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Repulsive force of twin boundary on curved dislocations and its role on the yielding of twinned nanowires

Chuang Deng[a,b] and Frederic Sansoz[a,*]

[a]School of Engineering and Materials Science Program, The University of Vermont, Burlington, VT 05405, USA
[b]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

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The effects of twin size and sample diameter on yield stress and surface dislocation emission in twinned metal nanowires deformed uniformly were studied using classical dislocation theory and the concept of image force from twin boundaries. This theoretical study is shown to quantitatively capture the linear increase in yield stress as twin size decreases in periodically twinned Au nanowires predicted by atomistic simulations. The implication of this model as a yield criterion for realistic metal nanostructures with nanoscale growth twins is discussed.

Keywords: Nanowires; Twin grain boundary; Yield phenomena; Size effects; Dislocation theory

Predicting the yielding behavior of face-centered cubic (fcc) metal nanowires (NWs) is essential to determining the mechanical integrity of nanoscale devices. Both geometric and microstructure effects strongly influence the yield stress of fcc metal NWs under deformation [1–5]. Past experimental and theoretical studies have suggested that the process of dislocation emission from free surfaces plays a key role in size effects in nanoscale plasticity [6–9], which is fundamentally different from yielding mechanisms commonly observed in bulk metals. Equally important for the yield of metal NWs are nanoscale twins, which naturally form during synthesis [10–12], and can significantly increase the elastic limit of fcc metal nanowires in experiments [2,12]. Using molecular dynamics (MD) simulations, it has been found that coherent twin boundaries (CTBs) can act either to increase or decrease the stress required to nucleate new surface dislocations in comparison to that in twin-free NWs of corresponding diameter [13–20]. In an earlier work, we have also predicted by MD simulation that the critical resolved shear stress (CRSS) for the emission of surface dislocations in periodically twinned Au NWs, similar to that shown in Figure 1a, increases linearly with the number of CTBs per unit length [19]. In particular, such linear dependence on twin size was found more pronounced when the wire diameter decreases as shown in Figure 1b. It is therefore critically important to gain predictive understanding of the synergy between twin size and sample diameter on yield stress in twinned NWs for applications.

In this paper, using linear elastic theory, we examine the image force on a planar curved dislocation due to CTBs. We show that this model enables quantitative prediction of size effects on elastic limit in circular NWs with periodic distribution of CTBs for different values of diameter (D) and twin boundary spacing (TBS). We also discuss the implication of this image force-based model for the yield behavior of more realistic twinned nanostructures.

Chen et al. [21] have proposed an analytical model based on linear elasticity theory for the interaction of a straight screw dislocation of infinite length with a CTB in Al and Cu metals, in terms of image dislocations. In this model, the interaction is characterized by a repulsive force between the dislocation and its virtual image of negative Burgers vector with respect to the CTB given by

$$f_{CTB} = -\lambda \frac{\mu b^2}{4\pi x}, \qquad (1)$$

where f_{CTB} is the force per unit length exerted by the CTB on the screw dislocation ($f_{CTB} < 0$), x is the distance between dislocation and CTB, μ is the shear modulus in the slip direction of the crystal, b is the magnitude of the Burgers vector, and λ is a dimensionless

* Corresponding author. E-mail: frederic.sansoz@uvm.edu

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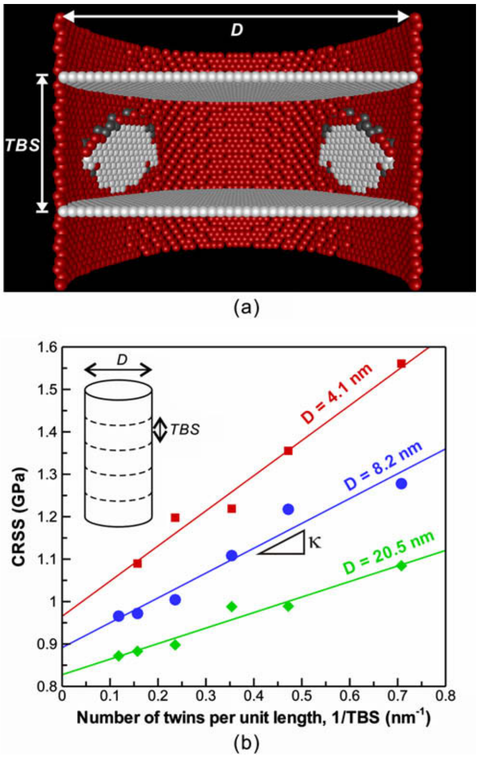

Figure 1. Molecular dynamics simulations of yielding in periodically twinned [1 1 1]-oriented Au nanowires under tensile strain. (a) Snapshot of surface dislocation emission at the junction of twin boundaries and the free surface. Atoms in white are stacking faults from twins and partial dislocations. Other non-coordinated atoms appear in red and gray. *D* and *TBS* are 12.3 and 4.2 nm, respectively. (b) Linear dependence of critical resolved shear stress (*CRSS*) on number of twin boundaries per unit length $1/TBS$ for different diameters. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

measure of the intrinsic strength of the CTB corresponding to the elasticity mismatch between parent and twin grains in terms of shear modulus [21]. Eq. (1), however, cannot be directly used to model the interaction force between CTBs and general dislocations of arbitrary shape, which exist in realistic NWs. For example, Figure 1a shows that the yielding of twinned cylindrical NWs of Au deformed in tension with $D = 12.3$ nm and $TBS = 4.2$ nm proceeds via the nucleation of curved {1 1 1}<1 1 2> Shockley dislocations at specific sites where CTBs intersect the free surface.

A representative model of surface dislocation emission on a $\{11\bar{1}\}$ slip plane inside a twinned NW with circular cross-section is presented in Figure 2. A snapshot of the slip nucleus at the free surface obtained from atomistic simulation and its schematic illustration are shown in Figure 2a and b, respectively. These figures clearly show that the slip plane is elliptical and intersected by several CTBs separated by the same distance L_b (here $L_b = TBS/\sin\theta$ with θ the angle between the glide plane and the CTBs). It is important to note that the dislocation nucleation site is also positioned at a distance L_b from the closest CTB (Fig. 2a), because dislocation emission always occurs at the intersection between CTB and free surface [19]. In the following, we assume that the predominant interaction force acting on the slip nucleus is manifested by the closest CTB (CTB1 in Fig. 2b) and therefore other CTB–slip interactions are neglected.

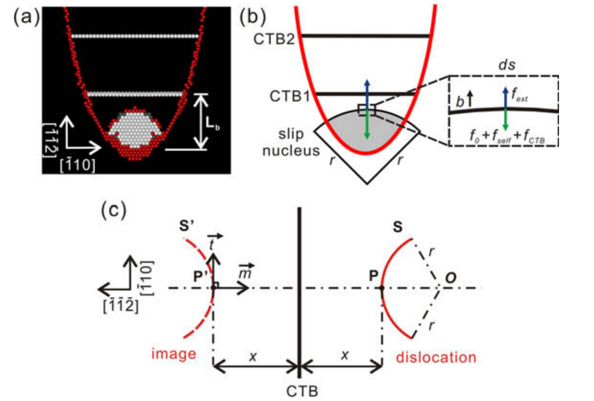

Figure 2. Model of nucleation of a curved (partial) dislocation on a $\{11\bar{1}\}$ slip plane inside a twinned NW with circular cross-section. (a) Top view of dislocation on its elliptical glide plane from atomistic simulation and (b) its schematic illustration. The inset in (b) represents the balance of forces acting on the dislocation segment of Burgers vector $\vec{b}$, radius r and length ds. (c) Schematic of the curved dislocation (S) and its mirror image (S') across a coherent twin boundary (CTB).

First, let us rewrite Eq. (1) by considering the stress field of an image screw dislocation of infinite length (τ_{img}) located at a distance $2x$ away from the dislocation line ($x > 0$), such that

$$f_{CTB} = -\lambda \cdot \tau_{img} \cdot b, \tag{2}$$

with

$$\tau_{img} = \frac{\mu b}{2\pi} \cdot \frac{1}{2x}. \tag{3}$$

Eq. (3) shows that the stress field τ_{img} decreases as the distance away from the image dislocation increases. Also, any points on the image dislocation line ($x = 0$) should have a stress equal to zero due to symmetry. Therefore, it is more convenient to rewrite Eq. (3) as follows:

$$\tau_{img} = \tau(\varepsilon)\frac{\varepsilon}{2x}\Big|_{\varepsilon\to 0}, \tag{4}$$

with

$$\tau(\varepsilon) = \frac{\mu b}{2\pi} \cdot \frac{1}{\varepsilon}. \tag{5}$$

According to Eq. (4), the stress field τ_{img} monotonically decreases from a maximum value $\tau(\varepsilon)$ as the distance $2x$ away from the dislocation line increases (see Fig. S1 provided as Supplementary data). Here $\tau(\varepsilon)$ can be interpreted as the maximum stress at a distance $\varepsilon \sim 0$ close to the core of the image dislocation.

Likewise, we propose that the interaction force between a curved dislocation and a CTB can be calculated by considering the stress field of a curved image dislocation in the twin grain on the other side of the CTB. For that purpose, Figure 2c schematically represents a circular dislocation S of radius r and its mirror image S' with respect to the CTB. Similar to Eq. (4), the stress at point $\boldsymbol{P}$ on dislocation S due to its image S' can be expressed as

$$\tau_{img}(P) = \tau_{S'}(\varepsilon)\frac{\varepsilon}{2x}\Big|_{\varepsilon\to 0}, \tag{6}$$