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Stochastic effects in plasticity in small volumes

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Recent studies of micro- and nano-scale metallic structures have exposed considerable statistical distribution, in addition to significant size dependencies, in the yield strength. This intrinsic statistical variation is particularly evident in the micro-compression and micro-tension thin film tests. This work investigates the relationship between the initial dislocation density, the heterogeneous initial spatial dislocation distribution, and the resulting localized deformation with multiscale discrete dislocation dynamics simulations. This relationship is examined separately from commonly reported external factors affecting observed strength, such as variations in specimen geometry and base support. Towards this end, we performed multiscale dislocation dynamics simulations of geometries commonly employed in micro-scale testing techniques, including micro-pillar compression, microtensile thin film, and microbulge tests. The statistical variation of yield strengths from all three simulation geometries is in agreement with experimental data from the corresponding loading techniques. We show that the onset of plasticity is stochastic in small volumes containing a small density of dislocations: a contrast to classical deterministic plasticity theory. The yield stress in these small volumes is stochastic, not deterministic, because of statistical variation of the initial dislocation content. The numerical results exhibit a localized deformation process and demonstrate a strong dependence of the yield stress on the initial dislocation density, the initial dislocation spatial distribution, and the specimen geometry size. Leveraging nucleation theory, a stochastic model for the onset of plasticity in micro- and nano-scale structures is developed based on these results.

1. Introduction

Micro scale metallic structures, e.g. micro-pillars and thin films, demonstrate significantly higher yield strengths than their bulk counterparts and exhibit very strong size dependencies accompanied with a jerky deformation process (Uchic et al., 2004; Nix, 1989). This higher strength has been explained by researchers using different theories depending on the various loading techniques. For loading conditions that can impose a strain gradient on specimens, e.g. bending or torque, the size effect can be attributed to geometrically necessary dislocations (GND) (Fleck et al., 1994; Ma and Clarke, 1995; Nix and Gao, 1998; Stolken and Evans, 1998; Zhang and Aifantis, 2011). However, in both experimental and numerical studies, the size dependency of strength has also been observed in macroscopically homogenous loading conditions, e.g. in micro-compression tests (Uchic et al., 2004; Lee and Nix, 2012; Dimiduk et al., 2005; Kiener et al., 2009; Schneider et al. 2011; Tang et al., 2007; Akarapu et al., 2010; Zbib and Akarapu, 2009; Gao et al., 2010; Ng and Ngan, 2008a,b,c; Ngan and Ng, 2010; Zhou, et al., 2010), in thin film microbulge, and microtension tests (Xiang et al., 2006; Yu and Spaepen, 2004; Jaeger et al.,

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2006; Hommel and Kraft, 2001; Nix, 1989; Gruber et al., 2008; Huang and Spaepen, 2000). The theory of GND is not applicable in these cases because of the absence of macroscopic strain gradients. Rather the high strength and size dependence can be attributed to the scarcity of dislocations in small volumes, and the strong interactions of dislocations with obstacles and surfaces (Rhee et al., 1994; Uchic et al., 2004; Akarapu et al., 2010; Zbib and Akarapu, 2009; El-Awady et al., 2011). The size effect on the strength of micro-pillars and thin films has been studied quite extensively over the past few years (Lee and Nix, 2012; Akarapu et al., 2010; Zbib and Akarapu, 2009; Hommel and Kraft, 2001; Nix, 1989; Gruber et al., 2008; Brotzen, 1994; El-Wady et al., 2011), and different scaling models for the size effects have been proposed. The compressive strength of micro-pillars generally decreases as a power law with increasing pillar diameter (Lee and Nix, 2012):

$$\tau_{CRSS} = \tau_0 + A \cdot D^{-n} \tag{1}$$

where τ_{CRSS} is critical resolved shear stress required to activate a dislocation arm in micro-pillars, τ_0 is the shear strength in bulk material, D is the diameter, and A and n are model parameters. Commonly thin films are polycrystalline materials, so the presence of grain boundaries also affects the thin film strength (Lawrence et al., 2012). Therefore, the tensile strength for thin films is more complex and depends on both the film thickness and grain size (Hommel and Kraft, 2001; Nix, 1989). However many investigators have also shown that the strength-thickness relationship in a thin film geometry follows Eq. (1) (Gruber et al., 2008; Brotzen, 1994).

In the literature, modeling of the size effect in microscale metallic structures treated the onset of plasticity as a deterministic event. In striking contrast to this assumption is the large amount of microscale experimental data: the data display a significant amount of statistical variation and a jerky flow process regardless of how careful and elegantly the experiments are performed (Dimiduk et al., 2005; Kiener et al., 2009; Schneider et al., 2011; Yu and Spaepen, 2004; Jaeger et al., 2006; Hommel and Kraft, 2001; Gruber et al., 2008; Huang and Spaepen, 2000; Rinaldi et al., 2012; Lawrence et al., 2012; Li et al., 2012). For instance, Kiener et al. (2009) have observed a variation of about 200 MPa (maximum difference) in the yield shear strength corresponding to micro-pillars with diameters under 1 micron. In other experimental work, including microcompression tests, microbulge tests, and microtension tests on various FCC and BCC materials, a conspicuous amount of variation is present in the data. The cause of this significant variation was largely categorized into the similar systematic errors as listed by Kiener et al. (2009) and Kraft et al. (2010). These studies suggest the strength in metals at small length scales is strongly dependent on the underlying dislocation mechanisms: how dislocations interact with grain boundaries, interfaces, and various defects which may be present in the crystal. The size effect on small scale metal strength can be addressed rigorously by means of discrete dislocation dynamics (DD).

The DD method is suited for tackling problems where size effects and interfaces are important for two reasons: First the constitutive behavior of a small material volume is captured naturally within the DD simulations, reflecting the effect of both the microstructure and the internal/external geometry of the material e.g., Groh et al. (2009); Second the dynamics of an individual dislocation can be sensitive to any changes in the scale describing the problem, and these changes are directly determined in DD. For example, Deshpande et al. (2005), Benzerga and Shaver (2006), Guruprasad and Benzerga (2008) have performed two dimensional (2D) dislocation dynamics simulations on a planar single crystal both under tension and compression. These studies examined the underlying dislocation mechanisms responsible for the macroscopic response of micro-pillars. Although the 2D dislocation analyses provided useful insights, these analyses lack many key three dimensional (3D) dislocation interactions. 3D-DD analyses of micro-pillars have been performed by an number of investigators. For example, the works of Tang et al. (2007, 2008), Rao et al. (2008), Zbib and Akarapu (2009), El-Awady et al. (2009), Zhou et al. (2010), and El-Awady et al. (2011) show that 3D-DD can capture the dependence of the yield stress on the specimen size, initial dislocation density, and loading conditions. Furthermore through the use of 3D-DD analyses, the large statistical variation in the flow stress was attributed to several factors: loading direction (Zhou et al., 2010), initial dislocation content and boundary conditions (Zbib and Akarapu, 2009; El-Alwady et al., 2009), and density pre-straining (Schneider et al., 2013; El-Awady et al., 2013).

In order to investigate the plastic deformation in finite sizes such as in the cases of micro-pillars and thin films, the conventional dislocation dynamics framework needs to account for surface effects and heterogeneous deformation fields. Experiments show that the deformation field in micro-pillars and thin specimens is heterogeneous and becomes highly localized with increased strain. Yasin et al. (2001) coupled 3D-DD with the finite element method and showed that surface effects cannot be ignored regardless of size, and may result in errors as much as 10%. Akarapu et al. (2010) showed that slip bands with local strains approaching 50% occur in micro-pillars, highlighting the extreme heterogeneity in the strain fields.

Surface effects within the DD framework have been addressed by a number of investigators using the concept of image stresses when dislocations are in finite volumes, while heterogeneous deformation is addressed by coupling DD with continuum plasticity (see a recent review article by Groh and Zbib, 2009). Generally, the solution to the surface effects in DD is based on the superposition method proposed by Van der Giessen and Needleman (1995). The solution is obtained as the sum of two contributions. The first represents the solution for dislocations in an unbounded crystal and the other is the complementary elastic solution needed to satisfy equilibrium at external and internal boundaries. The second solution can be solved in a continuum mechanics way, such as finite element methods, see for example, Van der Giessen and Needleman (1995), Yasin et al. (2001), Martinez and Ghoniem (2002), Zbib and de la Rubia (2002), or the boundary element method, see, for example Fivel et al. (1996) and El-Awady et al. (2008). Khraishi and Zbib (2002) developed a rigorous method to handle the issue of image stresses. The method is semi-analytical/numerical in which they enforce either traction or