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Stochastic behaviors in plastic deformation of face-centered cubic micropillars governed by surface nucleation and truncated source operation

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ABSTRACT

Three dimensional dislocation dynamics (***DD***) simulations are performed to investigate the governing mechanism of size dependent plastic deformation in submicron face-centered cubic (***fcc***) micropillars under uniaxial loading. Based on previous atomistic simulations, we introduce an algorithm for dislocation nucleation at the free surface as a function of stress and temperature in the ***DD*** simulation. The simulation results show stochastic behaviors in agreement with experimental observations, and reveal that dislocation nucleation at the free surface is the dominant mechanism of plastic flow in small pillars with diameters less than 200 nm, while the operation of truncated dislocation sources is the governing mechanism in large pillars with diameters exceeding 1 μm. In between, both mechanisms come into play in a stochastic way.

1. Introduction

With the advent of micro-scale devices for engineering applications, mechanical properties of materials at small scales have attracted progressively more attention. Since it is now known that many mechanical properties at the sub-micron scale differ from those at the bulk scale, a fundamental understanding of such size dependence is required for further development.

Recent micromechanical experiments have revealed that the flow stress (τ) of metallic micropillars correlates with the pillar diameter ($\boldsymbol{d}$), with a scaling law of $\tau \propto \boldsymbol{d}^{-0.5}$ to $\boldsymbol{d}^{-1.0}$ for a wide variety of face centered cubic (***fcc***) metals, even in the absence of strain gradients [1–7]. The reader is referred to the literature [8–10] for recent reviews on size effects in small structures. Among proposed models for these 'smaller is stronger' phenomena in metals, commonly accepted explanations include the dislocation starvation (***DS***) model [11,12] and the single arm source (***SAS***) model [13–18]. According to the ***DS*** model, smaller samples contain fewer dislocation sources making it easier for dislocations to escape, so that higher stresses are required to generate new dislocations for sustained plastic deformation. In the ***SAS*** model, the lengths of the truncated sources are shorter in smaller samples, so that higher stresses are required to operate them. Recent *in situ* ***TEM*** observations provided support for both dislocation source exhaustion [19] and truncated source operation [20], and showed that both mechanisms could contribute to higher strengths in smaller volumes simultaneously rather than exclusively [21]. In both models, dislocation sources play a critical role in controlling the deformation behavior.

To achieve a better understanding of size dependent plasticity at the sub-micron scale, it is necessary to explore the details of dislocation behavior in small crystals. For this task, dislocation dynamics (***DD***) simulation provides a unique opportunity both to study the motion of individual dislocations, and to understand the mechanical behavior of materials in terms of the collective behavior of dislocations [17,22–29]. Fertig and Baker summarized the main features of widely used ***DD*** codes in their recent review [30]. Using ***DD*** simulations, Tang et al. showed that mobile dislocations in smaller micropillars could escape more quickly than in larger ones, so that the flow stress increases due to fewer sources [31,32], thus providing a strong support for the ***DS*** model. On the other hand, it has also been shown that activation of truncated sources can successfully explain the size dependent flow behavior in both ***fcc*** and ***bcc*** crystals [18,20,33]. To model realistic situations, it is necessary to account for both internal sources from dislocation

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interaction and those in the vicinity of the free surface where dislocation nucleation is expected to occur. It is necessary to account for dislocation sources at the free surfaces especially in submicron crystals where the surface-to-volume ratio is very high. To our knowledge, most existing ***DD*** models consider only the internal sources while ignoring those associated with dislocation nucleation at the surface, and tend to underestimate the role of surface nucleation [14,25,29,33,34].

With regard to external dislocation sources, the dislocation nucleation rate, a fundamental quantity of interest, has been calculated by continuum [35,36] and atomistic models [37–41]. However, these approaches both have limitations. Continuum models are usually based on the linear elastic constitutive relation, which may not be valid under the high strain and nonlinear conditions of dislocation nucleation. On the other hand, direct molecular dynamics (***MD***) simulations are limited to exceedingly high strain rates. To overcome these limitations, a recent approach is to combine reaction rate theories with atomistic models, wherein atomistic simulations are used to compute the activation barrier which then serves as an input parameter for the reaction rate theory to predict the dislocation nucleation rate [42,43].

In this paper, we investigate the plastic flow behavior of single-crystal copper specimens under uniaxial loading using a dislocation dynamic model. In particular, attention will be given to the ***fcc*** metals in which perfect dislocations have a dominant role in the process of plastic deformation. We develop an algorithm within the ***DD*** framework to account for dislocation nucleation at the free surfaces, based on both atomistic modeling and reaction rate theory. Using this model, we explore its application to the plastic flow behavior of ***fcc*** metal micropillars under uniaxial loading. Our ***DD*** simulation results, when compared to both experiments [21,44,45] and theoretical models [13,46] on micropillar deformation, show that exhaustion hardening and truncated source operation can play significant roles simultaneously .

2. Simulation methods

2.1. Three dimensional dislocation dynamics in a cylinder

Dislocation dynamics simulations were performed using a modified version of ***ParaDiS*** (***Para****llel* ***Di****slocation* ***S****imulator*), a ***DD*** code originally developed at the Lawrence Livermore National Laboratory [22]. In ***ParaDiS***, arbitrarily curved dislocations are discretized to a series of straight dislocation segments connected by nodes. To keep track of dislocation motion, we computed the force on each node based on the *Peach–Koehler* (***PK***) formula. The local stress is determined from contributions from the applied loading, interactions with other dislocations, and corrections due to the existence of free surfaces. Once the force has been evaluated at each node, the dislocation velocity is computed using a mobility function [47]. In this work, we consider the over-damped regime in which the velocity of each dislocation is linearly proportional to the nodal force, subjected to glide plane constraints. Finally, dislocation movements are computed and updated with the consideration of topological changes and remesh requirements [22].

In order to model a micropillar compression experiment, the effect of the free surface on the stress field needs to be taken into account. To this end, various methods have been proposed to satisfy the traction-free boundary condition on the free surface [34,48,49]. In this work, we consider the effect of the image stress using the *Yoffe* correction field of semi-infinite segments for computational efficiency, which has been shown to be a good approximation, especially for segments intersecting the surface [50,51]. To check the validity of this approach, we compared a ***DD*** result using the *Yoffe* solution with the one using the spectral method [48], and did not observe a significant qualitative difference. Using a surface nucleation algorithm to be described in the next section in detail, a series of ***DD*** simulations of uniaxial tension were performed on ***Cu*** single crystal micropillars with diameters ranging from 150 nm to 1000 nm. For all the samples, the ratio of height to diameter is fixed at 5. The material properties and controlling parameters are listed in Table 1.

Table 1
Material properties and operating parameters.

Material and parameters	Dimension	Value
Shear modulus	[GPa]	48
Poisson ratio		0.34
Edge mobility	[Pa^{-1} s^{-1}]	10^5
Screw mobility	[Pa^{-1} s^{-1}]	10^5
Burgers vector length (b)	[m]	2.556×10^{-10}
Temperature	[K]	300
Attempt frequency (ν_0)	[s^{-1}]	1×10^{13}
Mean value of SCF ($\bar{\alpha}$)		1.0
Standard deviation (β) in SCF		1.0
Friction stress in Cu [61]	[MPa]	34.6

2.2. Dislocation nucleation at the free surface

At the small scale of interest here, all possible dislocation sources need to be taken into account. Most existing ***DD*** models focus only on internal dislocation sources which mainly result from dislocation–dislocation interactions, cross-slip or artificial pinning points [29,52]. However, artificially created pinning points are not physically realistic and cross-slip does not occur easily in metals with low stacking fault energy. Internal dislocation sources from the interaction of dislocations can be naturally formed within the ***DD*** framework, while external sources due to dislocation nucleation at the free surface have not been carefully considered yet. Here, we develop a simple algorithm to implement surface nucleation in the ***ParaDiS*** cylinder code.

To accommodate dislocation sources associated with surface nucleation within the ***DD*** framework, we have adopted the nucleation rate from atomistic models [42,43], usually expressed as a function of stress and temperature. The computed dislocation nucleation rate (ν) is expressed as

$$\nu = \nu_0 \exp\left(-\frac{Q(\sigma,T)}{k_B T}\right), \tag{1}$$

where ν_0, k_BT are the attempt frequency, the thermal energy, respectively, and Q is the activation free energy which is obtained from the previous study for dislocation nucleation from a ***Cu*** nanorod [42,43]. Even though the nanorod considered in the atomistic model has a square cross section, which is different from the circular cross section considered here, the tabulated $Q(\sigma,T)$ function in [42] is used here given the various approximations already invoked in the present model. Furthermore, the previous work [42] considered nucleation of *Shockley* partial dislocations, while here we consider perfect dislocations, under the assumption that the trailing partial will quickly follow once the leading partial is nucleated. In this work, we focus on plastic flow at room temperature only, while noting that other temperatures could be treated in the same way. At given nucleation rate, we implement the surface dislocation nucleation in ***DD*** by adopting an algorithm commonly used in the kinetic *Monte Carlo* method [53], which can provide a simple yet powerful tool to obtain information about the statistical behavior of kinetics in many physical phenomena. To mimic the surface roughness, N possible nucleation sites on the surface are randomly distributed on the surface with different stress concentration factors (***SCF***s), which follow a normal distribution with a mean of $\bar{\alpha}$, and a standard deviation of β. These values were chosen to fit the experimental values, as listed in Table 1. At a given stress and