ARTICLE IN PRESS

International Journal of Plasticity xxx (2016) 1–16

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Numerical study of the size-dependent deformation morphology in micropillar compressions by a dislocation-based crystal plasticity model

Peng Lin, Zhanli Liu**, Zhuo Zhuang*

Applied Mechanics Lab., School of Aerospace Engineering, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 17 June 2016
Received in revised form 2 September 2016
Available online xxx

Keywords:
A. Dislocations
B. Crystal plasticity
C. Finite elements
Size effect

ABSTRACT

In recent years, size-dependent deformation morphology has been observed in uniaxial micropillar compression experiments. After deformation, large pillar shows a barrel shape while small pillar shows a clear shear band. Meanwhile, one or more slip systems are activated at different sizes. In order to reveal the underlying mechanism of this size-dependent phenomenon, a dislocation-based crystal plasticity model is developed in this paper to simulate the uniaxial compression tests for different sizes of pillars with material imperfection. The simulation results show that: (1) The transition from barrel shape to severe shear with decreasing pillar size is well captured by the newly developed model. Two slip systems operate equally in large pillar and only one slip system is activated in small pillar. (2) The back stress induced by dislocation mutual interactions plays an important role in size-dependent deformation morphology. High back stress in small pillar impedes the second slip system to operate. (3) The critical size of transition from double slip (or multiple slip) to single slip is obtained and it is quantitatively comparable with experiments in a specific case. (4) Material softening is necessary to trigger slip band. It can be concluded that the competition between the short range back stress and the external resolved shear stress results in the transition from barrel shape to shear band during the micropillar compression tests.

1. Introduction

Size-dependent phenomena appear when the sample dimension falls into small scale. These phenomena can be considered at two aspects. Firstly, for overall response, size-dependent flow stress and serrated stress–strain curves of crystal micropillars are observed in uniaxial compression tests (Greer et al., 2005; Kiener and Minor, 2011; Uchic et al., 2004; Volkert and Lilleodden, 2006). Secondly, the local deformation of the pillar, for example, the deformation morphology and microstructure evolution are also size-dependent. Greer (2006) pointed out that small pillars under compression were lack of Stage II work-hardening, that was, small samples tended to deform on an individual slip system instead of activating multiple slip systems. After deformation, large pillars were in barrel shapes with almost homogenous deformation, while small one showed severe shear bands (Dimiduk et al., 2005), see Fig. 1(a). Even loaded in a high-symmetry orientation <100> (Kiener and Minor, 2011), the pillars also revealed a transition from multiple slip to single slip with decreasing diameter, see Fig. 1(b).

---

* Corresponding author. Fax: +86 10 62783014.
** Corresponding author. Fax: +86 10 62783014.
E-mail addresses: liuzhanli@tsinghua.edu.cn (Z. Liu), zhuangz@tsinghua.edu.cn (Z. Zhuang).

http://dx.doi.org/10.1016/j.ijplas.2016.09.001

Please cite this article in press as: Lin, P., et al., Numerical study of the size-dependent deformation morphology in micropillar compressions by a dislocation-based crystal plasticity model, International Journal of Plasticity (2016), http://dx.doi.org/10.1016/j.ijplas.2016.09.001

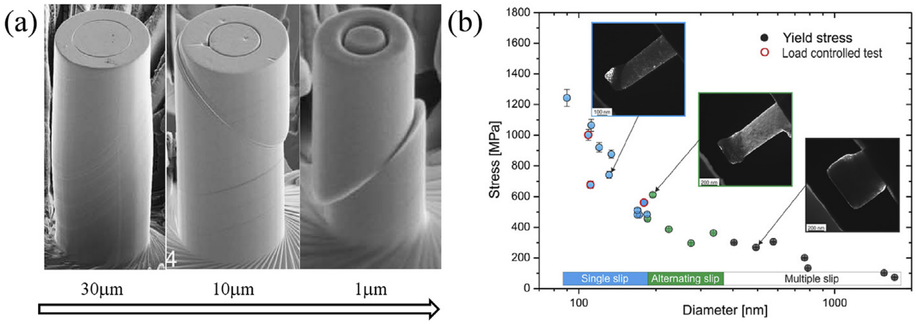

Fig. 1. (a) The transition from barrel shape to shear band with decreasing pillar size, from experiments of Dimiduk et al. (2005); (b) Besides a size effect on strength, a change in the deformation morphology is shown, indicated by differently colored symbols and color bars indicating the regimes, from experiments of Kiener and Minor (2011). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Many researchers have lent their efforts to study the underlying mechanism of the size-dependent flow stress and serrated stress–strain curve. Lots of theoretical and numerical models have been proposed (Akarapu et al., 2010; Akasheh et al., 2007; Csikor et al., 2007; Cui et al., 2014; Greer et al., 2005; Lin et al., 2015; Ohashi et al., 2007; Parthasarathy et al., 2007; Tang et al., 2007) and the size-dependent flow stress and serrated stress–strain curve have been well understood by these models. On the other hand, the size-dependent deformation morphology has not gained enough attention. So far, most studies are focused on the external factors. For example, lateral constraint of the test system had a positive effect on the activation of multiple slip systems (Greer, 2006; Shade et al., 2009) and the deformation mode was observed to be dependent on the aspect ratio of the pillar (Milne et al., 2011; Ouyang et al., 2009). However, the influence of these external factors is not size-dependent and cannot reveal the underlying internal deformation mechanism. The discrete dislocation dynamics (DDD) simulations of Kiener et al. (2011), in which no lateral constraint was involved and the aspect ratio remained the same for different diameters, showed that the discreteness of source distribution could lead to the localization on one slip system in smaller pillars even oriented for multiple slip, while the dislocation density built up in both slip systems from the onset of plastic deformation in larger pillars. Therefore, it is worth studying the internal mechanism causing the size-dependent deformation morphology.

Although DDD simulations mentioned above have shed some light on the size-dependent deformation morphology, they remain a computationally demanding technology for large-scale problems. Besides, DDD simulations involve a relatively high strain rates, which are several orders of magnitude higher than the strain rates found in experiments. These difficulties can be overcome by dislocation-based continuum crystal plasticity theories. Moreover, the continuum crystal plasticity model can be easily implemented by finite element codes, which are more applicable to engineering problems. However, due to the lack of characteristic length, the conventional continuum crystal plasticity theories are unable to describe the size-dependent phenomena. In the last decades, a number of strain gradient plasticity theories have been proposed to describe the plastic behavior at micron scales, for example, Fleck et al. (1994), Fleck and Hutchinson (1997) and Gao et al. (1999). In addition to these isotropic theories, there are two kinds of higher-order crystal plasticity theories, which include the inherent anisotropy of crystal lattice. One involves the evolution equation of crystal slip (Bittencourt, 2014; Gurtin, 2000; Han et al., 2005; Hurtado and Ortiz, 2012; Shu and Fleck, 1999) and the other involves the evolution equation of dislocation density (Arsenlis et al., 2004; Bayley et al., 2006; Evers et al., 2004; Kuroda and Tvergaard, 2006; Yefimov et al., 2004). Most of the theories are based on the introduction of geometrically necessary dislocations (GNDs), which are related to strain gradient. These theories have successfully explained size effects in torsion (Fleck et al., 1994), indentation (Nix and Gao, 1998), and passivated thin films (Xiang and Vlassak, 2005). In these cases, GNDs obviously existed due to the non-uniform deformation. But few were used to explain size-dependent phenomena in uniaxial compression tests. The reason was that strain gradient was thought to be absent in uniaxial compression tests at the early stage (Greer et al., 2005). However, this was not the case highlighted by the recent numerous experiments (Kiener et al., 2011). In particular, in-situ synchrotron work by Maass and Uchic (2012) revealed that both elastic and plastic strain gradients developed during micro-compression testing. Although the strengthening entirely based on GNDs was not sufficient to rationalize size effect in strength, higher-order crystal plasticity theories were capable to explain size-dependent phenomena in small-scale compression tests with some particular considerations, for example, Hurtado and Ortiz (2012), which revealed size-dependent strength of compressed pillars by considering the self-energy of GNDs and the formation energy of dislocation steps on free surface. In ultra-fine grain polycrystals, simulations by strain gradient plasticity have shown that intense slip bands being promoted in smaller specimens (Cordero et al., 2012a,b). So it encourages us to use a strain gradient plasticity model to study the size-dependent morphology in micropillar compressions.

Motivated by the continuum description of the collective behavior of dislocations from Groma et al. (2003), a new dislocation-based crystal plasticity model is developed in this paper. Compared with conventional crystal plasticity models, a micro force equilibrium equation is involved by combining the equation of dislocations motion and Orowan's law. The micro force equilibrium equation contains a GND-related back stress to consider the short range interactions of dislocations. The resulting equation is for crystal slip instead of dislocation density, so it is more convenient when coupling with the macro

Please cite this article in press as: Lin, P., et al., Numerical study of the size-dependent deformation morphology in micropillar compressions by a dislocation-based crystal plasticity model, International Journal of Plasticity (2016), http://dx.doi.org/10.1016/j.ijplas.2016.09.001