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Trapping and escape of dislocations in micro-crystals with external and internal barriers

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ABSTRACT

We perform three-dimensional dislocation dynamics simulations of solid and annular pillars, having both free-surface boundary conditions, or strong barriers at the outer and/or inner surfaces. Both pillar geometries are observed to exhibit a size effect where smaller pillars are stronger. The scaling observed is consistent with the weakest-link activation mechanism and depends on the solid pillar diameter, or the annular pillar effective diameter, $D_{eff} = D - D_i$, where D and D_i are the external and internal diameters of the pillar, respectively. An external strong barrier is observed to dramatically increase the dislocation density by an order of magnitude due to trapping dislocations at the surface. In addition, a considerable increase in the flow strength, by up to 60%, is observed compared to simulations having free-surface boundary conditions. As the applied load increases, weak spots form on the surface of the pillar by dislocations breaking through the surface when the RSS is greater than the barrier strength. The hardening rate is also observed to increase with increasing barrier strength. With cross-slip, we observe dislocations moving to other glide planes, and sometimes double-cross-slipping, producing a thickening of the slip traces at the surface. Finally the results are in qualitative agreement with recent compression experimental results of coated and centrally-filled micropillars.

1. Introduction

Recently, Uchic et al. (2004) developed a new experimental technique to study the flow behavior of micron-sized crystals. In this methodology, micron scale samples were fabricated using Focused Ion Beam (FIB) milling, and tested under uniaxial compression using a nano-indentation system equipped with a flat ended diamond tip (Uchic et al., 2003, 2004; Uchic and Dimiduk, 2005). Moreover, Greer et al. (2005) have extended this technique into the nano-scale regime. These experiments have sparked a wide interest in plasticity and size effects at micron-scales, from both experimental and modeling perspectives. A myriad of adaptations to this methodology have been applied to study a variety of materials, and to address different aspects of the plasticity at such small scales (Uchic et al., 2009; Oh et al., 2009; Shim et al., 2009; Ng and Ngan, 2009; Shade et al., 2009).

From these experimental results, a consistent size-dependency of the flow strength on the sample diameter was observed (Uchic et al., 2009). In addition, the flow strength was observed to be stochastic in nature, with the micro-samples deforming

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