Materials and Design 45 (2013) 292–299

Contents lists available at SciVerse ScienceDirect

Materials and Design

journal homepage: www.elsevier.com/locate/matdes

The effect of the angle between loading axis and twin boundary on the mechanical behaviors of nanotwinned materials

Shu Zhang [a], Jianqiu Zhou [a,b,*], Lu Wang [a], Ying Wang [a]

[a] Department of Mechanical Engineering, Nanjing University of Technology, Nanjing, Jiangsu 210009, China
[b] Department of Mechanical Engineering, Wuhan Institute of Technology, Wuhan, Hubei 430070, China

ARTICLE INFO

Article history:
Received 6 July 2012
Accepted 31 August 2012
Available online 20 September 2012

Keywords:
Nanotwinned materials
Model
Shear deformation
Mechanical behaviors

ABSTRACT

This paper proposes a computational mechanical model to evaluate the effect of the angle between loading axis and twin boundary (TB) on the deformation behaviors of nanotwinned materials. In this model, the shear deformation across the TBs and the shear deformation parallel to the TBs were considered. The model correctly predicted the experimentally observed tendency of the influence of twin density on flow strength. Besides, the mechanical behaviors of nanotwinned Cu with different angle were studied. However, as twin density increases, the effect of the angle on the stress–strain relations was weakening. This analysis can offer some useful information for optimizing of strength and ductility.

1. Introduction

Nanocrystalline (nc) metals, which have grain sizes smaller than 100 nm, have drawn considerable interest because of their unique mechanical properties [1–5]. They exhibit increased strength/hardness [6–8] and reduced ductility in comparison with their ultrafine crystalline (ufc) and microcrystalline (mc) counterparts, with grain sizes on the order of 100 nm $\sim$ 1 μm and greater than 1 μm, respectively. The strengthening originates from the fact that grain boundaries (GBs) act as barriers to dislocation motion, thereby making plastic deformation more difficult at smaller grain sizes. Lu and co-workers [9–11] have synthesized ultrafine-grained Cu containing controlled concentrations of nanoscale growth twins by the pulsed electrodeposition technique. The nanotwinned Cu also shows the same characteristics of high tensile strength and hardness. These strengthening trends are found to be very similar to those of nc Cu that has experienced grain size refinement when the twin lamellar thickness is comparable to the grain size [12]. However, the reduction in grain size in the nanometer regime leads to a severely compromising tensile ductility of nc Cu, while the nanotwinned Cu possesses desired ductility as a consequence of decreasing twin lamellar thickness [11]. These results suggest that twin boundaries (TBs) are equivalent to conventional GBs in strengthening materials [13,14] but quite different from them in controlling ductility.

Atomistic simulations [15–18] revealed detailed TB-mediated dislocation mechanisms and these studies were central to understanding the influence of TBs on strain hardening and ductility. Work by Froseth et al. [17] focused on the effect of grown-in TBs on the plastic deformation mechanisms in nc Ni and Cu. The results were talked over in terms of the different ratios of the extrema of the generalized planar fault curves. Yamakov et al. [18] analyzed in detail the mechanisms of dislocation-dislocation and dislocation-TB reactions that took place under sufficiently high stress. Moreover, some researchers presented a variety of analytical models to describe the mechanical behaviors of nanotwinned materials. Dao et al. [12] developed a computational mechanical model based on the experimental observations to describe the effects of twin density on flow strength and rate sensitivity of plastic flow. Moreover, they predicted the ductility of nanotwinned Cu via a failure criterion as a function of twin lamellar thickness. Zhu et al. [19] put forward a mechanistic framework that describes the origin of ductility in the nanotwinned samples in terms of the interaction of dislocations with the interfaces. They attributed the relatively high ductility to the gradual loss of coherence of TBs during plastic deformation. The dislocation mechanics analysis performed by Asaro and Kulkarni [20] provided insights into how processes like cross-slip lead to high strength and rate sensitivity in nanotwinned fcc metals.

These models can help us to understand the deformation processes related to nanotwinned materials. However, most attention had been paid on the twin density effect on the properties and microstructure evolutions. Actually, the angle θ between the loading axis and TB also plays an important part for nanotwinned materials on the mechanical behaviors. It is known that the

* Corresponding author at: Department of Mechanical Engineering, Nanjing University of Technology, Nanjing, Jiangsu 210009, China. Tel.: +86 25 83588706; fax: +86 25 83374190.
E-mail address: zhouj@njut.edu.cn (J. Zhou).

0261-3069/$ - see front matter
http://dx.doi.org/10.1016/j.matdes.2012.08.080

submicron-sized grains are subdivided into nano-meter thick twin/matrix lamellar structures by the TBs. Dislocations glide/accumulation in the direction parallel to TBs is different from that in the direction perpendicular to TBs due to the multi-model distributions of length scales, Therefore the strength and ductility of nanotwinned materials will change according to the value of θ. This may offer helpful information for optimizing of strength and ductility, and make it possible for potential industry applications.

The paper is organized as follows: Section 2 provides a description of the model and the deformation mechanisms (shear deformation across the TBs and shear deformation parallel to TBs). Section 3 presents the microstructure in which the value (in degrees) of each θ is given. The effect of θ on the plastic deformation response of nanotwinned Cu is discussed in Section 4. The contour plots of the equivalent plastic strain are also shown at that time to provide quantitative support and insight into the underlying mechanisms. Finally, conclusions are drawn from all these results.

2. Model setup

Only three slip systems are considered within each grain and the slip directions are constrained to be in the plane on account of the two-dimensional characteristic of the model, as shown in Fig. 1. Once nucleated, dislocations glide along the slip system $\langle 1 1 \bar{2}\rangle(1 1 1)$ which runs parallel to the TBs and along the alternating mirrored slip systems $\langle 1 1 2\rangle(1 1 \bar{1})$ and $\langle 5 5 2\rangle(\bar{1}\,\bar{1}\,5)$ which intersect the TB at an angle of 70.53. The length scale parallel to the TBs is several hundreds of nanometers while the length scale perpendicular to the TBs is of the order of tens of nanometers. Apparently, the former is significantly larger than the latter. Therefore, there exists a significant plastic anisotropy: dislocations moving along the TBs experience no barriers until they encounter the GBs, so the shear deformation is effortless; however, dislocations are hindered by the TBs in the other two slip systems. Hence, the shear deformation is relatively harder.

As illustrated in Fig. 2a, the three slip systems are arranged in an isosceles triangle. The reference base vectors i_1 and i_2 of the local coordinates as well as j_1 and j_2 of the global coordinates are aligned as shown. θ is the angle from j_1 to i_1, where j_1 is along the loading

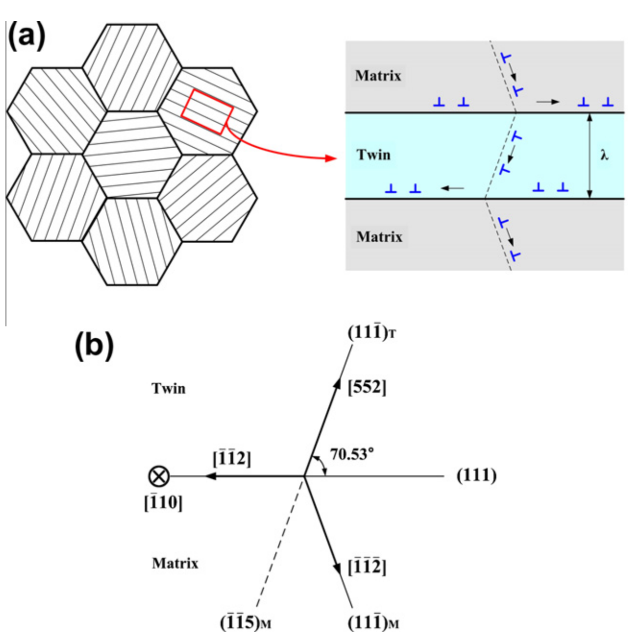

Fig. 1. Model setup (a) illustration of dislocation-TB interaction, and (b) diagram for slip systems.

direction and i_1 is along $[1 1 \bar{2}]$ direction. According to the Schmid law, the resolved shear stress τ_s for sth slip system is defined as

$$\tau_s = m_s \cdot \sigma \tag{1}$$

where σ is the applied stress, m_s is the Schmid factor given by

$$m_s = \cos\phi^{(s)} \cdot \cos\lambda^{(s)} \tag{2}$$

Here, $\phi^{(s)}$ is the angle between the slip plane normal and the loading axis, $\lambda^{(s)}$ is the angle between the slip direction and the loading axis.

During plastic deformation, the displacement of a point in crystal is the sum of the displacements caused by all three slip systems at the point and it can be written as follows:

$$\boldsymbol{u} = \sum\nolimits_{s=1}^{3} \boldsymbol{u}_s = u_1\boldsymbol{i}_1 + u_2\boldsymbol{i}_2 \tag{3}$$

where $\boldsymbol{i}_1$, $\boldsymbol{i}_2$ are the reference base vectors of the local coordinates, u_1, u_2 are the shadows that $\boldsymbol{u}$ casts on the local coordinates, respectively. u_s is the displacement on the sth slip system, as shown in Fig. 2b, which can be expressed as

$$\boldsymbol{u}_s = \gamma^{(s)}(\boldsymbol{R}\boldsymbol{n}^{(s)})\boldsymbol{b}^{(s)} \tag{4}$$

where $\boldsymbol{R}$ is the radius vector of X which is a casual point, $\gamma^{(s)}$ is the shear strain on the sth slip system which is defined by orthogonal pair of unit vectors $(\boldsymbol{b}^{(s)}, \boldsymbol{n}^{(s)})$. $\boldsymbol{b}^{(s)}$ is along the sth slip direction and $\boldsymbol{n}^{(s)}$ is normal to the sth slip plane.

Therefore, the strain tensor can be obtained by Eqs. (3) and (4):

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)(i, j = 1, 2) \tag{5}$$

Further more, the equivalent strain ε_e can be expressed as

$$\varepsilon_e = \frac{\sqrt{2}}{3}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + \varepsilon_1^2 + \varepsilon_2^2 + 6\varepsilon_{12}^2} \tag{6}$$

2.1. Shear deformation across the TBs

A constitutive model related to dislocation density is used to describe the constitutive behavior across the TBs. During the deformation process, the evolution of the dislocation density ρ_s takes into account the athermal storage of dislocations ρ_s^+ as well as the annihilation of dislocations ρ_s^-

$$\rho_s = \rho_s^+(\gamma) + \rho_s^-(\gamma) \tag{7}$$

where γ is the plastic strain. Capolungo et al. [21] put forward a model accounting for the athermal storage of dislocations based on the statistical approach proposed by Kocks and Mecking [22]. The relationship between $d\rho_s^+$ and $d\gamma$ can be obtained by

$$\frac{d\rho_s^+}{d\gamma} = \frac{M}{b}\left(\frac{1}{\lambda_T} + \xi\sqrt{\rho_s}\right) \tag{8}$$

where M, b, λ_T and ξ are the Taylor factor, Burger vector, twin lamellae thickness and proportionality factor, respectively. The dynamic recovery process controlled by the annihilation of stored dislocations is expressed by

$$\frac{d\rho_s^-}{dot\gamma} = -C_{20}\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{-1/m} \cdot \rho_s \tag{9}$$

Here, C_{20} is a constant as well as $\dot{\gamma}_0$, m is inversely proportional to the temperature T. Combining Eqs. (8) and (9), the evolution of dislocation density with the increasing of $\dot{\gamma}$ can be written as follows:

$$\frac{d\rho_s}{d\gamma} = \frac{d\rho_s^+}{d\gamma} + \frac{d\rho_s^-}{d\gamma} = \frac{M}{b}\left(\frac{1}{\lambda_T} + \xi\sqrt{\rho_s}\right) - C_{20}\left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^{-1/m} \cdot \rho_s \tag{10}$$