TWINNING AND DETWINNING MECHANISMS IN NANOTWINNED MATERIALS

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Abstract

The theoretical models are suggested which describe specific plastic deformation mechanisms in nanotwinned materials. Materials containing high-density ensembles of nanoscale twins (nanotwinned materials) exhibit the outstanding mechanical and physical properties - simultaneously high strength and functional ductility at room temperature. These characteristics are achieved due to operating of the specific deformation modes in nanotwinned materials. The theoretical models are suggested which describe specific plastic deformation mechanisms in nanotwinned materials. In the framework of the suggested models, micromechanism of nanotwin widening and micromechanism of combined action of lattice dislocation slip and twin boundary migration in nanotwinned materials are considered. In addition, the detwinning mechanism in ultrafine-grained nanotwinned metals through stress-driven migration of incoherent boundaries of nanoscale twins is examined. It is demonstrated that detwinning of ultrathin twins can occur at very low stresses, while detwinning of thicker twins requires high applied stresses. The theoretical results and their comparison with corresponding experimental data in the exemplary case of nanotwinned cooper (Cu) are discussed.

Keywords: Nanotwinned materials, nanotwins, plastic deformation, twinning, detwinning

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]. It is considered that micromechanism for stress-driven migration of twin boundaries in nanotwinned metals is glide of partial dislocations along twin boundaries. This factor should be definitely taken into account in analysis of plastic flow in nanotwinned metals. Also, recently, using transmission electron microscopy, several research groups observed detwinning of nanotwinned Cu occurring via migration of incoherent twin boundaries (ITBs) under indenter loading [10-12]. In particular, Liu et al. [12] observed migration of an ITB with the length of 5.5 nm in nanotwinned Cu at ultralow indentation stress of 0.1 GPa, well below the stress needed for macroscopic yielding. Wang et al. [10], using molecular dynamics simulations, confirmed that in the case of ultrathin twins with a thickness below 2 nm, ITB migration can proceed at low shear stresses below 0.3 GPa. At the same time, the reasons for easy detwinning of thin twins in nanotwinned Cu are not yet fully understood.

Thus, the main aim of this paper is to suggest the theoretical models which describe plastic deformation through widening of nanoscale twins and detwinning process in nanotwinned metals with subsequent comparison with the experimental data.

2. MODEL OF STRESS-DRIVEN MIGRATION OF TWIN BOUNDARIES

Let us consider a two-dimensional model of an ultrafine-grained metal sample with periodic nanotwinned structure subjected to external tensile stress σ (**Figure 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 (**Figure 1a**). Let us consider an individual grain containing N+1 identical nanotwins of the same thickness λ and length d distributed periodically (**Figure 1b**). Therefore, these nanotwins are restricted by N twin boundaries, with the same distance λ in between (**Figure 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 $\tau = k\cdot\sigma$, 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.

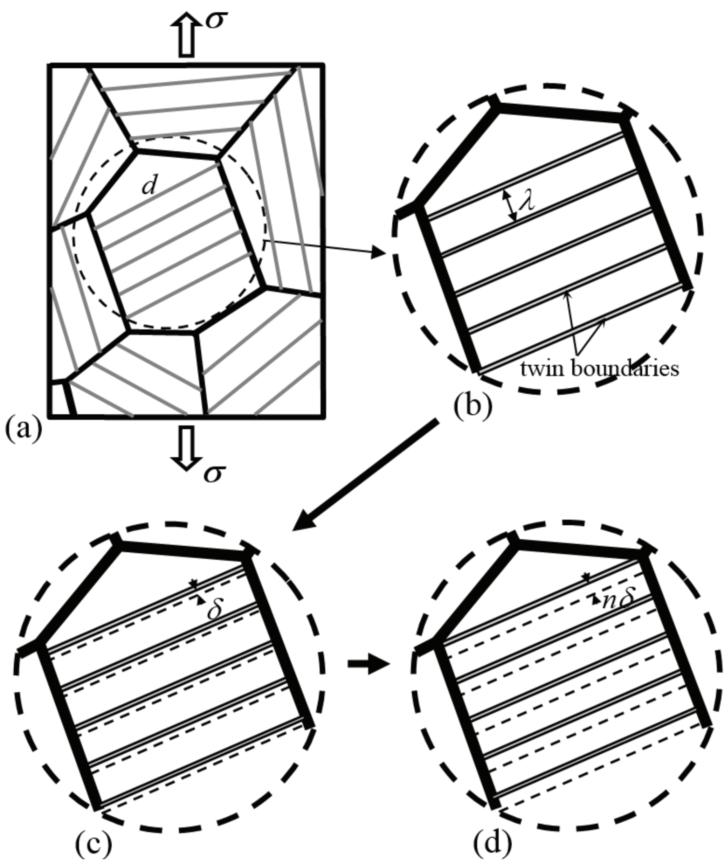

Figure 1 Model of plastic deformation of ultrafine-grained material due to twin boundary migration. A ultrafine-grained specimen with nanotwinned structure (a general view). (a) The grain contains structure from *N* periodically arranged identical nanotwins. (b) The elementary act of twin boundary migration.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

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** (**Figure 1c**). Therefore, the process of simultaneous migration of N twin boundaries can be described by formation of N dipoles of partial ±b-dislocations (**Figure 1c**). 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 (**Figure 1c**). 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·δ (**Figure 1d**).

3. ENERGETIC CHARACTERISTICS OF STRESS-DRIVEN MIGRATION OF TWIN BOUNDARIES

Let us consider energetic characteristics of the n^{th} elementary act of twin boundary migration (**Figure 1d**). The n^{th} elementary act of twin boundary migration is characterized by the energy change $\Delta W_n = W_n - W_{n-1}$, where W_{n-1} and W_n are energy of the defect system in the $(n-1)^{th}$ and n^{th} 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:

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

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:

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

where $D = G / 2\cdot\pi\cdot(1-\nu)$, G is shear modulus, $\nu$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:

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

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

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

The energy E_τ of elastic interaction with external shear stress τ is given by standard equation:

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

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

4. DEPENDENCE OF THE YIELD STRESS ON THE DISTANCE BETWEEN NANOTWINS

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 $\varepsilon = 0.02$.

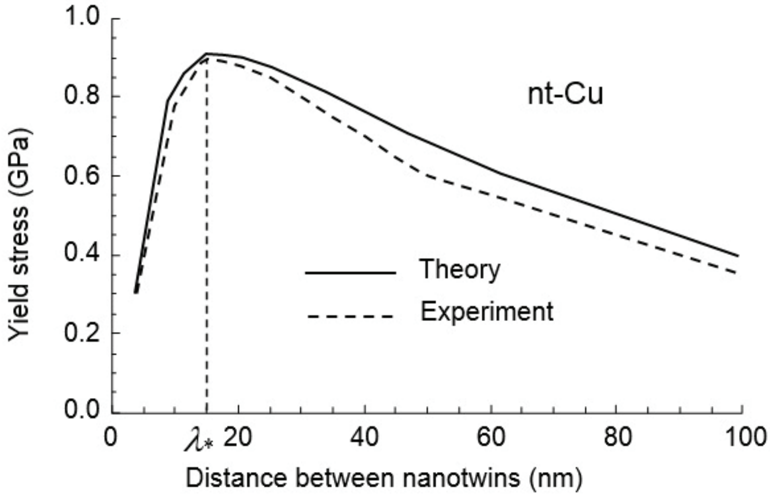

Figure 2 The dependencies of theoretical (the solid line) and experimental (the dashed line) yield stress on the distance λ between nanotwins in the exemplary case of ultrafine-grained copper (Cu) with nanotwinned structure

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 [13], σ_0 = 200 MPa, K_{HP} = 1750 MP [14]. Parameters of defect structure are taken as: d = 500 nm, $\alpha = 0.4$, $\beta = 0.6$ and $\lambda_* = 15$ nm [1,2]. In **Figure 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 λ between the twin boundaries are shown. As is clear from **Figure 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.

5. MECHANISM OF DETWINNING IN NANOTWINNED METALS

Let us consider a model grain in a deformed nanotwinned metal with a face-centered cubic (fcc) lattice (**Figure 3**). Within our model, the grain is composed of growth twins divided by CTBs. We assume that an applied shear stress τ acts in the examined grain as shown in **Figure 3**. In the initial state, the model grain contains a rectangular twin CEFD bounded by grain boundary (GB) segments CD and EF and CTB CE and BF. We consider the situation where an incoherent twin boundary (ITB) AB is generated at the GB segment CD and moves along the CTBs CE and DF (**Figure 3**). In doing so, the motion of the ITB AB is accompanied by the disappearance of the CTB fragments AD and BC, thus leading to the shrinking of the twin AFEB. If the ITB approaches the GB EF, the twin AFEB completely disappears, thus promoting local detwinning in the nanotwinned solid. Now consider the geometry of the formation and motion of the ITB AB. It is known that, in fcc solids, CTBs are located at {111} crystal planes, while ITBs commonly lie in {112} planes. For definiteness, we suppose that CTBs AF and BE occupy (111) crystal planes, while the ITB AB is located at a $(11\bar{2})$ crystal plane. Within our model, the formation and motion of the $(11\bar{2})$ ITB (accompanied by the shrinkage of the CTBs BE and AF) can be realized by the formation and simultaneous motion of the Shockley partial dislocations along all the (111) planes of the twin CEFD [11,12]. Each Shockley partial has the line direction $[\bar{1}10]$ and the Burgers vector $\mathbf{b}_1$, $\mathbf{b}_2$ or $\mathbf{b}_3$, where $\mathbf{b}_1 = (a/6)[11\bar{2}]$, $\mathbf{b}_2 = (a/6)[1\bar{2}1]$ and $\mathbf{b}_3 = (a/6)[\bar{2}11]$ (**Figure 3**), with a being the crystal lattice parameter. The dislocations specified by the Burgers vector $\mathbf{b}_1$ represent edge dislocations, while those with the Burgers vectors $\mathbf{b}_2$ and $\mathbf{b}_3$ are 30° mixed dislocations. The vector sum of the three Burgers vectors $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ is zero, that is, $\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = 0$.

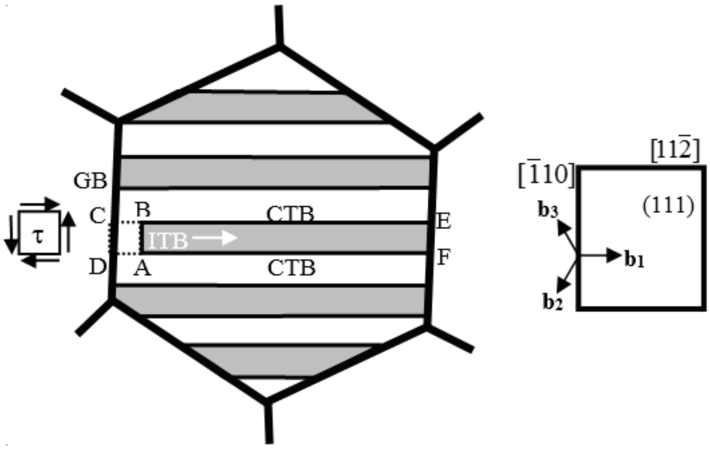

Figure 3 Model grain of a nanotwinned solid under the action of an applied shear stress τ. An incoherent twin boundary (ITB) nucleates at a grain boundary and moves under the action of the applied shear stress along coherent twin boundaries (CTBs)

Define the critical stress τ_c^d as the minimum non-negative stress (for a given twin thickness h) at which detwinning via the formation and migration of an ITB is favored at least for some values of the disclination strength ω. In other words, τ_c^d corresponds to the minimum value of τ' at $h \geq h_c$, and $\tau_c^d = 0$ at $h < h_c$. The dependence of the critical stress τ_c^d on twin thickness h for nanotwinned Cu is presented in **Figure 4**. From **Figure 4** it follows that the critical stress τ_c^d quickly increases with the twin thickness h at $h > h_c$ until h reaches 5-10 nm. After that, τ_c^d only slightly increases with increasing h. Also, **Figure 4** shows that, if the twin thickness lies in the interval 5-25 nm, the critical shear stress is around 0.7-0.8 GPa. These values are higher than the typical values of the resolved shear stress during the uniaxial deformation of nanotwinned Cu, but they can be reached at some regions of nanotwinned Cu due to stress concentration or in the regions near the indenter in the case of indenter loading.

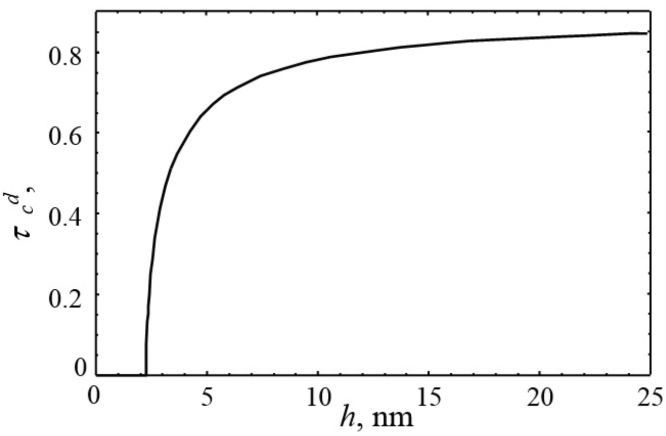

Figure 4 Dependences of the critical shear stress $\tau_c{}^d$ on twin thickness *h* in nanotwinned Cu

6. CONCLUSION

The theoretical models have been developed describing peculiar aspects of plastic deformation of ultrafine-grained materials with nanotwinned structure. In the first model, 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. In parallel with deformation twinning, stress-induced detwinning also occurs in nanocrystalline and ultrafine-grained metals. In particular, in nanotwinned metals detwinning can occur through stress-driven migration of ITBs (**Figure 3**). It was found that the formation and migration of the incoherent boundaries of ultrathin nanotwins (characterized by $h < h_c$, where the critical twin thickness $h_c \approx 2.2$ nm for Cu) is favored even in the situation with the zero net Burgers vector of the ITB. This result is well consistent with the experimental observation [12] of the motion of an ITB containing a dislocation array characterized by a zero net Burgers vector in nanotwinned Cu under indenter loading in the case of twin thickness being around 2 nm.

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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