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PLASTIC DEFORMATION MODES IN ULTRAFINE-GRAINED METALS WITH NANOTWINNED STRUCTURES

I.A. Ovid'ko[1,2,3], N.V. Skiba[1,2,3] and A.G. Sheinerman[1,2,3]

[1]Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198504, Russia
[2]Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg 199178, Russia
[3]Research Laboratory for Mechanics of New Nanomaterials, Peter the Great St. Petersburg Polytechnical University, St. Petersburg 195251, Russia

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Abstract. A theoretical model is suggested which describes basic deformation modes – stress-driven migration of twin boundaries and lattice dislocation slip – in ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains (nanotwinned metals). In the framework of the suggested model, the micromechanism for stress-driven migration of twin boundaries in nanotwinned metals is glide of partial dislocations along twin boundaries. The energy and stress characteristics of this micromechanism are calculated. With the assumption that stress-driven migration of twin boundaries and lattice dislocation slip concurrently operate in nanotwinned metals, we calculated the dependence of the yield stress on the distance between twins in nanotwinned metals. Our theoretical results are well consistent with corresponding experimental data reported in the literature.

1. INTRODUCTION

Ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains exhibit outstanding mechanical properties (first of all, simultaneously high strength and functional ductility at room temperature) and enhanced electrical conductivity due to their specific structural features; see, e.g., [1–11]. These characteristics of ultrafine-grained metallic materials containing high-density ensembles of nanoscale twins within grains (hereinafter called nanotwinned metals) are very promising for a range of technologies. Despite the recent progress in the research efforts focused on simultaneously high strength and functional ductility of nanotwinned metals, the fundamental nature of plastic deformation processes in these metals is not fully understood and represents the subject of intensive discussions; see, e.g., [1–11]. In particular, the specific deformation modes operating in nanotwinned metals are of crucial interest for understanding the role of the nanotwinned structure in optimization of strength and ductility. One of the specific modes in nanotwinned metals is viewed to be plastic deformation occurring through widening of nanoscale twins [2,9,12–15]. In previous description of this deformation mode, the focuses were placed on dislocation reactions resulting in formation of the twinning partial dislocations that move along twin boundaries and provide twin boundary migration [2,9,12–15]. At the same time, in parallel with dislocations, grain boundaries (whose amounts are rather large in nanotwinned metals having ultrafine grains) can significantly influence plastic deformation carried by twins. For instance, grain boundaries can serve as plane defects where deformation twins are generated and/or stopped; see, e.g., [16–20]. When twins are generated and stopped by grain boundaries, the ensembles of Shockley dislocation

Corresponding author: I.A. Ovid'ko, e-mail: ovidko@nano.ipme.ru

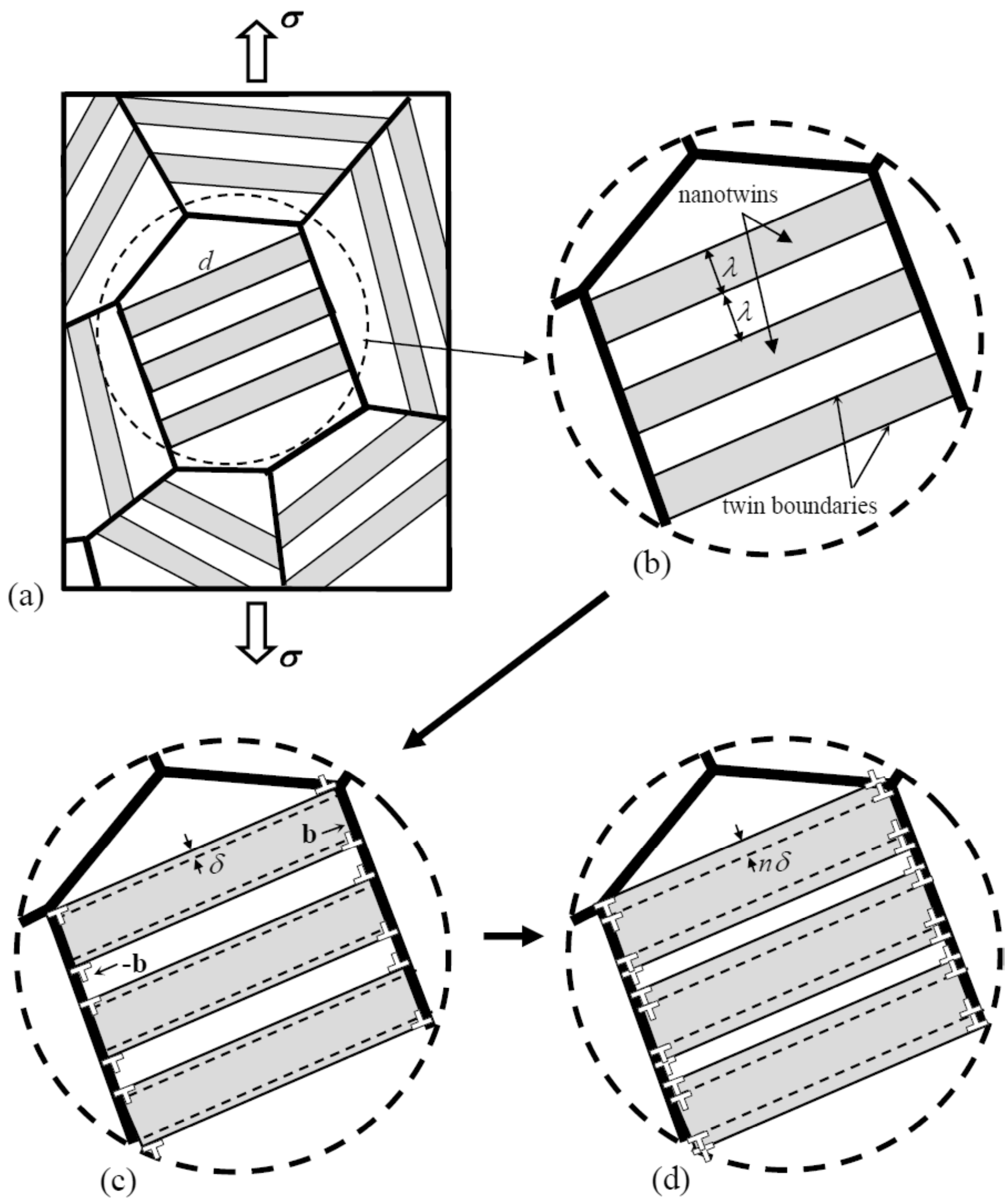

Fig. 1. Twin boundary migration in a deformed nanotwinned solid. (a) Nanotwinned specimen (general view). (b) The magnified region from (a) containing a grain with a regular twinned structure. (c) All the twin boundaries in the examined grain migrate by the interplane distance δ. (d) The positions of twin boundaries after their migration by the distance $n\delta$.

dipoles are typically formed at the junctions of grain and twin boundaries. Such defects create stress fields, and their ensemble is often characterized by a rather high elastic energy which can crucially influence the yield and flow stresses of a nanotwinned metal. This factor should be definitely taken into account in analysis of plastic flow in nanotwinned metals. The main aim of this paper is to suggest a theoretical model which describes plastic deformation through twin boundary migration in nanotwinned metals, with special attention being paid to the effects of the Shockley partial dislocations (formed at the junctions of twin and grain boundaries) on the yield stress characterizing these metals.

2. MIGRATION OF TWIN BOUNDARIES UNDER AN APPLIED MECHANICAL LOAD. MODEL

Consider a two-dimensional model of an ultrafine-grained metallic specimen with a periodic nanotwinned structure, loaded by a uniaxial tensile load σ (Fig. 1a). We assume that the grains of the nanotwinned specimen with an average size d are composed of rectangular nanotwins bounded by coherent twin boundaries and grain boundaries (Fig. 1a). Let us examine an individual model nanograin that contains $N/2$ nanotwins with the same thickness λ and the same length d (Fig. 1b). The action of the applied tensile load σ creates a resolved shear stress τ at the twin boundaries. It is known (e.g., [1,12,21]) that if the resolved shear stress τ is high enough, it can lead to twin boundary migration. In the face-centered cubic (fcc) metals, which we consider below, migration of coherent twin boundaries is realized through the emission of Shockley partials from the junctions of grain and twin boundaries, followed by their motion across the grain over the twin boundaries towards the opposite grain boundaries. Within our model, where no Shockley partials pre-exist at the junctions of the twin and grain boundaries, each emitted partial Shockley dislocation leaves an opposite-sign partial dislocation at the junction of the twin and grain boundaries. As a result, the emission of a Shockley partial with the Burgers vector **b** and its motion across the grain over a twin boundary produces a dipole of the Shockley partials with the Burgers vectors ±**b** at the junctions of the twin and grain boundaries (Fig. 1c). At the same time, a single slip of a Shockley partial over a coherent twin boundary across the grain leads to the movement of this twin boundary in the direction normal to the twin plane by one interplane distance.

Now let us suppose that all N twin boundaries in the examined grain simultaneously migrate under the action of the resolved shear stress τ by one interplane distance δ (Fig. 1c). The geometry of twins requires that the adjacent twin boundaries should migrate in the opposite directions, as shown in Fig. 1c. As a result, some twins widen while others shrink. Simultaneous migration of N coherent twin boundaries is accompanied by the formation of N dipoles of Shockley partial dislocations (Fig. 1c). In the examined case of the nanotwinned specimen with the fcc crystal lattice, twin boundaries occupy the {111} planes, which yields the following relation for the interplane distance δ: $\delta=a/\sqrt{3}$, where a is the crystal lattice parameter. Also, the Shockley partials represent the $(a/6)\langle 11\bar{2}\rangle$ dislocations with the Burgers vector magnitude $b=a/\sqrt{6}$.

The simultaneous migration of all the coherent twin boundaries by the interplane distance δ can repeat many times. As a result of n such events of twin boundary migration, all the twin boundaries migrate by the distance $n\delta$ (Fig. 1d). Since each event of the simultaneous migration of all the coherent twin boundaries by the interplane distance δ leads to the formation of N dislocation dipoles, n such events create $n\times N$ dipoles. Twin boundary migration can proceed if the applied load is high enough to drive it and stops when the applied load becomes insufficient or when the adjoining twin boundaries merge, leading to the complete detwinning of the examined grain. In particular, if we do not consider the case of the complete detwinning, then the realization of the nth event of twin boundary migration is possible provided that the resolved shear stress τ exceeds some critical value τ_n^{crit}. The critical stress τ_n^{crit} can be defined as the minimum resolved shear stress at which the nth event of twin boundary migration becomes energetically beneficial. To calculate τ_n^{crit}, in the next session we will examine the energetics of twin boundary migration under the action of the resolved shear stress τ.

3. ENERGY CHANGE ASSOCIATED WITH TWIN BOUNDARY MIGRATION DRIVEN BY AN APPLIED MECHANICAL LOAD

Consider the energy variation associated with the nth event of twin boundary migration (Fig. 1d). The nth event of twin boundary migration is characterized by the energy change $\Delta W_n=W_n-W_{n-1}$, where W_n and W_{n-1} are the energy of the examined system after the nth and (n-1)th event of twin boundary migration, respectively. The realization of the n th migration event is energetically favored if $\Delta W_n<0$. To calculate the critical stress τ_n^{crit} required for such a migration event, below we will derive the expressions for ΔW_n. To do so, we will model the nanotwinned specimen as an elastically isotropic solid with the shear modulus G and Poisson's ratio ν. Then the energy change ΔW_n can be presented as

$$\Delta W_n = E_N^b + E_n^{b-b} - E_{n-1}^{b-b} - A_N^{\tau}, \tag{1}$$

where E_N^b is the sum of all the self-energies of N Shockley dislocation dipoles, E_n^{b-b} and E_{n-1}^{b-b} are the total energies of the elastic interaction among all the Shockley dislocation dipoles after the nth and (n-1)th migration event, respectively, and A_N^{τ} is the work of the resolved shear stress τ on migration of all the twin boundaries by the distance δ.

The sum E_N^b of all the self-energies of N Shockley dislocation dipoles is given [22] by

$$E_N^b = NDb^2\left(\ln\frac{d}{b}+1\right), \tag{2}$$

where $D=G/2\pi(1-\nu)$.

For simplicity, let us focus on the situation where the number N of the migrating twin boundaries is even. Then the energy E_n^{b-b} of the elastic interaction among all the Shockley dislocation dipoles after the *n*th migration event (calculated as the sum of the strain energies of the dipole-dipole interaction over all the dipole pairs) follows as

$$E_n^{b-b} = Db^2\left[NF + \sum_{k=1}^{N/2-1}\left(N/2-k\right)\left(B_k + C_k + 2E_k\right)\right], \quad (3)$$

where

$$F = N\sum_{l=1}^{n-1}\left(n-l\right)f(l\delta),$$

$$B_k = nf\left[\lambda\left(2k-1\right)+\delta\left(n+1\right)\right] + \sum_{l=1}^{n-1}\left(n-l\right)\left(f\left[\lambda\left(2k-1\right)+\delta\left(n+1-l\right)\right] + f\left[\lambda\left(2k-1\right)+\delta\left(n+1+l\right)\right]\right),$$

$$C_k = nf\left[\lambda\left(2k-1\right)-\delta\left(n+1\right)\right] + \sum_{l=1}^{n-1}\left(n-l\right)\left(f\left[\lambda\left(2k-1\right)-\delta\left(n+1-l\right)\right] + f\left[\lambda\left(2k-1\right)-\delta\left(n+1+l\right)\right]\right), \quad (4)$$

$$E_k = nf\left(2\lambda k\right) + \sum_{l=1}^{n-1}\left(n-1\right)\left(f\left(2\lambda k - l\delta\right) + f\left(2\lambda k - l\delta\right)\right)$$

and

$$f(p) = \ln\frac{d^2+p^2}{p^2} - \frac{2d^2}{d^2+p^2}.$$

The energy E_{n-1}^{b-b} is obtained from formula (4) by the replacement of *n* by *n*-1.

The work A_N^τ of the resolved shear stress τ on migration of all the twin boundaries by the distance d follows as

$$A_N^\tau = N\tau bd. \quad (5)$$

Now the critical stress τ_n^{crit} (defined as the minimum resolved shear stress at which the *n*th event of twin boundary migration becomes energetically beneficial) can be found from formulae (1)–(5) and the relation $\Delta W(\tau=\tau_n^{crit})=0$. In turn, the critical resolved shear stress τ_n^{crit} is related to the critical applied tensile load σ_n^{crit} by the relation $\tau_n^{crit}=\kappa\sigma_n^{crit}$, where κ is the geometric factor ($0\leq\kappa\leq 0.5$) determined by the orientation of the Shockley dislocation slip system with respect to the direction of the applied load. Also, the parameter *n* is related to the shear deformation angle γ as follows: $n=\gamma d/(Nb)$. As a result, the expressions for τ_n^{crit} combined with the relations $\sigma_n^{crit} = \tau_n^{crit}/\kappa$ and $n=\gamma d/(Nb)$ give the critical applied load σ_n^{crit} as a function of the plastic shear deformation angle γ. To estimate the yields stress associated with twin boundary migration (labeled here as σ_{TBM}), we define it as the critical stress σ_n^{crit} corresponding to the shear deformation angle of 2 percent, that is, $\sigma_{TBM} = \sigma_n^{crit}$ ($\gamma=0.02$). In the next section, the critical stress σ_{TBM} associated with twin boundary migration will be used to calculate the overall yield stress of the nanotwinned solid deformed by various deformation mechanisms.

4. TWIN THICKNESS DEPENDENCE OF THE YIELD STRESS OF NANOTWINNED METALS

The critical stress σ_{TBM} determines the yield stress in an individual grain where plastic deformation is realized through twin boundary migration. At the same time, along with twin boundary migration, other deformation mechanisms can act in nanotwinned metals. The classical deformation mechanism involves the emission of partial dislocations from twin boundaries followed by their slip across the twins and their absorption by the adjacent twin boundaries. Another possible deformation mechanism is associated with the motion of jogged dislocations (accomplished via the slip of their threading segments in between the twins accompanied by the extension of their misfit segments along twin boundaries (e.g., [9])). This plastic deformation mechanism can be realized in the grains where twin thickness is small and twin boundary planes make low angles with the direction of the applied tensile load. However, for simplicity, we focus on the situation where this deformation mechanism is realized in a small fraction of grains, so that its effect on the yield stress of the nanotwinned solid can be neglected.

Thus, within our model, two principal deformation mechanisms act in the nanotwinned solid. These mechanisms represent twin boundary migration and dislocation motion across twins. To calculate the overall yield stress of the nanotwinned solid, one can introduce the yield stress of an individual grain. The rigorous calculation of the yield stress of the nanotwinned solid with a fixed twin thickness should account for the distributions of twin boundary orientations with respect to the direction of the applied load. In this case, the yield stress of a specified grain should represent the lower of the critical stresses, σ_{TBM} and σ_{HP}, for the start of either of the principle deformation mechanisms, and the volume fraction of the grains where the yield stress corresponds to either the critical stress σ_{TBM} (for twin boundary migration) or the critical stress σ_{HP} (for dislocation motion across twins) would gradually vary with a change in twin thickness. However, for simplicity, in a zero approximation, we will not compare the critical stresses for the action of the two deformation mechanisms in a specified grain and postulate the following:

(i) If the twin thickness is small (below some critical thickness λ_*), plastic deformation occurs only via twin boundary migration (at least, at the initial stages of plastic deformation). In this case, the yield stress of each grain is determined by the critical stress σ_{TBM} for twin boundary migration.

(ii) If the twin thicknesses is sufficiently large (above some critical thickness λ_*), plastic deformation can occur either through twin boundary migration or via dislocation motion across twins. In this case, we introduce the volume fraction α of the grains where the yield stress is equal to the critical stress σ_{TBM} (for twin boundary migration) and the volume fraction 1-α of the grains where the yield stress is equal to the critical stress σ_{HP} (for dislocation motion across twins). Here we do not require that the yield stress of a specified grain should correspond to the lower of the two critical stresses, σ_{TBM} and σ_{HP}, and postulate that the volume fraction α does not depend on twin thickness λ.

(iii) The critical stress σ_{HP} for the onset of dislocation motion across twins obeys the classical Hall–Petch law [23,24]: $\sigma_{HP}=\sigma_0+K\lambda^{-1/2}$, where σ_0 and K are the materials parameters.

(iv) The yield stress σ_y of the nanotwinned solid is related to the yield stresses of individual grains using the mixture rule [25,26]:

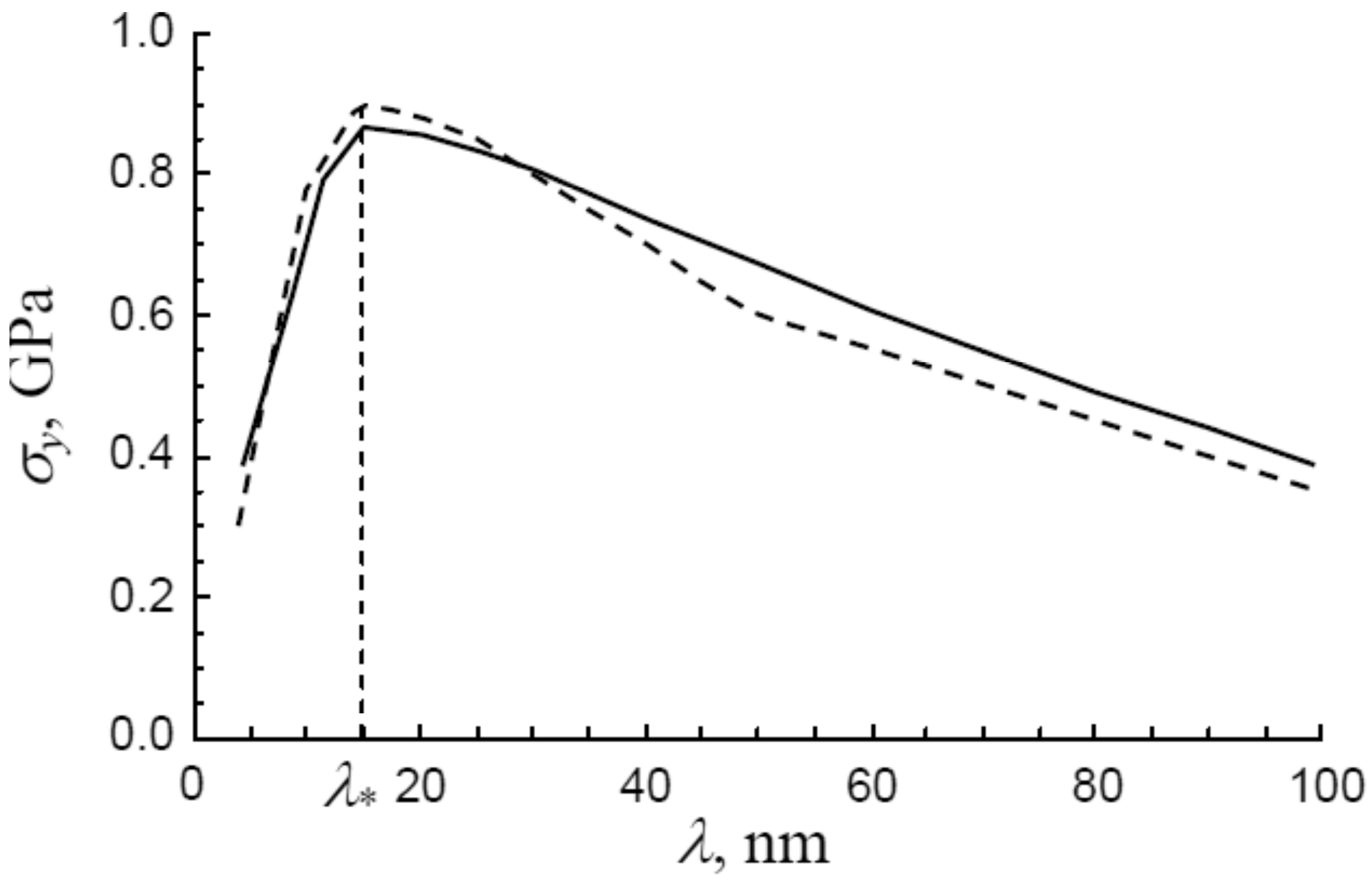

Fig. 2. Dependences of the yield stress σ_y of nanotwinned Cu on twin thickness λ. The solid line shows the calculated dependence while the dashed line depicts the experimental dependence from refs. [1,2].

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

Using formula (6), let us plot the dependence of the yield stress σ_y on twin thickness λ for the case of nanotwinned Cu characterized by the following parameter values: G = 44 GPa, ν = 0.38, a = 0.352 nm [27], σ_0 = 200 MPa and K_{HP} = 1750 MPa [25]. We also put d = 500 nm, α = 0.4, $\kappa = \sqrt{3}/4$, λ_*=15 nm [1,2], $N = 2N'$, $N' = \lfloor d/2\lambda \rfloor$, where $\lfloor X \rfloor$ means an integer part of a rational number X. The calculated dependence $\sigma_y(\lambda)$is shown in Fig. 2 as a solid line. The dashed line in Fig. 2 depicts the experimental dependence of the yield stress on twin thickness obtained in refs. [1,2]. Fig. 2 clearly demonstrates very good agreement between the theoretical and experimental curves, both of which show the transition from softening to hardening (with decreasing twin thickness λ) at λ = 15 nm. In other words, at λ < 15 nm, the yield stress σ_y decreases with decreasing twin thickness λ while at λ > 15 nm it increases with decreasing λ. The dependences in Fig. 2 also confirm that at optimum twin thickness of 15 nm, the yield stress of nanotwinned Cu can be very high, reaching the value of 0.9 GPa.

5. CONCLUSIONS

Thus, in this paper, we have suggested a model that describes the strengthening and softening of nanotwinned metals. Within the model, the principal deformation mechanisms in nanotwinned metals represent twin boundary migration and dislocation motion across the twins. We have calculated the critical stress for the onset of each deformation mechanism, which allowed us to estimate the yield stress of nanotwinned Cu. The results of the calculations demonstrate the existence of the transition from the strengthening to the softening of nanotwinned metals with decreasing twin thickness at a critical twin thickness λ_*, which is observed experimentally (e.g., [1,2,12]). The transition is attributed to a change of the principal deformation mechanism from twin boundary migration (at small twin thicknesses) to dislocation motion across the twins (at large enough twin thicknesses). The calculated twin thickness dependence of the yield stress of nanotwinned Cu agrees well with the corresponding experimental data [1,2] and confirms the existence of an optimum twin thickness (equal, in our case, to 15 nm) at which nanotwinned Cu demonstrates ultrahigh yield strength (around 0.9 GPa). This provides the possibility for the fabrication of superstrong nanotwinned solids by varying their twin thickness.

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