Plasticity of Nano- and Micro-pillars

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ABSTRACT

We review unique mechanisms of plastic deformation in nano- and micropillars. At the nanoscale, it is shown that plastic deformation is asymmetric with respect to direction of mechanical loading, as a result of specific relationships between the normal and resolved shear stress on active slip planes. This is attributed to the dependence of shear wave speed on the stress state acting on slip planes. Plastic deformation of nano-twinned copper pillars show a mechanism transition from dislocation nucleation to twin boundary migration. The flow strength σ_f of micropillars is shown to be size-dependent, and scales with the diameter, D as: $\sigma_f \propto D^{-0.69}$, in agreement with experiments. For micropillars of diameter larger than $\approx$ 100 nm, a 'weakest-link'dislocation activation mechanism accounts for the size effect. Aspects of work-hardening in discrete steps can be explained to result from cross-slip and sub-division of screw segments.

1. Introduction

At the atomic level, plastic deformation is facilitated by several basic mechanisms involving grain boundary sliding, diffusional creep, slip through dislocation motion, and twin boundary migration. It is generally associated with the irreversible deformation of solid crystals, because processes such as atomic diffusion and defect nucleation require an energy barrier, and as such, atomic motion cannot be reversed. The mechanical deformation of nanopillars beyond the elastic regime shows unusual characteristics that are not observed in bulk materials. Recent Molecular Dynamics (MD) simulations show that the primary yielding mechanism under uniaxial compression is by nucleation of Shockley partial dislocations from the surface. However, when considering polycrystalline nanopillars, the interaction of grain boundaries and dislocations produces a yet more complex picture. Deformation mechanisms in nanopillars containing multiple grains can be accommodated by either grain boundary migration, grain boundary sliding, motion of existing dislocations, and nucleation of new dislocations from surfaces and grain boundaries. The preferred mechanism can depend on a variety of conditions ranging from the orientation and direction of the crystallography relative to the deformation, the availability of slip planes, or the lattice energies of the respective defects. The effects of free surfaces on yielding was studied by Li and Ghoniem[1] for twinned copper. For micro-pillars, one of the key issues discussed in the literature recently is the dependence of the flow strength on the pillar size, and the mechanisms that control work hardening

One objective of the present work is to explore conditions that control two important modes of plastic deformation in copper nanopillars: dislocation nucleation from the surface and twin boundary migration. The main aim here is to show that a transition from reversible to irreversible plastic flow can be induced in axially loaded nano-pillars, and that a tension-compression asymmetry is inherent in plastically deforming nanopillars. A second objective is to investigate the effect of size on the strength of micropillars, and the nature of work hardening. The present review is based on the recent work of Brown & Ghoniem[2], and El-Awady et. el[3].

2. Computational Method

Atomic interactions in MD simulations here were modeled using an Embedded Atom Method (EAM) potential for copper using the Mishin potential. A twin boundary was then constructed by performing 180° rotation of the half-grain above a selected slip plane (111) relative to the other half. For each simulation, the angle θ formed between the load axis and the twin boundary normal controls the shear load ratio, R, defined as the ratio between the resolved shear stress and normal stress acting on the slip plane. In addition to the rotation, in-phase shifts lateral to the rotation plane were also performed on the half-grains. Finally, all atoms outside a cylinder with a diameter of 9 nm and of a height between 27 and 30 nm were removed from the simulation block, thus leaving an atomically smooth cylindrical surface behind.

The computational method adopted for micropillars follows the formulation developed by El-Awady et al.[3]. In this formulation, the Boundary Element Method (BEM) is coupled with the 3-D Parametric Dislocation Dynamics (PDD) to incorporate the influence of free and internal interfaces on dislocation motion, and hence to describe microscopic plastic flow in finite volumes. In this methodology, the effects of surfaces and boundary conditions are modeled with the BEM, while the computational structure of the PDD is unchanged. In the PDD, all dislocation loops are discretized into curved parametric segments and the elastic field, forces, and motion of the dislocation segments in an infinite medium are computed.

3. Reversible-Irreversible Plasticity Transition

Plastic deformation of twinned fcc crystals has been shown by Li and Ghoniem to proceed via two main channels: (1) nucleation and propagation of dislocations; and (2) twin boundary migration[1]. Nucleation of Shockley partial dislocations takes place at free surfaces[4], or at twin boundaries themselves[1], and as such, will lead to irreversible plastic deformation. On the other hand, if surface dislocation nucleation is somehow prevented, and twin boundaries are subjected to sufficient shear displacement, twinning dislocations can form at these boundaries allowing them to migrate normal to the shear plane displacement. The atomic mechanisms of this twin boundary motion (TBM) “coupled”to shear deformation have recently been described within the framework of stick-slip dynamics[4]. Hu, Li and Ghoniem found that the “stick”phase of the dynamics is associated with accumulated strain in the crystal, and that such strain is suddenly released by the nucleation of $1/6[112]$-type twinning partial dislocations[4].

The yield locus for twinned copper nanopillars is shown in Fig. 1. When the local shear stress is below about 1 GPa, and the normal stress on twin planes is very large (e.g. above $\approx$ 2.5 GPa), TBM cannot be sustained anymore, and another plastic deformation channel opens up in the form of dislocation nucleation from the surface. We select here the two stress components, $< \sigma_R >$ and $< \sigma_N >$, to depict the yield surface of copper nano-pillars loaded in tension and in compression. The state of plastic reversibility at local shear stresses in the range $0.5 \leq < \sigma_R > \leq 1$ GPa can be attained with a corresponding increase in the compressive normal stress, up to $\approx$ 2.5 GPa. Beyond these limits, twinned copper nanopillars make a transition to a state of plastic irreversibility attained by surface dislocation nucleation and TBM. The critical transition from reversible to irreversible plasticity is demonstrated in Fig. 2, where it is clearly shown that below a strain of about 3.3%, twinned copper nanopillars prefer to deform plastically by TBM, and thus the deformation is reversible since it is not associated with any surface dislocations.

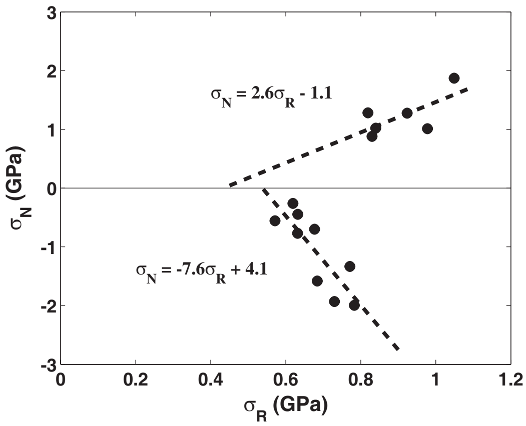

Figure 1: Yield locus for reversible plasticity for twinned nanopillars ($< \sigma_N >$ versus $< \sigma_R >$).

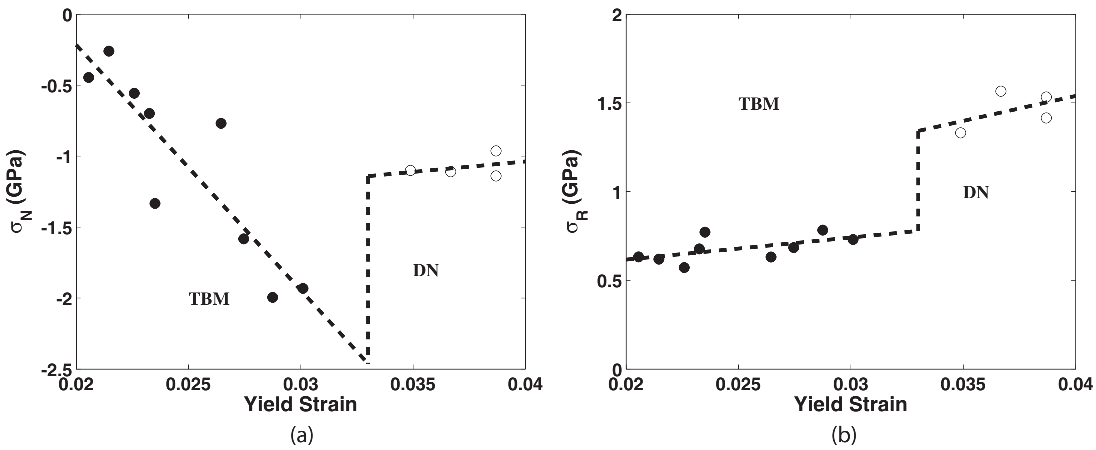

Figure 2: The normal stress, $< \sigma_N >$, (a) and the critical resolved shear stress, $< \sigma_R >$, (b) plotted as a function of the yield stain for twinned copper nanopillars under compression. At larger values of strain, plastic deformation becomes irreversible.

4. Tension-Compression Asymmetry

A tension-compression asymmetry is observed[2] in simulations of nanopillars. Fig. 1 shows the yield locus for reversible plasticity controlled by TBM. Under compression, a lower value of the local shear stress is needed to initiate yield by TBM, as compared to the same conditions under tension. Twinning dislocation nucleation and motion is facilitated when the twin boundary is under compression, as compared to being under tension. However, and in both cases, a larger value of local shear is required to initiate TBM when any normal stress is additionally operating on the twin plane. Analysis of the simulations show that the speed of dislocation motion on twin boundaries is reduced whether the normal stress is tensile or compressive.

5. Flow Strength Size Dependence of Micro-pillars

To develop scaling laws for the strength of micropillars, PDD computer simulations coupled with a statistical analysis have been performed on the range of diameters from 0.25 to 5.0m[3]. For each of the micropillar sizes, the initial dislocation density was statistically varied in the range $\rho = 1 - 50 \times 10^{12}$ m^{-2}. The scaling relationship for the flow strength, σ_f , with the micropillar diameter is seen to be of a power law type, with an exponent of -0.69. This is in close agreement with the exponent produced by the experimental results[3]. A best fit of simulated results for Ni micropillars is $\sigma_f \approx 222\, D^{-0.69}$, where D (μm) and σ_f (MPa). Plastic deformation beyond the yield point of micropillars shows work-hardening that has two characteristics: (1) it shows nearly perfect plasticity, with intermittent steps in the stress-strain relationship, and (2) large deformation results in geometric instabilities. The work-hardening in discrete steps can be explained in the simulations[3] to result from cross-slip and sub-division of screw segments

6. Summary & Conclusions

Plastic deformation of twinned copper nanopillars shows behavior that is not observed in the deformation of bulk copper. The unique features of this deformation stem from the small size and the ability to control the type and nature of dislocation nucleation and motion inside these nano-systems. The yield locus for twinned copper nanopillars is an approximate linear relationship between the shear and normal components of the average atomic stress on twin planes. The critical transition from reversible to irreversible plasticity is shown to take place at a strain of $\approx 3.3\%$. We also show here that reversible plastic yield under tension is not the same as under compression, which indicates a clear "tension-compression asymmetry"in the reversible plasticity of twinned nanopillars. The reversible-irreversible plasticity transition is found to be the result of a competition between the nucleation and growth of twinning dislocations for reversible plasticity, versus dislocation emission from free surfaces for irreversible plasticity. For micropillars, the probability of a single pinned or double pinned dislocation of length $0.1\ \mu$m existing in a micropillar is found to be very small. Thus, for a micropillar having a diameter D $\leq 0.16\ \mu$m, most pre-existing dislocations would be close to the surface, and also junction formation would be very unlikely because of the low initial dislocation density. Thus, surface-nucleated dislocations would escape from the pillar leaving it dislocation free, giving rise to a possible dislocation-exhaustion mechanism. For larger micro-pillars, however, there is a higher probability of having pinned dislocations, and thus a 'weakest link'mechanism would control the strength and work-hardening of the pillar.

References

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