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International Journal of Plasticity 22 (2006) 2091–2117
INTERNATIONAL JOURNAL OF Plasticity
www.elsevier.com/locate/ijplas

Discrete dislocation dynamics simulations to interpret plasticity size and surface effects in freestanding FCC thin films

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Received 26 June 2005; received in final revised form 27 December 2005
Available online 6 March 2006

Abstract

Strong size effects have been experimentally observed when microstructural features approach the geometric dimensions of the sample. In this work experimental investigations and discrete dislocation analyses of plastic deformation in metallic thin films have been performed. Columnar grains representative of the film microstructure are here considered. Simulations are based on the assumptions that sources are scarcely available in geometrically confined systems and nucleation sites are mainly located at grain boundaries. Especially, we investigated the influence on the mesoscopic constitutive response of the two characteristic length scales, i.e., film thickness and grain size. The simulated plastic response qualitatively reproduces the experimentally observed size effects while the main deformation mechanisms appear to be in agreement with TEM analyses of tested samples. A new interpretation of size scale plasticity is here proposed based on the probability of activating grain boundary dislocation sources. Moreover, the key role of a parameter such as the grain aspect ratio is highlighted. Finally, the unloading behavior has been investigated and a strong size dependent Bauschinger effect has been found. An interpretation of these phenomena is proposed based on the analysis of the back stress distribution within the samples.

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doi:10.1016/j.ijplas.2006.01.007

Keywords: Size effects; Discrete dislocation dynamics; Thin films; Plasticity; Grain boundaries; Frank–Read sources; Bauschinger effect

1. Introduction

Thin film plasticity is currently an active field of research essentially for two reasons: (i) metallic thin films are widely used in electronic components; (ii) the plastic properties of thin films differ significantly from the properties of the corresponding bulk materials due to the reduced length scales of the microstructure, which become comparable to the geometric structural dimensions. Metallic thin films on substrates usually exhibit a flow stress which is an order of magnitude higher than the same material in bulk form and this flow stress increases with the decrease of the film thickness (Arzt, 1998; Spaepen, 2000; Arzt et al., 2001).

So far, thin film plasticity has mostly dealt with films (essentially Al and Cu) deposited on Si substrates. Following the pioneering work of Nix (1989) for single crystalline films, several authors analyzed the response of polycrystalline thin films; they focused on the effect of film thickness, grain size and orientation, on the stress/strain response and other important features like the level of thermal stresses as a function of the thickness and the effect of passivation layers (Venkatraman and Bravman, 1992; Yu et al., 1997; Keller et al., 1998; Baker et al., 2001; Hommel and Kraft, 2001). Recently, Baker et al. (2003) found an "anomalous" large Bauschinger effect for thin Cu films on substrates when the films were exposed to air.

For polycrystalline *free-standing* thin films, the experimental data and setups are more limited (Keller et al., 1996; Huang and Spaepen, 2000; Espinosa et al., 2003; Haque and Saif, 2004). Espinosa and co-workers (Espinosa and Prorok, 2001; Espinosa et al., 2003, 2004), using the membrane deflection experiment (MDE), identified major size effects in the mechanical properties of free-standing submicron FCC thin films (electron beam evaporated Au, Cu, and Al). These films were polycrystalline in nature with thicknesses ranging from 200 nm to 1 μm and were tested by applying macroscopic *pure homogeneous uniaxial tension*, i.e., in the absence of any *macroscopic strain gradient*. The average grain size (about 200 nm) was independent of the film thickness. This feature is quite important to eliminate the so-called Hall–Petch effect. The reader should note that for the case of electron-beam evaporated Cu, similar results concerning the deviation from linear elasticity and onset of plastic flow were obtained using a micro-tensile device with in situ TEM by Keller et al. (1996). These authors did observe dislocation nucleation and emission from grain boundaries consistent with current understanding of plastic flow in metals.

Haque and Saif (2004) also explored size effects in FCC metal films such as sputtered pure Al and Au, by measuring the tensile stress–strain response of submicronic (down to a thickness of 0.1 μm) free-standing films subjected to loading and unloading. However, in their experiments, the grain size varied with film thickness, which makes the interpretation more complex. The average grain size in the investigation was 100 nm or smaller. Upon performing in situ TEM observations, they did not notice dislocation activity for an average grain size lower than 50 nm, and they concluded that a grain boundary-based mechanism was the dominant contribution to deformation. These observations are in agreement with the results obtained for "bulk" nanocrystalline materials, either through in situ TEM, or by means of large scale molecular dynamics simulations, which are usually performed as a "guide" to experiments (Kumar et al., 2003).