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TWINNING MECHANISM AND YIELD STRESS IN NANOTWINNED MATERIALS

N.V. Skiba[1,2,3] and S.V. Bobylev[1,2,3]

[1]Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg 199178, Russia
[2]Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198504, 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. Nanotwinned materials are ultrafine-grained materials which contain high-density ensembles of nanoscale twins. They exhibit simultaneously high strength and good ductility. A brief review of the theoretical models which describe specific twinning mechanism and dependence of yield stress in nanotwinned materials is presented. In the framework of the model, new micromechanism through nanotwin widening in nanotwinned materials is considered. In addition, dependence of the yield stress on twin thickness in nanotwinned cooper (Cu) is theoretically described. The theoretical results and their comparison with corresponding experimental data in the exemplary case of nanotwinned cooper (Cu) are discussed.

1. INTRODUCTION

Nanostructured materials often exhibit the outstanding physical and mechanical properties such as high strength and hardness. At the same time, practical utility of nanostructured materials is limited by the fact that most of them have disappointingly low ductility and fracture toughness. However, recently, several examples of functional ductility and good toughness have been reported [1-9]. 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 [1-9]. These characteristics of nanotwinned metals are very desirable for practical applications. However, the micromechanisms responsible for the experimentally observed unique combination of high strength and plasticity of nanotwin materials are not fully understood and represents the subject of intensive discussions. 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 due to stress-driven migration of twin boundaries [1,2,10-13]. It is considered that micromechanism for stress-driven migration of twin boundaries in nanotwinned metals is glide of partial dislocations along twin boundaries [1,2,10-13]. This factor should be definitely taken into account in analysis of plastic flow in nanotwinned metals.

Thus, the main aim of this paper is to suggest the theoretical models which describe plastic deformation through widening of nanoscale twins and dependence of the yield stress on nanotwin width in nanotwinned metals with subsequent comparison with the experimental data.

Corresponding author: N.V. Skiba, e-mail: nikolay.skiba@gmail.com

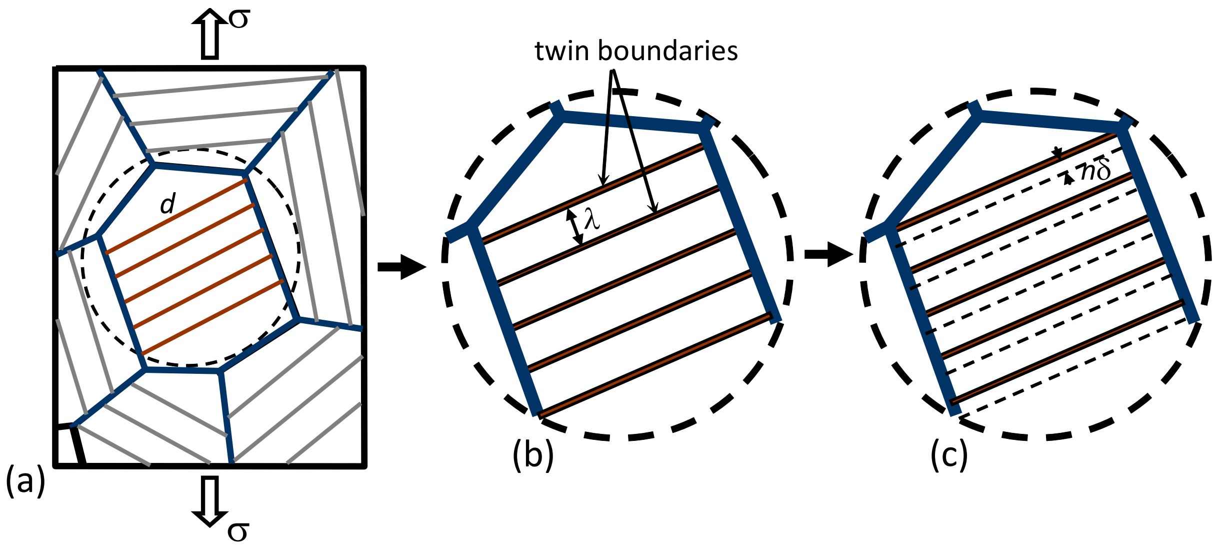

Fig. 1. Model of plastic deformation of ultrafine-grained material due to widening of nanoscale twins. A ultrafine-grained specimen with nanotwinned structure (a general view). (a) The grain contains structure from *N* periodically arranged identical nanotwins. (b) The defect structure after realization of the *n*-th elementary act of twin boundary migration. (c).

2. MICROMECHANISM OF NANOTWIN WIDENING IN NANOTWINNED MATERIALS

Let us consider a two-dimensional model [10-12] of an ultrafine-grained metal sample with periodic nanotwinned structure subjected to external tensile stress s (Fig. 1a). It is assumed that in the grains of nanotwinned material with average dimension d, rectangular nanotwins restricted by coherent twin boundaries are arranged continuously (Fig. 1a). Let us consider an individual grain containing $N+1$ identical nanotwins of the same thickness λ and length d distributed periodically (Fig. 1b). Therefore, these nanotwins are restricted by N twin boundaries, with the same distance λ in between (Fig. 1b). Action of external tensile stress σ causes shearing stress τ along the twin boundaries. The shear stress τ is related to the applied tensile load σ by the relation $\tau = k\times\sigma$, where k is the geometric factor ($0 \leq k \leq 0.5$) determined by the orientation of the Shockley dislocation slip system with respect to the direction of the applied load. It is well known that slip of partial dislocations (for FCC materials – the Shockley dislocations) on the planes parallel to twin boundaries serves as the primary mechanism of migration of twin boundaries. For our model, action of shear stress τ causes the partial dislocations with Burgers vectors **b** (partial b-dislocations) to slip along the planes parallel to the twin boundaries.

Slip of the partial b-dislocations cause moving the twin boundaries in the direction perpendicular to the boundary plane to the distance between adjacent planes parallel to the plane of the twin boundary. Migration of all twin boundaries in the grain is assumed to occur simultaneously. The process of generation and slip of partial b-dislocation can be simulated by formation of a dislocation dipole with Burgers vectors ±**b**. Therefore, the process of simultaneous migration of N twin boundaries can be described by formation of N dipoles of partial ±b-dislocations. As a result, an elementary act of plastic deformation of the nanotwinned sample is represented by simultaneous migration of twin boundaries to the same interplanar distance. The elementary act of twin boundary migration to the distance δ may occur repeatedly. Sequential n acts of plastic deformation result in migration of twin boundaries to the distance $n\delta$ (Fig. 1d).

3. ENERGETIC CHARACTERISTICS OF NANOTWIN WIDENING

Let us consider energetic characteristics of the n-th elementary act of twin boundary migration (Fig. 1d). The n-th elementary act of twin boundary migration is characterized by the energy change $\Delta W_n = W_n - W_{n\text{-}1}$, where $W_{n\text{-}1}$ and W_n are energy of the defect system in the (n-1)-th and n states, respectively. The n-th elementary act of plastic deformation is energetically favorable, if $\Delta W \leq 0$. The energy change W_n can be written as follows [11]:

$$\Delta W_n = E_b + E_{\text{int}\,2} - E_{\text{int}\,1} + E_\tau, \tag{1}$$

where E_b - is the proper energies of N dipoles of Shockley ±b-dislocations; E_{int1} and E_{int2} - are the energy of elastic interaction between all dipoles of Shockley ±b-dislocations in the (n-1)-th and n-th states, respectively, and E_τ - is the work spent by the external shear stress τ on movement of N twin boundaries over the distance δ.

The proper energy E_b is given by the standard expression [10,11]:

$$E_b = NDb^2\left(\ln\frac{d-b}{b}+1\right), \quad (2)$$

where $D = G / 2\pi\times(1-\nu)$, G is shear modulus, ν is Poisson ratio.

The energies E_{int1} and E_{int2} of elastic interaction between all dipoles of ±b-dislocations in (n-1)-th and n-th states are calculated as the total work on generation of each dipole of ±b-dislocations in the summary stress field of all other dipoles, and can be written for the (n-1)-th and n-th states, respectively, as follows [11]:

$$E_n^{b-b} = Db^2\sum_{z=1}^{n}\sum_{j=1}^{k-1}\sum_{i=1}^{n-z+1}\left(\ln\left[1+\frac{d^2}{y_n^2}\right]-\frac{2d^2}{d^2+y_n^2}\right), \quad (3)$$

$$E_{n-1}^{b-b} = Db^2\sum_{z=1}^{n-1}\sum_{j=1}^{n-z}\sum_{i=1}^{k}\left(\ln\left[1+\frac{d^2}{y_{n-1}^2}\right]-\frac{2d^2}{d^2+y_{n-1}^2}\right), \quad (4)$$

where $y_n = \lambda\cdot(i\text{-}1)+\delta\cdot(k\text{-}j)$ and $y_{n\text{-}1} = j\cdot\lambda - \delta\cdot(i\text{-}1)$.

The energy E_τ of elastic interaction with external shear stress τ is given by standard equation [10,11]:

$$E_\tau = -N\tau\delta d. \quad (5)$$

With help of Eqs. (1)-(5), we obtain the expressions for total energy change ΔW_n.

4. THE YIELD STRESS OF NANOTWINNED MATERIALS

The n-th elementary act of plastic deformation becomes possible when the external shear stress τ reaches some critical value τ_{cn}, which can be determined from the condition $\Delta W_n = 0$. Use the value of the critical shear stress τ_{cn} to determine the yield stress σ_y. Let us assume that the yield stress σ_y agrees with the value of critical stress $\tau_{0.02}$ required to reach the plastic deformation $\varepsilon = 0.02$.

Calculate the dependence yield stress σ_y on the distance λ between the twin boundaries in the exemplary case of ultrafine-grained nanotwinned copper (Cu). For material constants, let us select the following values: $G = 44$ GPa, $\nu = 0.3$, $a = 0.352$ nm [14], $\sigma_0 = 200$ MPa, $K_{HP} = 1750$ MP [15]. Parameters of defect structure are taken as: $d = 500$ nm, $\alpha = 0.4$, $\beta = 0.6$ and $\lambda_* = 15$ nm [1,2]. In Fig. 2, the theoretical $\sigma_y(\lambda)$ (the solid line), and experimental (the dashed line, from experimental papers [1,2]) dependencies of the yield stress σ_y on the distance l between the twin boundaries are shown. As is clear from Fig. 2, theoretical dependence $\sigma_y(\lambda)$ of the yield stress on the distance between the twin boundaries is in good agreement with the experimental data.

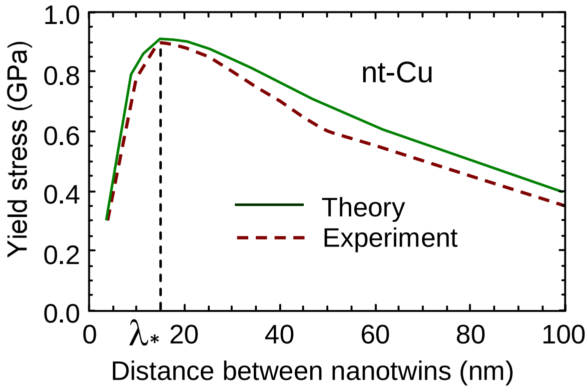

Fig. 2. The dependencies of theoretical (the solid line) and experimental (the dashed line) yield stress on the distance λ between nanotwins in the exemplary case of ultrafine-grained copper (Cu) with nanotwinned structure.

5. CONCLUSION

The theoretical models have been developed describing twinning micromechanism and dependence of the yield stress in ultrafine-grained materials with nanotwinned structure. In the models, plastic deformation occurs due to sequential migration of the twin boundaries and lattice slip within the spaces between the twin boundaries. The critical external stress and plastic deformation degree characterizing each elementary act of twin boundary migration accompanied by lattice slip have been calculated. Theoretical dependence of the yield stress on the distance between the twin boundaries for nanotwinned copper (Cu) has been calculated. Theoretical dependence of the yield stress on the distance between the twin boundaries has been compared with similar experimental dependencies in the exemplary case of ultrafine-grained copper with nanotwinned structure. Theoretical results well agree with the experimental data.

The results of this theoretical investigation can be used in practice to form specific nanotwin structure in ultrafine-grained materials to provide recommendations on optimization of their mechanical properties, which allow for simultaneous combination of high strength and functional plasticity of such materials. In particular, the theoretical model developed allows for determination of the yield stress in nanotwinned materials depending on width of the nanotwins.

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