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Thickness effects in polycrystalline thin films: Surface constraint versus interior constraint

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ABSTRACT

The uniaxial tension behavior of polycrystalline thin films, in which all grain boundaries (GBs) are penetrable by dislocations, is investigated by two-dimensional discrete dislocation dynamics (DDD) method with a penetrable dislocation-GB interaction model. In order to study thickness effect on the tensile strength of thin films with and without surface treatment, three types of thin films are comparatively considered, including the thin films without surface treatment, with surface passivation layers (SPLs) of nanometer thickness and with surface grain refinement zones (SGRZs) consisting of nano-sized grains. Our results show that thickness effects and their underlying dislocation mechanisms are quite distinct among different types of thin films. The thicker thin films without surface treatment are stronger than the thinner ones; however, opposite thickness effects are captured in the thin films with SPLs or SGRZs. Moreover, the underlying dislocation mechanisms of the same thickness effects of thin films with SPLs and SGRZs are different. In the thin films with SPLs, the thickness effect is caused by the sharp increase of dislocation density near the film-passivation interface, while it is mainly due to the sharp decrease of dislocation density within the refined surface grains of the thin films with SGRZs. No matter in what type of thin films, thickness effect gradually disappears when the number of grains in the thickness direction is large enough. Our analysis reveals that general mechanism of those thickness effects lies in the competition between the exterior surface-constraint and interior GB-constraint on gliding dislocations.

1. Introduction

With the startlingly rapid development of micro-technology, especially in micro-forming and micro-manufacturing, the ever-continuing miniaturization of various components/devices becomes an unstoppable trend. Once the leading sizes of the micro-components/devices decrease to the same order as the intrinsic lengths of materials, size effects appear and the mechanical behavior of small-sized materials remarkably deviates from that of bulk counterparts. Generally speaking, the intrinsic lengths of materials are usually at the micron or submicron scale (Arzt, 1998). For this reason, various thin films with micron/nanometer thicknesses, which are widely used in many micro-electronic and micro-electro-mechanical systems, commonly display strong size effects. A thorough understanding of the size dependent plasticity in thin films and its inherent mechanism is not only of academic significance, but also of great urgency to the reliability design and security assessment of various micro-electric and micro-electro-mechanical systems.

Recently, the micro-plasticity of thin films becomes an active research field (Keller et al., in press; Lee et al., 2011; Liang et al., 2009; Nicola et al., 2005b, 2006; Xiang et al., 2006; Xiang and Vlassak, 2006) due to the increasing application of thin films in micro-electric and micro-electro-mechanical systems. Different from single crystalline thin films, there are usually several grains in the thickness direction of polycrystalline thin films (Espinosa et al., 2006, 2004). At least two characteristic lengths (i.e., grain size and film thickness) strongly influence the tensile strength of polycrystalline thin films. The effect of grain size is associated with the interior grain boundary (GB)-constraint on dislocations (i.e., Hall–Petch effect); however, the thickness effect is mainly because of the weak exterior surface-constraint on dislocations. Both "GB engineering" method, i.e., manipulating GB structures or strengthening GBs in polycrystalline metals, and "surface engineering" method, i.e., refining surface grains or passivating surfaces of thin films can obtain the desired high strength. Obviously, the former method enhances the strengths of polycrystalline thin films by strengthening their interior constraint; however, the latter stiffens thin films by strengthening their exterior constraint. In recent years, these two methods have been broadly used to increase the strength of polycrystalline thin films (Geers et al., 2006; Nicola et al., 2006; Xiang and Vlassak, 2006).

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