DISCRETE DISLOCATION ANALYSES OF SIZE EFFECTS IN PLASTICITY

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Summary We analyze plasticity size effects by means of computational discrete dislocation dynamics. Using an enhanced method capable of simulating hardening and millions of interacting dislocations, we explore behavior transitions under compression in the space of meaningful structural parameters. We also analyze the response in pure bending and the contribution of GNDs to dissipation versus energy storage as the size of the bent crystals approaches the micron.

INTRODUCTION

Continuum modeling of plasticity requires constitutive statements on hardening and energy partitioning between stored and dissipated [1]. In particular, when continuum concepts are extended to the micron scale the role of geometrically necessary dislocations (GNDs) in dissipation and energy storage is debated [2, 3], often based on beliefs. Among other tacit assumptions of continuum plasticity, including strain-gradient plasticity, two are worth mentioning. First, theories assume that sources of plasticity are available: upon attainment of a stress-based "yield" criterion, plastic flow sets in. Such an assumption misses a physical length scale related to dislocation source size or spacing. Second, theories assume that plastic flow occurs at random in the elementary volume: the emergence of a substructure under macroscopically homogeneous deformation is impossible to model beyond its effect on, say hardening via a set of internal variables. This misses a spectrum of evolving length scales, e.g., the cell size. To investigate plastic behavior when deviations from the above assmuptions take place, we employ an enhanced version of a discrete dislocation dynamics simulation method [4]. The method also enables calculations of the stored energy in geometrically similar crystals subject to bending.

FORMULATION

Crystals having dimensions $L \times D$ are potentially oriented for double slip and loaded in compression or bending. Initial dislocation sources are randomly distributed with fixed density ρ_0. To maintain a near-zero net Burgers vector in the initial state, forest dislocations are used as "centers" of multiplication [5]. Critical conditions for source operation are derived from a line tension model [6]. The source size distribution has natural higher and lower cutoffs. A superposition framework [7] is used to compute Peach-Koehler glide forces as

$$f^i = \mathbf{m}^i \cdot \left[\hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \boldsymbol{\sigma}^j \right] \cdot \mathbf{b}^i \qquad (1)$$

where $\mathbf{m}^i$ is the slip plane normal, $\mathbf{b}^i$ the Burgers vector, $\boldsymbol{\sigma}^j$ the self-stress and $\hat{\boldsymbol{\sigma}}$ an image stress field. Overdamped dislocation motion is modeled through: $Bv^i = f^i$ with B the drag factor and v^i the dislocation velocity. The superposition procedure does not apply to dislocation cores where nonlinear effects are prominent. These are accounted for through a set of "2.5-D" rules describing the short-range dislocation interactions such as junctions [8]. The method has recently been enhanced through code parallelization and an implmentation of a fast multipole method allowing to simulate a few millions of dislocations [4].

RESULTS

Compression

The regime of low initial dislocation density leads to behavior dominated by source-size and spacing effects (exhaustion hardening) [5]. By way of contrast, if the initial dislocation density is sufficiently large all crystals exhibit some steady size-dependent strain-hardening, Fig. 1a. The results of many such calculations are compared with experiments in Fig. 1b. The asymptotic limit of $\Theta \to \Theta_{\text{bulk}}$ has recently been met thanks to computational enhancements allowing multi-million dislocation simulations [4].

In this high dislocation density regime, the average dislocation spacing is much smaller than D and any size effect must be related to the evolving dislocation structure. Following a method developed in [9] maps of GND densities were generated, an example of which is shown in Fig. 2a. An effective measure of GND density is then defined as the volume average of the GND density over the specimen (note that the net GND density vanishes irrespective of size). As

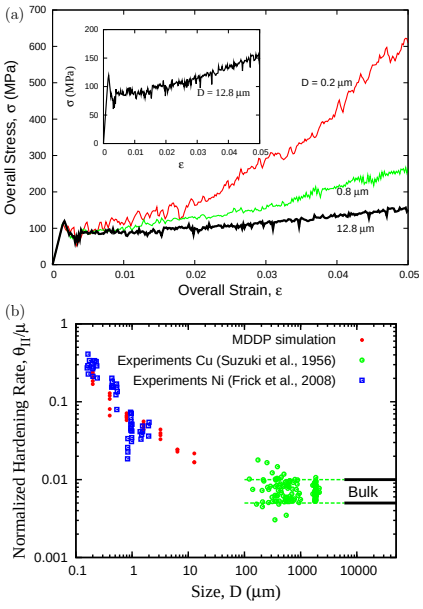

Figure 1. Results of 2.5D simulations in a specimen with initial source density of $1.5\,10^{14}\text{m}^{-2}$ and $L/D = 3$. (a) Sample stress versus strain curves; (b) Hardening rate (in units of shear modulus) versus specimen width D.

shown in Fig. 2b the effective GND density consistently increases with decreasing specimen size. The size effect on hardening is therefore due to the emergence of deformation-induced dislocation structures with a characteristic length comparable with specimen dimensions.

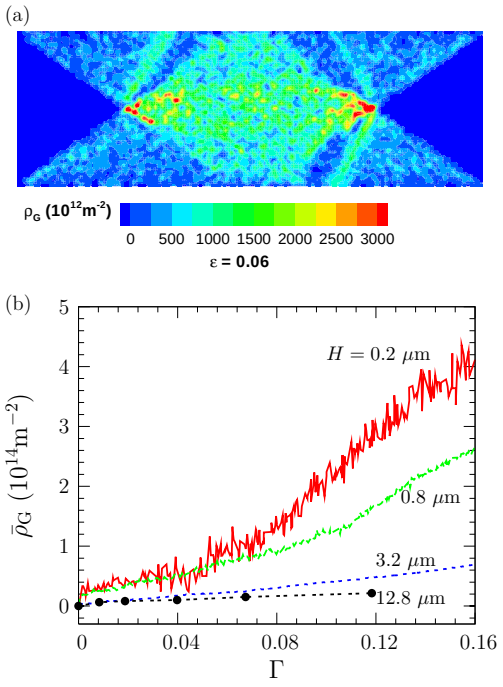

Figure 2. (a) Contour of GND density, ρ_G, at $\varepsilon = 0.06$ and a resolution of 50×50 nm^2 for crystal width $H \equiv D3.2$ μm. (b) Effective GND density (integral measure over specimen) versus overall strain in four different specimens.

Bending

In bending, we obtained size-dependent moment (M) versus rotation (θ) responses, as would be expected based on net GND densities. Here, we focus on stored energy calculations. Consider a loading program from initial $t = 0$ (stress-free state) to time t. Then:

$$\int_0^t \mathcal{D}dt = \int_0^t \dot{\mathcal{W}}dt - \Phi(t) \tag{2}$$

where $\mathcal{D}$ is the rate of dissipation and $\Phi(t)$ is the free energy of the body computed as strain energy knowing all dislocation positions at t. Also, $\mathcal{W}$ is the work expended:

$$\mathcal{W} = \int_0^t M\dot{\Theta}dt \tag{3}$$

The energy locked in the dislocation structure is computed from $\Phi(t)$ after subtracting out the work of tractions:

$$E^s(t) = \Phi(t) - \frac{L}{2D^*}M^2 \tag{4}$$

with D^* the bending modulus.

Fig. 3 shows sample results of $E^s/\mathcal{W}$ for two crystal sizes. Two sets of physical rules were used in the simulations, basic 2D rules (no junctions) and 2.5-D rules (with junctions). Irrespective of such details, the results indicate a strong increase in the proportion of stored energy upon decreasing specimen size.

CONCLUSIONS

Continuum plasticity theories assume availability of sources and spatial randomness of plastic flow within the RVE. The breakdown of either assumption may lead to size effects. Exhaustion hardening is active at low dislocation density and is rooted in the initial dislocation structure. Size-dependent strain hardening is active at high dislocation density and is rooted in the evolving dislocation structure. Analyses of bending indicate size dependence of energy storage in microcrystals.

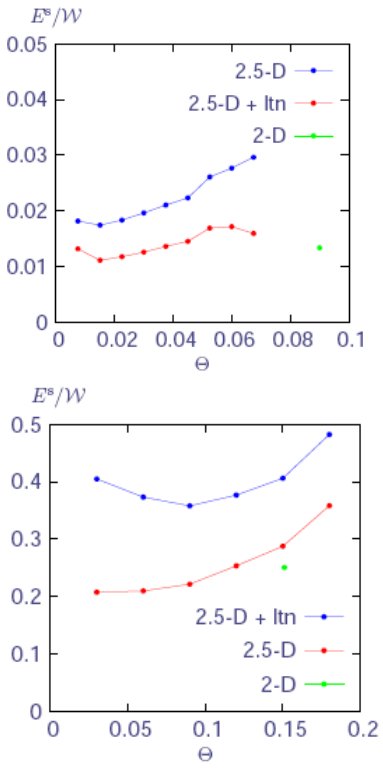

Figure 3. Energy stored per unit of work expended in bending (a) large 4μm$\times 12\mu$m crystal; (b) small 1μm$\times 3\mu$m crystal.

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