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A Brief Review on Plastic Deformation Mechanisms in Nanotwinned Materials

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Abstract

A brief review of the theoretical models which describe mechanisms of the plastic deformation in bulk nanotwinned materials, nanotwinned films and bimodal composites with nanotwinned structure is presented. The first model considers the mechanism of the plastic deformation due to the stress-driven high-angle grain boundary migration which is accompanied by migration of twin boundaries in ultrafine-grained metals with nanotwinned structure. In the framework of the second model, the micromechanism of the plastic deformation in nanotwinned films is widening of nanoscale twins due to migration of twin boundaries. In the third model, the plastic deformation of bimodal composites occurs due to the lattice dislocation slip and the grain boundary sliding in nanocrystalline/ultrafine-grained matrix, and the lattice dislocation slip and the migration of the twin boundaries in large grains with nanotwinned structure.

Keywords: Plastic deformation; Nanotwinned materials; Nanotwins; Twin boundaries; Twin widening

1. INTRODUCTION

Nanostructured materials often exhibit the outstanding physical and mechanical properties such as high strength and hardness, but, in most cases, at the expense of low ductility and low fracture toughness. However, recently, several examples of functional ductility and good toughness have been reported [1–7]. For example, novel nanotwinned metals (ultrafine-grained metallic materials with high-density ensembles of nanoscale twins within grains) exhibit simultaneously high strength and good ductility at room temperature [1–7]. The properties of nanotwinned materials are dramatically influenced by specific deformation mechanisms which effectively operate in these materials.

One of the specific modes in nanotwinned metals is viewed to be plastic deformation occurring through widening of nanoscale twins due to stress-driven migration of twin boundaries [1,8–12]. Another mode that causes a special interest is stress-driven migration of grain boundaries (GBs) [13,14]. The theoretical model [15] shows that the stress-driven high-angle GB migration accompanied by the twin boundary migration can facilitate the process of the GB migration in ultrafine-grained materials with the nanotwinned structure.

According to the recent experimental [1,2] and theoretical [8–12] works, the main micromechanism responsible for the unique combination of high strength and plasticity of nanotwinned materials is viewed to be plastic deformation occurring through widening of nanoscale twins due to migration of twin boundaries. The theoretical work [16] presents a model that describes the plastic deformation through widening of nanoscale twins in nanotwinned films with the ultrafine-grained structure.

Recently, a new class of bimodal metal-graphene composites with a nanotwinned structure has been actively developed. Experimental studies [17,18], theoretical models [19–22] and computer simulations [23,24] demonstrate that composites with a bimodal structure simultaneously exhibit high strength and ductility. In such composites,

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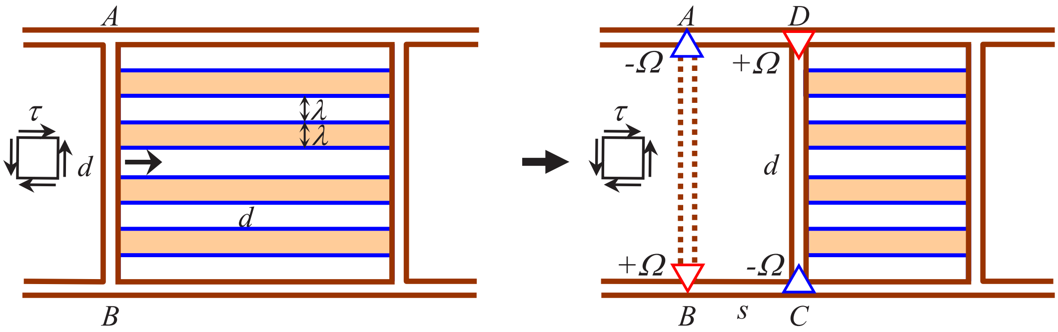

Fig. 1. Model of the stress-driven GB migration accompanied by the twin boundary migration in ultrafine-grained materials with nanotwinned structure. (a) An initial defect configuration containing high-angle GB *AB* and nanoscale twins which adjoin the GB *AB*. (b) Migration of GB *AB* by a distance *s* in a new position *CD*. Reproduced from Ref. [15] under the terms of CC BY-NC-ND 4.0 license.

the nanocrystalline/ultrafine-grained metal-matrix is responsible for high strength, while coarse grains provide good ductility. It should be noted that the formation of a nanotwinned structure in the large grains is accompanied by an additional increase in the strength and the plasticity of bimodal composite [2,9,19]. The theoretical model [25] describes the implementation of the plastic deformation in bimodal composites with nanotwinned structure.

2. MODEL OF STRESS-DRIVEN GB MIGRATION ACCOMPANIED BY TWIN BOUNDARY MIGRATION

Consider a two-dimensional model of an ultrafine-grained specimen containing ensembles of nanotwins bounded by coherent twin boundaries and GBs [15]. We assume that the nanotwinned specimen has rectangular grains with an average size d (Fig. 1a). Let us consider an individual grain containing n identical growth nanotwins of the same thickness λ and length d distributed periodically and restricted by twin boundaries, with the same distance λ in between (Fig. 1a). The nanotwins adjoin the GB *AB* representing a high-angle tilt boundary which characterized by the tilt misorientation parameter Ω. It is assumed that under action of an external shear stress τ, the GB *AB* migrates a distance s in a new position *CD* (Fig. 1b). It is well known [18] that stress-driven GB migration is accompanied by formation of wedge disclinations at GB junctions (Fig. 1b). Let us consider this process in detail. In the initial state (Fig. 1a), triple junctions *A* and *B* are supposed to be geometrically compensated. In other words, the sum of GB misorientation angles at each of these junctions is equal to zero. After GB *AB* migration the angle gaps $\pm\Omega$ appear at the GB junctions *A* and *B*, and at two new GB junctions *C* and *D*. In the theory of defects in solids, these angle gaps are defined as partial wedge disclinations having strength $\pm\Omega$ (Fig. 1b). Thus, stress-induced migration of high-angle tilt GB *AB* results in the formation of a quadrupole of wedge disclinations *ABCD* with strength $\pm\Omega$ (quadrupole $\pm\Omega$-disclination) (Fig. 1b).

In the frame of the work, the GB *AB* migration is accompanied by migration of twin boundaries which adjoin the GB *AB* (Fig. 1b). The migration of the twin boundaries leads to a decrease in the length of nanotwins by a value which equal to the distance s of the GB *AB* migration (Fig. 1b). Decrease in the length of nanotwins reduces elastic energy of the defective system and, therefore, facilitates the process of the GB *AB* migration. In other words, the GB migration accompanied by the twin boundary migration becomes possible at lower values of the external shear stress τ in comparison with the stresses necessary for GB migration in the absence of nanotwins.

Further, we consider the energy characteristics and estimate the critical stresses of the stress-driven GB migration in ultrafine-grained materials with nanotwinned structure. Let us calculate the energy difference ΔW specifying the GB migration (Figs. 1a,b) under consideration. To do so, we assume that the ultrafine-grained specimen represents an isotropic solid characterized by the shear modulus G and the Poisson's ratio ν. The GB *AB* migration is characterized by the energy change $\Delta W = W_2 - W_1$, where W_1 is the energy of the defect configuration in its initial state (Fig. 1a), and W_2 is the energy of the defect configuration in its final state after GB *AB* migration (Fig. 1b). The transformation is energetically favorable, if $\Delta W < 0$. In terms of the theory of defects in solids, the energy change ΔW is written as follows:

$$\Delta W = E_s^{\Omega} + \Delta E_{TB} - A_{\tau}, \qquad (1)$$

E_s^{Ω} is the proper energy of the quadrupole $\pm\Omega$-disclination; ΔE_{TB} is the difference in the energy of twin boundaries between the final and initial states; A_{τ} is the work spent by the external shear stress τ on movement of the GB *AB* over the distance s. A detailed calculation of the energies in Eq. (1) is presented in the theoretical work [15].

With the help of the expression for total energy change ΔW, let us calculate the dependence of the ener-

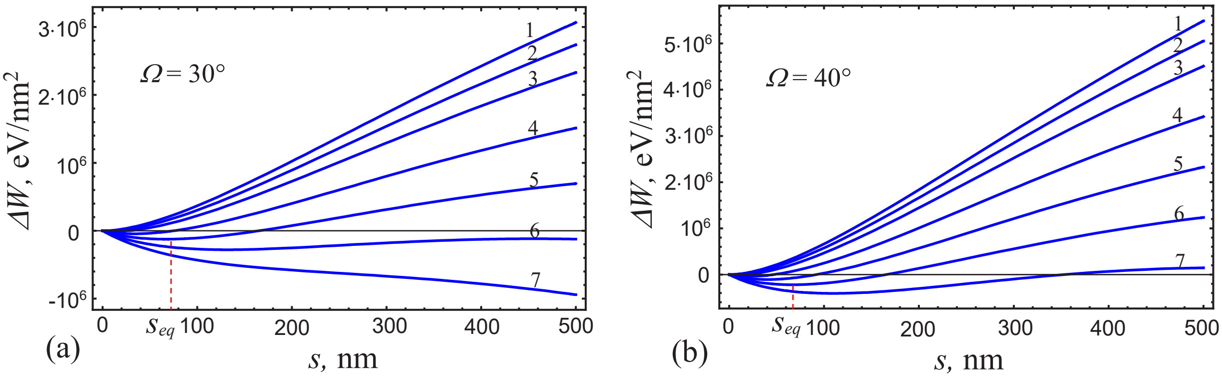

Fig. 2. Dependences the energy change ΔW on the migration distance s, for misorientation parameter $\Omega = 30°$ (a) and 40° (b), at various values of the external shear stress $\tau = 0.1$, 0.5, 1, 2, 3, 4 and 5 GPa (curves 1, 2, 3, 4, 5, 6 and 7, respectively). Reproduced from Ref. [15] under the terms of CC BY-NC-ND 4.0 license.

gy difference ΔW on the GB AB migration distance s in exemplary case of ultrafine-grained nanotwinned copper (Cu) characterized by the following parameter values: $G = 48$ GPa, $\nu = 0.34$ and $\gamma_{TB} = 24$ mJ/m^2. The twin thickness λ and the grain size d are taken as $\lambda = 15$ nm and $d = 500$ nm.

The dependences $\Delta W(s)$ are presented in Figure 2, for various values of the external shear stress τ and the misorientation parameter $\Omega = 30°$ (the strength of quadrupole of ±Ω-disclinations) (Fig. 2a) and 50° (Fig. 2b). These values of Ω correspond to the case of high-angle GB AB. As it follows from Fig. 2, there are three types of function $\Delta W(s)$ behavior, depending on the external stress τ. For low values of the external shear stress τ, the energy change $\Delta W(s)$ first decreases, reaches its minimum, and then grows monotonously with rising of the distance s (Fig. 2a, curves 1–5; and Fig. 2b, curves 1–7). In this case the initial stage of the GB AB migration is energetically favorable (the energy change is negative $\Delta W(s) < 0$ and monotonically decreases) at some critical value τ_{c1} of the external shear stress (Fig. 2). Thus, the critical stress τ_{c1} is the lowest stress at which stable migration of GB AB starts to occur. The GB AB can migrate until the point of minimum which determines the equilibrium migration distance s_{eq} (Fig. 2). The distance s_{eq} of the equilibrium migration of the GB AB is set by the level of the external stress τ, than higher value of the external shear stress τ the more equilibrium GB migration distance s_{eq} (Fig. 2). With rising the external shear stress τ, the energy change $\Delta W(s)$, after reaching its minimum, increases and achieves its maximum, and then decreases monotonously (see Fig. 2a, curve 6). The point of maximum determines the energy barrier for further GB migration. When the external shear stress τ is high enough, the energy change is always negative and decreases monotonously with increasing the migration distance s at some critical value τ_{c2} of the shear stress (Fig. 2a, curve 7). For the external shear stress $\tau > \tau_{c2}$, there exist no stable equilibrium position and/or energy barriers for GB migration. In this situation where $\tau > \tau_{c2}$, unstable migration of GB AB occurres. Thus, the critical stress τ_{c2} determines the transition from stable to unstable GB migration. As it can be seen from the curves in the Figure 2, the decrease in the misorientation parameter Ω (the strength of quadrupole of ±Ω-disclinations) reduces the level of the external shear stress τ required for the GB AB migration.

Let us calculate the values of the critical stresses τ_{c1} and τ_{c2} which determine stable and unstable GB migration, respectively. The start of GB AB migration is possible, if $\Delta W(s = s') < 0$, where $s' = 1$ nm. Thus, the equation $\Delta W(s = s') = 0$ determines the critical stress τ_{c1} as the stress required to start process of the GB AB migration.

The equilibrium migration length, which characterizes the stable GB migration, corresponds to the minimum points on the dependences $\Delta W(s)$ (Fig. 2). The minimum points (which specify the equilibrium migration length) can be found from equation for the energy change $\Delta W(s)$ and the mathematical conditions $\partial \Delta W(s) / \partial s = 0$ and $\partial^2 \Delta W(s) / \partial s^2 > 0$. Using these mathematical conditions and the formula for the energy change $\Delta W(s)$, let us write the dependence of the external shear stress on the equilibrium GB AB migration length s_{eq} in the following form:

$$\tau(s_{eq}) = \frac{F(s_{eq})}{\Omega d}, \tag{2}$$

where $F(s_{eq}) = \partial(E_s^{\Omega} - \Delta E_{\gamma}) / \partial s\big|_{s=s_{eq}}$.

Let us calculate the dependences $\tau(s_{eq})$ in exemplary case of nanotwinned Cu. The dependences $\tau(s_{eq})$ are presented in Figure 3, for various values of the misorientation parameter Ω. The point of maximum on dependences $\tau(s_{eq})$ corresponds to the maximum stress $\tau = \tau_{c2}$ at which stable GB migration is realized, and the distance s'_{eq} is the maximum equilibrium migration length of the GB AB (Fig. 3). Thus, in the situation where $\tau > \tau_{c2}$, the GB migration becomes unstable and the GB AB can mi-

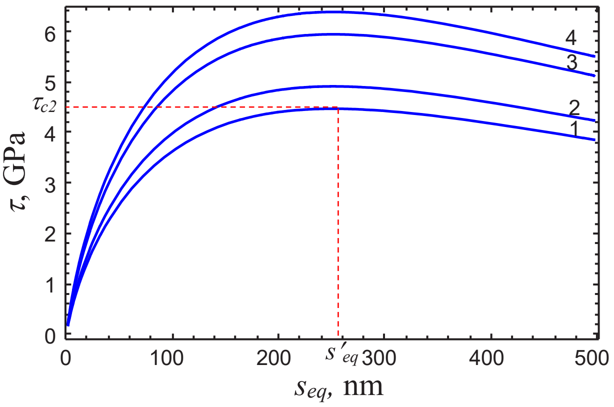

Fig. 3. Dependences of the external shear stress τ on the equilibrium migration length seq in the case of GB migration accompanied by twin boundary migration (curves 1 and 3) and GB migration in absence of nanotwins (curves 2 and 4), at various values of misorientation parameter $\Omega = 30°$ (curves 1 and 2) and 40° (curves 3 and 4). Correspondence τ and s_{eq} is correct to the left of the point (p'_{eq}, τ_{c2}). Reproduced from Ref. [15] under the terms of CC BY-NC-ND 4.0 license.

grate until it reaches the opposite GB. Figure 3 illustrates a comparison of dependences $\tau(s_{eq})$ (curves 1 and 3) corresponding to the stress-driven GB *AB* migration accompanied by the twin boundary migration with dependences $\tau(s_{eq})$ (curves 2 and 4) corresponding to the stress-driven GB *AB* migration in the absence of nanotwins (in the case $\gamma_{TB} = 0$). From Figure 3, it follows that the presence of nanoscale twins facilitates the process of the GB *AB* migration.

3. MODEL OF NANOTWINNED WIDENING IN ULTRAFINE-GRAINED FILMS

Let us consider a two-dimensional model of an ultrafine-grained film with a periodic nanotwinned structure which was formed by electrical deposition onto a semi-infinite substrate with the same chemical composition [16]. In the model, the film and the substrate are assumed to be elastically isotropic solids with the same shear modulus G and Poisson's ratios ν, and the same crystal lattice parameters a. Thus, the film-substrate interface does not create mismatch stresses. It is assumed that the grains of the nanotwinned film with an average size d are composed of rectangular nanotwins bounded by coherent twin boundaries and grain boundaries (Fig. 4a). The action of the applied tensile load creates a resolved shear stress τ at the twin boundaries. If the resolved shear stress τ is high enough, it can lead to the emission of a partial dislocation with the Burgers vector **b** (partial *b*-dislocation) and its motion across the grain over a twin boundary. As a result, a dipole of the partial dislocations *AB* with the Burgers vectors ±**b** is formed at the junctions of the twin and grain boundaries (Fig. 4b). At the same time, slip of the partial dislocation over a coherent twin boundary *AB* across the grain leads to the movement of this twin boundary *AB* in the direction normal to the twin plane by one interplane distance δ providing the twin widening (Fig. 4b).

Consider the energy difference associated with the twin boundary migration (Fig. 4b). The event of twin boundary migration is characterized by the energy difference $\Delta W = W_1 - W_0$, where W_1 and W_0 are the energy of the defect system after and before the twin boundary migration, respectively. The realization of the twin boundary migration event is energetically favored if $\Delta W < 0$. The energy difference ΔW is given as:

$$\Delta W = E_s^d - E_\tau, \tag{3}$$

where E_s^d is the proper energy of partial dislocation dipole *AB* and E_τ is the work of the resolved shear stress τ on migration of the twin boundary by the distance δ.

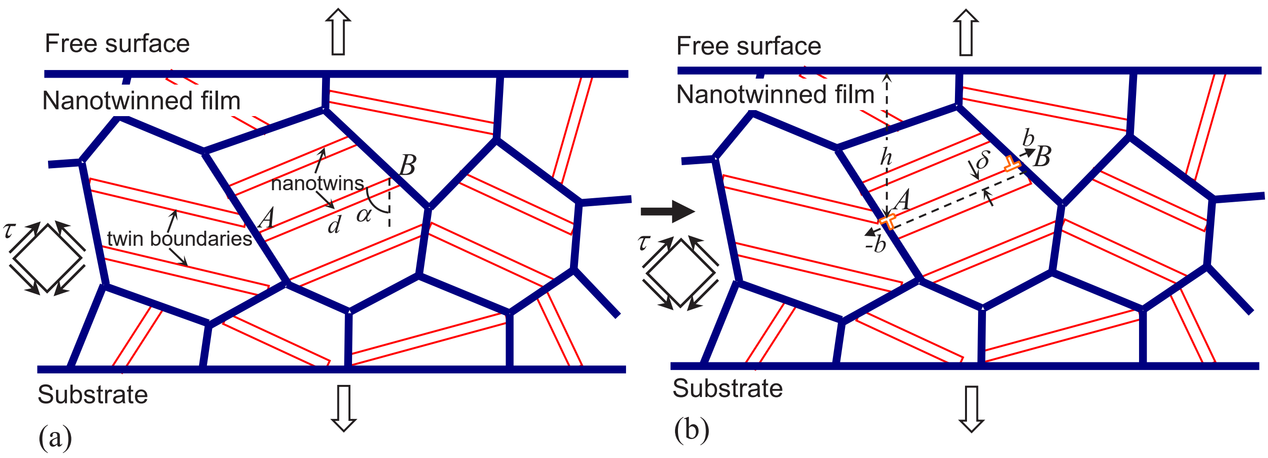

Fig. 4. A model of plastic deformation of an ultrafine-grained film with nanotwinned structure (with ultrafine-grained grains containing high-density ensembles of nanoscale twins). (a) A nanotwinned film specimen is under tensile load. (b) An elementary act of widening of nanotwin occurring through migration of a twin boundary *AB* in the result of emission of a partial *b*-dislocation and its motion across the grain over twin boundary *AB*. Reproduced from Ref. [16] under the terms of CC BY-NC-ND 4.0 license.

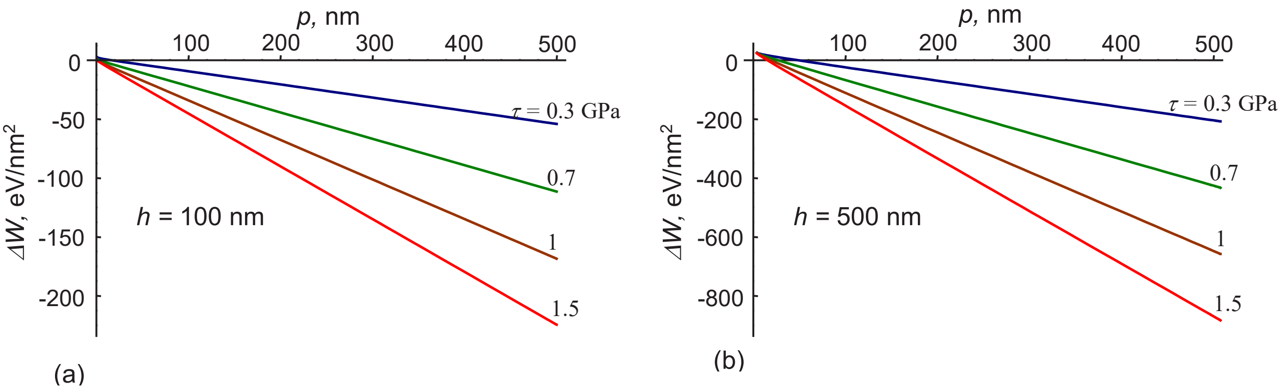

Fig. 5. Dependence of the energy difference ΔW on the distance p travelled by the partial b-dislocation, at various values of the shear stress τ and, for the distance $h = 100$ nm (a) and 500 nm (b). Reproduced from Ref. [16] under the terms of CC BY-NC-ND 4.0 license.

The proper energy E_s^d can be derived from the stress function of an edge dislocation located near a free surface and follows as

$$E_s^d = \frac{Db^2}{2}\left[\ln\frac{s^2+(h+h')^2}{p^2} + \ln\frac{4hh'}{b^2} + \frac{4hh'}{s^2+(h+h')^2}\left(\frac{s^2-(h+h')^2}{s^2+(h+h')^2} + 2\sin^2\alpha\cos 2\alpha\right) - 1\right], \quad (4)$$

where $D = G/2\pi(1-\nu)$, $h' = h - p\cos\alpha$, $s = p\sin\alpha$, α is the angle between twin boundary plane and normal to the free surface (Fig. 4a), p is the distance traveled by the partial b-dislocation.

The work E_τ of the resolved shear stress τ on migration of the twin boundary by the distance δ follows as

$$E_\tau = \tau b\, p \sin 2\alpha. \quad (5)$$

Eqs. (3)–(5) allow us to calculate the energy difference ΔW characterizing the elementary act of plastic deformation occurring through widening of nanoscale twin. Using expression for the energy difference ΔW, let us consider how ΔW changes when the partial b-dislocation slip along the twin boundary AB. We perform such calculations in the exemplary case of a nanotwinned copper film characterized the following values of parameters: $G = 44$ GPa, $\nu = 0.38$, $a = 0.352$ nm, $d = 500$ nm and $\alpha = 45°$. The dependences of $\Delta W(d)$ are presented in Figure 5, at various values of the shear stress τ and distance $h = 100$ nm (Fig. 5a) and 500 nm (Fig. 5b) between the nanotwin and the free surface. As it follows from Fig. 5 the dependences $\Delta W(d)$ monotonously decrease when the distance p traveled by the partial b-dislocation increases. The dependences $\Delta W(d)$ presented in Fig. 5 are indicative the fact that the nanotwin widening becomes energetically favorable ($\Delta W(d)$ is negative and monotonously decreases) when the external stress τ reaches some critical value $\tau_c \approx 0.7$ GPa, in the case $h = 100$ nm (Fig. 5a). Also, as it is seen from Fig. 5, when the distance h between the nanotwin and the free surface increases, the process of the nanotwin widening is hampered.

4. MECHANISMS OF PLASTIC DEFORMATION IN BIMODAL METAL-GRAPHENE COMPOSITES WITH NANOTWINNED STRUCTURE

Let us consider a two-dimensional model of a bimodal composite solid that consists of an nanocrystalline/ultrafine-grained (NC/UFG) metallic matrix with the inclusions in the form of graphene platelets and large grains with nanotwinned structure, loaded by an uniaxial tensile load σ (Fig. 6) [25]. According to experimental data [1,2] and theoretical models [8,22], two principal deformation mechanisms act in nanotwinned materials: twin boundary migration and dislocation motion across twins. The slip of the partial dislocations along the planes parallel to the twin boundaries serves as the primary mechanism of migration of the twin boundaries in the direction normal to the twin plane.

At the same time, according to work [21], the plastic deformation of the NC/UFG metallic matrix with the graphene inclusions occurs due to the emission of the lattice dislocations from GBs and their sliding in grain interiors, and GB sliding.

Taking into account the action of these deformation mechanisms, the yield stress of bimodal metal-graphene composites with nanotwinned structure was calculated [22]. Following theoretical model [8], the yield stress of nanotwinned solid is given by expression:

$$\sigma_y^{NT} = \begin{cases} \sigma_{TBM}, & \lambda < \lambda_*, \\ \alpha\sigma_{TBM} + (1-\alpha)\sigma_{HP}^{NT}, & \lambda \geq \lambda_*. \end{cases} \quad (6)$$

where σ_{TMB} is yield stress associated with twin boundary migration (see Ref. [8], for details), $\sigma_{HP}^{NT} = \sigma_0 + K\lambda^{-1/2}$ is the classical Hall–Petch law, σ_0 and K are the material parameters, α is the volume fraction of the large grains where the yield stress is equal to the σ_{TMB}.

According to the theoretical model [21], the yield stress of the UFG metal-matrix with graphene inclusions is given as

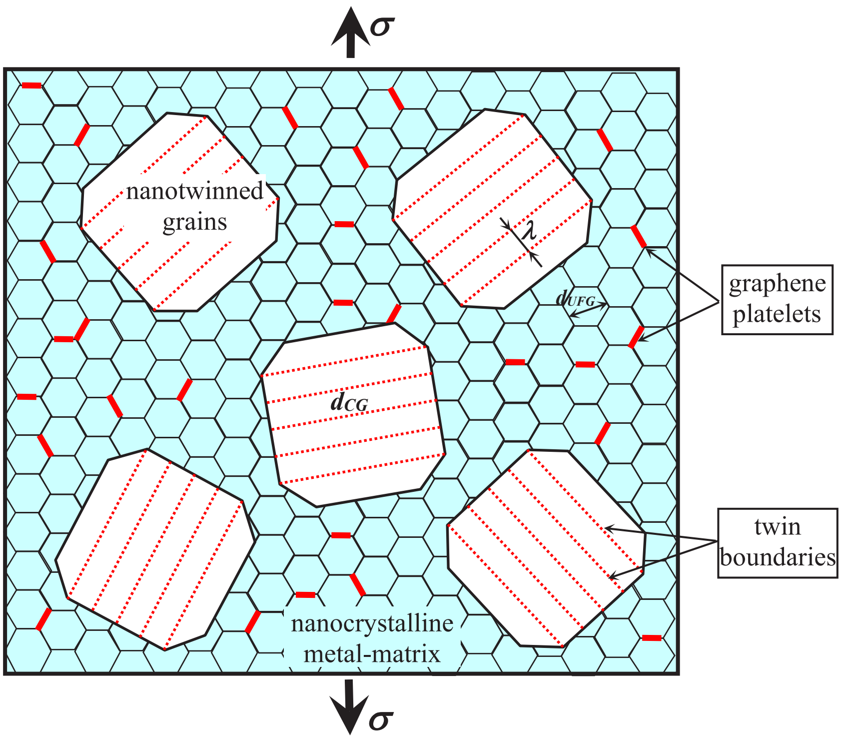

Fig. 6. Model of a bimodal metal-graphene composite consisting of large grains with nanotwinned structure embedded into NC/UFG metal matrix reinforced by graphene inclusions. Reproduced from Ref. [22] under the terms of CC BY-NC 4.0 license, © 2021 N.V. Skiba.

$$\sigma_y^{UFG} = f_{gr}\min(\sigma_{c1},\sigma_{c2}) + (1-f_{gr})\sigma_{c1}, \tag{7}$$

where $\sigma_{c1} = \sigma_{c0} + \sigma_{em}^{GB}$ is critical stress for emitting lattice dislocations from the GBs, $\sigma_{c0} = \sigma_0 + K d_{UFG}^{-1/2}$, d_{UFG} is mean grain size of the UFG matrix, $\sigma_{c2} = M_1\tau_{c2}$, $\tau_{c2} = 140$ MPa is the critical shear stress for slipping graphite monolayers, M_1 is the geometric factor, f_{gr} is the fraction of the GBs containing graphene and σ_{em}^{GB} is the stress necessary to free a dislocation segment pinned by obstacles (see Ref. [21], for details).

With the help of Eqs. (6) and (7) the yield stress of the bimodal metal graphene composites with nanotwinned structure can be expressed as follows [22]:

$$\sigma_y = \beta\sigma_y^{NT} + (1-\beta)\sigma_y^{UFG}, \tag{8}$$

where β is the volume fraction of the large grains with nanotwinned structure.

In the model [22], the dependences of the yield stress σ_y on the twin thickness λ for various values of the volume fraction β (0.3, 0.5 and 0.7, the solid lines 1, 2 and 3, respectively) of large grains in the case of bimodal Cu-graphene composite were calculated (Fig. 7). The dashed line 4 in Fig. 7 depicts the theoretical dependence of the yield stress on the twin thickness for UFG nanotwinned Cu obtained in paper [8]. The horizontal dashed line 5 defines the yield stress σ_y^{UFG} of UFG metal-graphene matrix without nanotwinned grains. The dependences $\sigma_y(\lambda)$ (curves 1–3) in Fig. 7 show the transition from softening to hardening and define that optimum twin thickness λ is equal to 15 nm as well as in the case of UFG nanotwinned Cu (curve 4). The dependences in Fig. 7 also demonstrate that the yield stress σ_y of bimodal metal-graphene composite with nanotwinned structure is higher of the yield stress σ_y^{UFG} of the UFG metal-graphene composite without nanotwinned grains in the range of the twin thickness $10 < \lambda < 40$ nm.

5. CONCLUSIONS

Theoretical model which describes the stress-driven GB migration accompanied by the twin boundary migration in

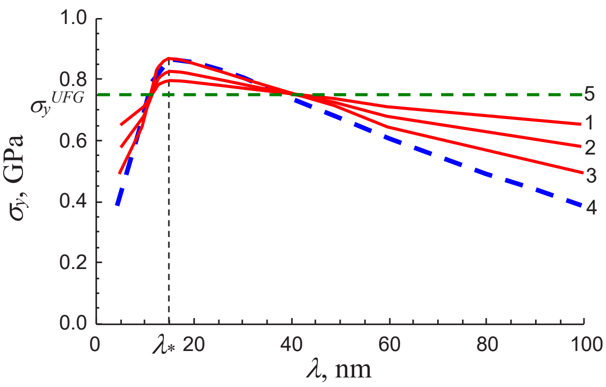

Fig. 7. The dependences of the yield stress σ_y on the twin thickness λ for bimodal nanotwinned Cu-graphene composite (curves 1–3), for UFG nanotwinned Cu (curves 4) and for NC/UFG metal-graphene composite (curve 5). Reproduced from Ref. [22] under the terms of CC BY-NC 4.0 license, © 2021 N.V. Skiba.

ultrafine-grained materials has been reviewed. It has been shown that there are two main regimes of GB migration depending on the level of the external shear stress τ: stable and unstable regime. When the external shear stress $\tau_{c1} \leq \tau < \tau_{c2}$, the GB migrates in a stable regime characterized by the equilibrium migration length s_{eq} which is determined by the level of τ. If $\tau > \tau_{c2}$, the GB migration becomes unstable and GB can migrate until it reaches the opposite GB.

Theoretical model has been reviewed that describes the micromechanism of the plastic deformation in ultrafine-grained metallic films with nanotwinned structure. In the framework of the model, the deformation mechanism in nanotwinned films represents the widening of the nanoscale twins due to the migration of the twin boundaries under the action of the mechanical load. It was shown that the nanotwin widening is energetically favorable in certain ranges of parameters of deformed metallic films with nanotwinned structure.

Also, the plastic deformation mechanisms in the bimodal composite with nanotwinned structure that are realized due to the twin boundary migration and the dislocation motion across the twins in the large nanotwinned grains, and the lattice dislocation slip and the grain boundary sliding in the UFG metal-graphene matrix have been described. It was shown that the presence of the large grains with nanotwinned structure increases the yield strength of the bimodal composite compared to the same composite with the large grains without nanotwinned structure.

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Краткий обзор механизмов пластической деформации в нанодвойникованных материалах

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Аннотация. Представлен краткий обзор теоретических моделей, описывающих механизмы пластической деформации в объемных нанодвойникованных материалах, нанодвойникованных пленках и бимодальных композитах с нанодвойникованной структурой. Первая модель рассматривает механизм пластической деформации, обусловленный миграцией высокоугловых границ зерен под действием внешнего напряжения, которая сопровождается миграцией границ двойников в ультрамелкозернистых металлах с нанодвойникованной структурой. В рамках второй модели микромеханизм пластической деформации в нанодвойникованных пленках представляет собой расширение наноразмерных двойников за счет миграции границ двойников. В третьей модели пластическая деформация бимодальных композитов происходит за счет скольжения решеточных дислокаций и зернограничного скольжения в нанокристаллической/ультрамелкозернистой матрице, а также скольжения решеточных дислокаций и миграции границ двойников в крупных зернах с нанодвойникованной структурой.

Ключевые слова: пластическая деформация; нанодвойникованные материалы; нанодвойники; границы двойников; расширение двойников