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Strain rate effects on the plastic flow in submicron copper pillars: Considering the influence of sample size and dislocation nucleation

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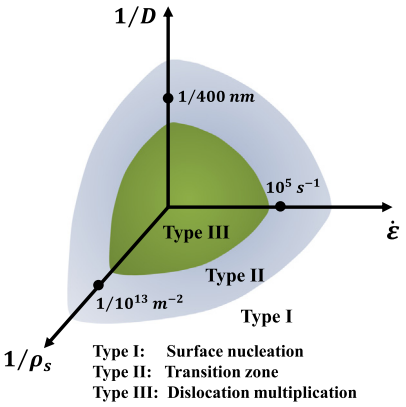
GRAPHICAL ABSTRACT



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ABSTRACT

Three-dimensional discrete dislocation dynamics (DDD) simulations are performed to investigate the plastic flow behaviors of submicron copper pillars under different loading rates, in which both inertial effect of dislocation motion and surface nucleation are taken into account. It is found that: (1) for pillars with a diameter below ~400 nm, there is a transition from internal dislocation multiplication to surface dislocation nucleation as the strain rate increases ($\geq 10^4$ s^{-1}); (2) for ~1 um diameter pillars, stable internal dislocation sources dominate for both low and high strain rates; (3) in general, a larger strain rate, smaller sample size and less internal dislocation sources make it more probable for a surface nucleation process to take the place of dislocation multiplication. Furthermore, a theoretical model is proposed to predict the submicron plastic behavior at different strain rates when internal dislocation sources prevail.

1. Introduction

It is well known that various aspects of mechanical behavior at submicron scales are quite different from those at the bulk scale. In addition to the widely known plasticity size effect [1–3], strain rate sensitivity at submicron scale has attracted much attention [4–6].

Recently, Jennings et al. [7] demonstrated strain rate effect emerging in the single crystalline copper pillars at submicron scales by experiments. By computing the activation volumes, as a function of pillar diameter at each strain rate, they postulated a plasticity mechanism transition from dislocation multiplication via the operation of single-arm sources to surface dislocation nucleation when the pillar size became smaller. The effects of both strain rate and sample size on the compressive strength of single crystalline copper were reported in their work while the quantitative investigations of dislocation sources and structures were quite

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limited. Lately, Gurrutxaga-Lerma et al. [8] investigated the dominant dislocation mechanism at different strain rates ranging from 10^1 s^{-1} to 10^{10} s^{-1} and illustrated the strain rate effect on both the activation time and the source strength of Frank–Read sources. They discussed Frank–Read sources and homogeneous nucleation processes which are essential in bulk deformation. However, in submicron and nano-sized samples, dislocation nucleation from the free surface has been observed to be a potent mechanism, e.g. [7,9].

Discrete dislocation dynamics (DDD) simulations have been reported in the literature that provide important insights into the mechanical behavior under different strain rates. They served as an effective method to study the dislocation based plasticity under low strain rates [10], high strain rates [11–14] and extremely high strain rates as shock compression [15–17]. The calculation procedure always follows the same general form. The forces acting on all the dislocation segments are evaluated at each time step, dislocation velocities are calculated by solving the equations of motion, and dislocation positions are updated for the next time step. In most applications of the DDD simulations, the equation of dislocation motion involves a linear force–velocity law, instead of the full dynamical formula which includes inertia. This assumption seems sufficient to describe dislocation motion at low deformation rates, but may be not appropriate in high strain rate deformation. Wang et al. [18] employed a full dynamical equation of dislocation motion to compare with the commonly assumed linear force–velocity dynamics. Through comparison and analysis, they indicated the inertial effect could not be ignored when the strain rate was 10^4 s^{-1} and larger.

In this paper, the plastic flow behavior of single crystalline copper pillars is investigated by 3D DDD simulations. We concentrate on the combined effect of sample size, strain rate and surface versus internal sources of dislocations on the mechanical behavior at submicron scales.

2. Methodology

The 3D DDD method used here has been described in detail in our previous paper [19]. Compared to the conventional DDD model, two new features are introduced. A full dynamical equation of dislocation motion including inertial effect is adopted and surface nucleation process is introduced.

The full dynamical equation of dislocation motion is

$$m_e \dot{v} + Bv = f, \tag{1}$$

where m_e is the effective mass of dislocation per unit length, $m_e = \rho_c b^2$, ρ_c is the material density and b is the magnitude of the Burgers vector. B is the viscous drag coefficient, f is the total Peach–Koehler force of the applied stress and interaction with other defects, line tension, as well as the image force by the free surface.

The introduction of dislocation sources associated with surface nucleation in the DDD computations is motivated by the atomistic model of Zhu et al. [20]. Their results suggest the free surface acts as an effective source of dislocations and the nucleation stress provides an upper bound to the strength of compressive nanopillars. Their probabilistic investigations revealed that the probability of dislocation nucleation from the free surface within a time span dt is given by

$$P = \nu_0 \exp\left[-\frac{Q(\sigma, T)}{k_B T}\right] \times \left(\frac{S}{b^2}\right) \times \mathrm{d}t. \tag{2}$$

Here, ν_0 is the attempt frequency, $Q(\sigma, T)$ is the activation free energy of dislocation nucleation from the free surface and $k_B T$ is the thermal energy, $\frac{S}{b^2}$ is the number of nucleation sites at the surface. In the DDD simulations, we expand the possible nucleation sites from sample corner to the whole surface, dislocation can nucleate at any point on the surface of the pillar and the stress $\sigma = |\sigma_{33}|$ is used in the simulations of compression test. A first approximation of the temperature effect on the activation free energy is introduced as

$$Q(\sigma, T) = \left(1 - \frac{T}{T_m}\right) \cdot Q_0(\sigma), \tag{3}$$

where T_m is the surface disordering temperature and is chosen to be 700 K. By taking the function form $Q_0(\sigma) = A(1 - \sigma/\sigma_{ath})^{\alpha}$ to fit the calculated activation energies at different stresses, $A = 4.8$ eV, $\sigma_{ath} = 5.2$ GPa, and $\alpha = 4.1$ are obtained [20]. The probability of surface nucleation is calculated at each time span. The number of nucleated dislocations N is as follows

$$N = \begin{cases} \text{Integer}[P], & \text{if } \int_{t_m}^{t_n} P \geq 1 \\ 0, & \text{if } \int_{t_m}^{t_n} P < 1. \end{cases} \tag{4}$$

Here, the probability of dislocation nucleation is accumulated from t_m to t_n because that once a dislocation nucleation process occurs, the probability starts from zero again, and an arc-shaped dislocation loop on a random slip system of all the twelve typical FCC is introduced at a stochastic site on the surface.

In the simulations, the cross sections of single crystalline copper pillars are set to be square. Side lengths are varied from 200 to 800 nm while the ratio of pillar height H to side length D is fixed to 2. These cuboid cells are used to mimic the cylindrical specimens used in the experiment [21], because it is easier to deal with the image force and it is known that the cross-section shape has only a weak effect [22]. All the pillars are loaded along $(00\bar{1})$ direction in a displacement-controlled manner and the lateral surfaces are traction free. A wide range of strain rates are performed in DDD simulation, ranging from 10^4 s^{-1} to 10^6 s^{-1}. The initial dislocation densities are around 4×10^{13} m^{-2}. The simulation for each pillar size is carried out for five different initial dislocation distributions to illustrate the stochastic scatter. The material properties of copper are as follows: shear modulus μ is 48 GPa, Poisson's ratio ν is 0.34, the density of Cu $\rho_c = 8.96 \times 10^3$ kg/m^3, and the viscous drag coefficient $B = 2 \times 10^{-5}$ Pa s. The attempt frequency ν_0 in Eq. (2) is set at 10^{13} s^{-1} [23] and the temperature $T = 300$ K. The time step used in the simulations is $\triangle t = 10^{-12}$ s which ensures that the numerical results are converged.

3. Results and discussions

The simulation results of pillars with different side lengths are shown in Fig. 1(a). The stress–strain curves exhibit three typical characteristics. For type I which is generally observed in small pillars ($D < 400$ nm), as marked in Fig. 1(a), the stress increases in an elastic way at the initial stage, then early yield events that are of short duration occur at various stress levels (varying between ~500 and ~1200 MPa), followed by an extensive elastic period, after which massive yield takes place at a stress level of around 1600 MPa. Despite the small oscillation, the flow stress is approximately stable in the end. Distinct from this, in type III plasticity, yield is massive right away and the stress remains roughly stable without obvious strain hardening. As a result, the flow stress is relatively low comparing with that in type I. Type II falls in between type I and III, it seems the stress remains stable after the initial yielding, but strain hardening can start at an unexpected time.

The evolution of representative dislocation structures corresponding to type I and III is shown in Fig. 1(b). For pillars as small as 200 nm, it is difficult for dislocations to form stable pinning points, and the initial dislocations will be driven out quickly by the subsequent external loading. After that, new dislocations emerge