Available online at www.sciencedirect.com
ScienceDirect
Scripta Materialia 63 (2010) 1096–1099
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Simulations of the effect of surface coatings on plasticity at small scales

Caizhi Zhou,[a,b] S. Biner[b] and Richard LeSar[a,b,*]

[a]Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, USA
[b]Ames Laboratory, Iowa State University, Ames, IA 50011, USA

Received 19 March 2010; revised 25 June 2010; accepted 6 August 2010
Available online 10 August 2010

Three-dimensional dislocation dynamics simulations were employed to examine how hard coatings affect plastic deformation in micron- and submicron-sized, single-crystal pillars ("micropillars") of nickel. Cross-slip of dislocations in the coated samples was found to be necessary for the formation of banded structures and subcells. Our simulations thus offer an explanation for both the significant increases in compressive strength and the higher strain-hardening rate as well as formation of banded structures in coated micropillars.

Keywords: Dislocation dynamics; Plastic deformation; Small scales; Cross-slip

Size-dependent deformation properties of single crystals have attracted much attention in the materials science community, in part because these properties are closely related to the reliability of such structures in technical applications. Microcompression testing of small face-centered cubic (fcc) single crystals (e.g., Ni or Au) with sizes of several microns and below shows that the flow stresses increase as sample sizes decrease. The dependence of flow stress (σ) on size (d) is generally fitted well with a power law, i.e., $\sigma \sim d^{-n}$, where n is around 0.6–1.0 [1–7].

Recently, Ng and Ngan [8] found that coating aluminum micro columns with tungsten significantly increased the compressive strength and depressed any strain bursts compared with the free-surface samples, agreeing with Greer's experimental results on Au micropillars coated by Al_3O_2 [9]. In addition, subcells and band structures formed in the coated samples, which have seldom been observed in micron-scale samples with free surfaces. However, the remarkable increase in strength and strain-hardening rate of micropillars with hard coatings could not be explained by standard mechanisms, e.g., the rule of mixtures (i.e., the strength of mixtures should be equal to the sum of the strength of each component multiplying their volume fractions) [8].

For the micron-scale systems described above, 3D dislocation dynamics (DD) simulations have provided important insights into the mechanisms that determine the mechanical response of small-scale materials. Recently, we found excellent correspondence between simulations and experiment only when we accurately modeled three elements of the physics:

1. we employed an experimental-like initial dislocation structure [10], which was created by cutting cylinders from larger simulations (representing a bulk sample) [11–17];
2. we included models that enabled the dislocations to cross-slip; and
3. we used the boundary element method to describe the image forces from the free surface.

In this study, we employed similar 3D DD simulations to examine the mechanical behavior and microstructural evolution in micropillars with a hard coating layer similar to the samples studied experimentally [8]. We compare the results from coated micropillars to those from free-surface micropillars to investigate how coatings affect the plastic deformation behavior in small volumes.

The 3D DDS framework described in Refs. [18,19] has been used in our study to simulate the mechanical behavior of Ni (fcc) single crystals under uniform compression. Experiment-like initial dislocation structures, containing FR sources, jogged dislocations, surface dislocations and spiral (single-armed) sources, were introduced into our DD simulations to study plastic

* Corresponding author at: Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, USA; e-mail: lesar@iastate.edu

1359-6462/$ - see front matter © 2010 Published by Elsevier Ltd. on behalf of Acta Materialia Inc.
doi:10.1016/j.scriptamat.2010.08.012

behavior micropillars under compression. We created these distributions by starting with a cubic cell (size $3 \times 3 \times 3\ \mu m^3$) with periodic boundary conditions (i.e., a bulk sample) containing dislocation sources on all 12 <0 1 1>{1 1 1} slip systems with random lengths, which was sheared to create a dislocation density of about $2.5 \times 10^{13}\ m^{-2}$. Then the "bulk" cubic sample was unloaded and cylinders of various sizes (representing micropillars) were cut out of the bulk sample along the [0 0 1] direction with the aspect ratio of D:H = 1:2, where D and H denote the diameter and height of micropillars, respectively. Subsequently, the deformed dislocation microstructures were relaxed under the influence of image and interaction forces. The dislocation densities after relaxation were all in the range of 1.0–$2.0 \times 10^{13}\ m^{-2}$ and consistent with conditions observed in experiments [20]. In the present study, samples with diameters $D = 0.5$ and $1.0\ \mu m$ were compressed in [0 0 1] direction for samples with both coated and free surfaces. In agreement with the experimental observations [8], the hard coating layer was considered as an impenetrable obstacle for dislocations, while free surfaces both served as a sink for dislocations and also generated image forces, which play a significant role in mechanical behavior of uncoated micro- and nanosamples [21]. The free surfaces were modeled using the boundary element method (BEM) [13]. We simulated the experimental loading conditions of Dimiduk and coworkers [1,2,20,22] in our computations, in which a mixture of constant displacement rate and creep-like loading conditions were employed; the applied stress was discretely increased by a small fixed value ($\delta\sigma$) every time the plastic strain rate approached zero.

For the simulations in this work, the applied strain rate was equal to $200\ s^{-1}$, and the materials properties of nickel were used: shear modulus $\mu = 76$ GPa, Poisson's ratio $v = 0.31$, and lattice constant $a = 0.35$ nm. Finally, a sophisticated thermally activated cross-slip model developed by Kubin and co-workers [23] was adopted in our DD simulations with Monte Carlo sampling to determine the activation of cross-slip. Detailed procedures can be found in our previous paper [10].

In Figure 1, the engineering stress–strain relationships of micropillars with diameters $D = 0.5$ and $1.0\ \mu m$ are shown. The size-dependent behavior, in which smaller samples have higher strength, is observed in both coated and free-surface samples. When starting from identical initial dislocation configurations, the flow stress of coated samples is approximately 110% higher than that of the free-surface samples with $D = 0.5\ \mu m$ and 60% higher with $D = 1.0\ \mu m$. In the coated samples, stress–strain curves exhibited larger-strain-hardening rates than those in samples with free surfaces, and the magnitude of strain bursts was decreased to a large degree, which agrees well with experiment results that coated samples demonstrated a significant increase in flow stress and the strain-hardening rate [8,9].

Figure 2a shows the comparison of the strain–stress curves and the corresponding variation of the dislocation density for a typical example of coated and free-surface micropillars with diameter $D = 1.0\ \mu m$. The same initial dislocation structure was used in the two simulations (shown in Figure 2b). The coated sample exhibited

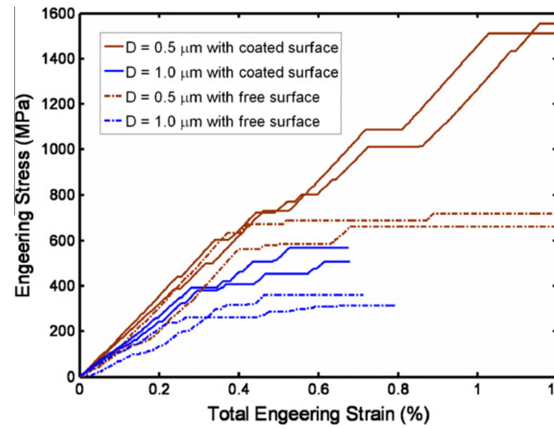

Figure 1. Stress–strain curves for both coated and uncoated samples.

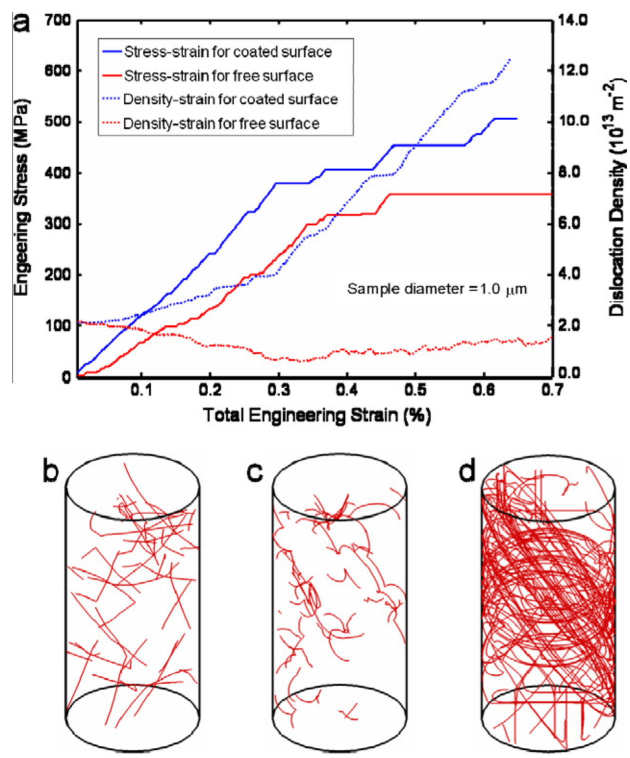

Figure 2. (a) Stress–strain and dislocation density–strain curves with diameter $D = 1.0\ \mu m$, (b) initial dislocation structure, (c) dislocation structure in free-surface sample at 0.6% strain, and (d) dislocation structure in coated sample at 0.6% strain.

not only higher flow stress, but also a higher hardening rate, i.e., at the same stress level, the total strain is smaller than that in free-surface sample. The large amount of "microplasticity" (plastic strain at low loads) in samples with free surfaces is the result of the weakly entangled dislocations from within the sample being driven out the free surfaces [10]. In the coated sample, however, dislocations are blocked by the coated layer and stored near the interfaces, inducing a strong back stress on subsequently activated dislocations. Thus, the plastic deformation induced by the movement of dislocations was smaller in the coated sample at low loads and showed a steeper slope of the strain–stress curves before