs in the range of φ from 45° to 90° is more preferred, as compared to that in the range of φ from 0 to 45°. When φ approaches 45° (this value characterizes plane where shear stresses are equal to 0 in the considered case of uniaxial tension), the critical

stress τ_c dramatically increases up to unrealistically high level.

4. CONCLUDING REMARKS

Thus, in this paper, we suggested a theoretical model describing a special micromechanism for generation of nanoscale deformation twins – the generation of nanotwin pairs at GB dislocation pile-ups (Fig. 1) - in nanocrystalline and ultrafine-grained materials. In the framework of the model, the generation of a pair of nanotwins is realized through simultaneously occurring events of stress-driven splitting of a gliding GB dislocation into two partial lattice dislocations (emitted to neighboring grains) and a sessile GB dislocation (Fig. 1). We calculated the energy and stress characteristics of the generation process in question. In particular, we found the total energy change (see formulas (1)-(10)) specifying the generation of nanotwin pairs at GB dislocation pile-ups (Fig. 1) in nanocrystalline and ultrafine-grained materials. In the exemplary case of copper, this energy and (for comparison) the energy of the generation of sole dislocations at GBs were calculated (Fig. 2). It was revealed that there is the critical shear stress τ_c for the generation processes under consideration to occur in the non-barrier way in copper and nickel. Typical values of τ_c are very high (the critical stress τ_c >0.1*G*, that is, >5 GPa in copper; and >7 GPa in nickel). Such a stress level is hardly realized in conventional quasistatic deformation tests. At the same time, stresses > 5–7 GPa are realized at high-strain-rate deformation [16–20], indentation loads and diamond anvil tests [21]. In addition, nanowires and micropillars with nanocrystalline structures can serve as solids where the generation of nanotwin pairs at GBs effectively occurs (because ultrahigh stresses can operate in nanowires and micropillars due to the free-surface and nanoscale effects [22–25]).

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