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Acta Materialia 59 (2011) 7673–7682

Acta MATERIALIA

www.elsevier.com/locate/actamat

Plastic deformation mechanisms of fcc single crystals at small scales

Caizhi Zhou [a,*], Irene J. Beyerlein [a], Richard LeSar [b,c]

[a] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
[b] Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011, USA
[c] Ames Laboratory, Iowa State University, Ames, IA 50011, USA

Received 29 March 2011; received in revised form 21 August 2011; accepted 22 August 2011
Available online 15 October 2011

Abstract

Three-dimensional (3-D) dislocation dynamics simulations were employed to examine the fundamental mechanisms of plasticity in small-scale face-centered cubic single crystals. Guided by the simulation results, we examined two distinct modes of behavior that reflect the dominant physical mechanisms of plastic deformation at small scales. We found that the residence lifetimes of internal dislocation sources formed by cross-slip decrease as the system size decreases. Below a critical sample size (which depends on the initial density of dislocations) the dislocation loss rate exceeds the multiplication rate, leading to the loss of internal dislocation sources. In this case nucleation of surface dislocations is required to provide dislocations for deformation and the "starvation hardening" mechanism becomes the dominant deformation process. When the sample is larger than a critical size multiplication of internal dislocation sources provides the dominant mechanism for plastic flow. As the strain is increased the rising dislocation density leads to reactions that shut off these sources, creating "exhaustion hardening".
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Keywords: Dislocation dynamics; Size effects; Small scales; Dislocation starvation; Cross-slip

1. Introduction

The mechanical properties of nano- and microscale materials have attracted much attention in recent years [1]. Starting with the pioneering microcompression measurements of Uchic et al. that reported an anomalous increase in the strength of micron-scale single-crystal pillars as their diameter decreased [2], numerous research groups have observed similar size effects in various face-centered cubic (fcc) single crystals [3–15]. An inverse relationship between sample size and flow stress was predicted by strain gradient models for small indentations, resulting from an increase in geometrically necessary dislocation densities to accommodate the lattice mismatch [16,17]. However, transmission electron microscopy (TEM) investigations [18] revealed that the dislocation structure on the active slip systems in micropillars with diameters larger than 2 μm is comparable with that found in bulk samples deformed to a similar state. Furthermore, the dislocation density in nanopillars smaller than 150 nm apparently approaches zero after deformation [19]. These experimental observations indicate that mechanisms other than the gradient-induced storage of geometrically necessary dislocations must be the cause of the observed size effects in microcompression tests on micropillars.

Two basic models have been used to explain the size effects on plasticity in fcc single crystals. The first is the "dislocation starvation" (DS) model [5–7,13,20,21], in which dislocations can easily escape from nearby free surfaces in a small sample prior to dislocation multiplication, leaving samples in a dislocation-free state. Continuous plastic flow would then require an increase in applied load to nucleate dislocations at the surface. Thus the principal idea behind the DS model is that plastic deformation at small scales is dislocation nucleation dominated. The other model is the "single arm dislocation" (SAD) model, which is based on the notion that size effects on the plasticity of

* Corresponding author. Tel.: +1 505 667 3216.
E-mail address: czhou@lanl.gov (C. Zhou).

1359-6454/$36.00 Published by Elsevier Ltd. on behalf of Acta Materialia Inc.
doi:10.1016/j.actamat.2011.08.032

small single crystals can be rationalized almost completely by considering the stochastics of single arm dislocation source lengths in the sample [22]. In contrast to the DS model, the SAD model assumes that plastic deformation is induced by multiplication of internal dislocation sources rather than nucleation of surface dislocations. To identify which of the two models best describes the dislocation behavior requires a better understanding of the evolution of dislocation structures with increasing strain and the details of the dynamic behavior of internal dislocation sources.

Three-dimensional (3-D) dislocation dynamics (DD) simulations, in which dislocations are the simulated entities, have been the primary modeling tool employed to study the various aspects of plastic behavior in nano- and microscale samples. The first applications of 3-D DD simulations to this problem employed a set of isolated Frank–Read sources (FR) with rigidly fixed ends as the starting dislocation populations [23–28]. To extend that simple (and limited) model Tang et al. [29] employed artificially generated jogged dislocations as the initial dislocation configuration for their simulations (although they neglected image stresses and cross-slip) and demonstrated that the shut-down of sources causes staircase behavior similar to that observed in experiments. Motz et al. [30] used the dislocation structures relaxed from a high density of closed dislocation loops as the initial input for their simulations. In our previous work [31] we employed initial dislocation structures similar to those determined experimentally, which were created by cutting a cylindrical sample from the results of simulations on larger bulk samples. Our goal was to mimic the physics of real systems as closely as possible. We found that the scarcity of available dislocation sources is indeed a major contributor to the higher flow stress in smaller sizes. Despite this progress, however, further studies are needed, both to determine the critical events for plastic deformation at small scales and to derive more accurate and reliable models to predict the mechanical properties of small-scale materials.

In this paper we extend our previous work using 3-D DD simulations to study the stability of dislocation sources in micropillars and explicitly examine the fundamental mechanisms of plasticity at small scales. Based on our simulation results analytical formulations of the DS model and a general SAD model were examined, from which we identify the relationship between nucleation-dominated and multiplication-dominated plastic deformation in small-scale fcc single crystals.

2. Simulation procedures

We employ the parametric DD method described in detail in Ghoniem and co-workers [32–34] to simulate the mechanical behavior of Ni single crystals under uniform compression. The material properties of Ni are used: shear modulus $\mu = 76$ GPa, Poisson's ratio $\nu = 0.31$, and lattice constant $a = 0.35$ nm. The dislocation drag coefficient was set to a typical value of $10^{-4}\,\mathrm{Pa}^{-1}\,\mathrm{s}^{-1}$ [35]. In this study the image stress field induced by the free surfaces has been evaluated by the boundary element method (BEM), further details of which can be found elsewhere [23,36].

The DD thermally activated cross-slip model developed by Kubin and co-workers [37,38] was adopted in our DD simulations to study the evolution of microstructures in small volumes. The probability of cross-slip of a screw segment with length L in a discrete time step is determined by an activation energy $V_{act}(|\tau| - \tau_{III})$ and the resolved shear stress on the cross-slip plane τ,

$$P = \beta \frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp\left[\frac{V_{act}}{kT}(|\tau| - \tau_{III})\right] \tag{1}$$

where β is a normalization constant, k is the Boltzmann constant, T is set to room temperature, V_{act} is the activation volume, and τ_{III} is the stress at which stage three hardening starts. In nickel V_{act} is equal to $420b^3$, with b the magnitude of the Burgers vector [39], and $\tau_{III} = 55$ MPa [40]. Parameters $L_0 = 1$ μm and $\delta t_0 = 1$ s are reference values for the length of the cross-slipping segment and for the time step. Eq. (1) describes the thermal activation of cross-slip expressed in terms of a probability function. A stochastic (Monte Carlo) method is used to determine whether cross-slip is activated for a screw dislocation segment. Accordingly, at each time step the probabilities of cross-slip of all screw segments are calculated using Eq. (1). For each screw segment the probability P is compared with a randomly generated number N between 0 and 1. If the calculated P is larger than N cross-slip is activated, otherwise, cross-slip is disregarded [41].

In our computations the experimental loading conditions of Dimiduk and co-workers [2,3,18] were simulated, 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 the applied strain rate. In all simulations compression loading was performed in the [0 0 1] direction. When the plastic strain rate was equal to 50 the applied load was increased by 1.0 MPa, i.e. $\delta\sigma = 1.0$ MPa for $\dot{\varepsilon}^p = 50$, while the applied stress was kept constant when the plastic strain rate was larger than 50, i.e. $\delta\sigma = 0$ for $\dot{\varepsilon}^p > 50$.

3. Results and discussion

In this section the results from our simulations will be used to address distinct aspects of dislocation behavior. We first discuss how the loss of dislocation sources through the free surfaces under larger deformations leads to what has been referred to as "starvation hardening", followed by development of a model for predicting under what conditions of system size and dislocation density that starvation hardening will occur. We then discuss how the dominant mechanism for the onset of plasticity seems to be the activation of a single (single armed) source, and that