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Theoretical and numerical investigations on confined plasticity in micropillars

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ABSTRACT

Multiscale dislocation dynamic simulations are systematically carried out to reveal the dislocation mechanism controlling the confined plasticity in coated micropillar. It is found that the operation of single arm source (SAS) controls the plasticity in coated micropillar and a modified operation stress equation of SAS is built based on the simulation results. The back stress induced by the coating contributes most to the operation stress and is found to linearly depend on the 'trapped dislocation' density. This linear relation is verified by comparing with the solution of the current higher-order crystal plasticity theory and is used to determine the material parameters in the continuum back stress model. Furthermore, based on the linear back stress model and considering the stochastic distribution of SAS, a theoretical model is established to predict the upper and lower bound of stress–strain curve in the coated micropillars, which agrees well with that obtained in the dislocation dynamic simulation.

1. Introduction

Crystal devices in micro-electromechanical systems (MEMS) often have a protective hard coating which makes them exhibit more excellent properties. For example, the coating can greatly improve the erosion or wear resistance, prevent stiction or electrical shorting (Hoivik et al., 2003), and improve thermal stability (Zhuang et al., 2006), etc. However, the deposition of coating also confines the free motion of dislocations in crystal, leading to ultra-high local flow stress during plastic deformation (Greer, 2007; Ng and Ngan, 2009; Gu and Ngan, 2012; Jennings et al., 2012; Lee et al., 2013). Such so-called 'confined plasticity' at microscale will bring new mechanical reliability issues to the MEMS. It is important to reveal the underlying dislocation mechanism and predict the flow stress.

The recent compression experiments for coated micropillars provided a good opportunity to investigate the confined plasticity problem. By carrying out compression tests for Au pillars with diameter 500 nm and 900 nm, Greer (2007) firstly reported that the coated pillar displayed much higher flow stress and a significant amount of linear strain-hardening, which differed substantially from that for pillars with free surfaces. During compression, numerous dislocations were trapped at the pillar-coating interface. Then, Ng and Ngan (2009) pointed out that the overall mechanical response was insensitive to the volume fraction of the coating V_{coating}, when V_{coating} varies from 0.07 to 0.32. These results suggested that load-sharing effect was not important in the considered coated pillars. Moreover, they found that the stress–strain behavior could be smoothened by coating, and strain bursts were effectively suppressed for micropillar with diameter ranging from 1.2 μm to

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6.0 μm and V_{coating} larger than about 0.26. The experimental results by Jenning et al. (2012) further showed that the coating could not fully suppress the strain burst in small pillars with diameter 200 nm and V_{coating} about 0.17, and plastic strain recovery occurred during unloading process.

To assess the microscopic mechanisms associated with the experimental observations, a lot of studies based on discrete dislocation plasticity have been carried out. Zhou et al. (2010) reported that the new mechanical response in the coated pillars was mainly caused by the dislocation pile-up, which could produce high back stress and significantly affect the operation of dislocation sources. At the same time, the role of dislocation cross-slip was emphasized in forming banded dislocation structures. Recently, by performing a series of dislocation dynamics simulations, Lee et al. (2013) reproduced the Bauschinger effect in coated pillars and compared with the experiment in detail. El-Awady et al. (2011) simulated the dislocation penetration process based on Koehler barrier strength criteria, and discussed the influence of barrier strength on strain hardening rate and strain burst. However, the character of dislocation sources in the coated pillar has not been investigated in detail in the studies above, that is very important in understanding and predicting flow stress in the submicron crystal (Benzerga and Shaver, 2006).

At the same time, some theoretical studies have also been performed to develop continuum model to describe the confined plasticity in coated pillars. Recently, Lee et al. (2013) used a simple numerical model to illustrate the coating effect on source operation. He introduced an additional stress term $\Delta\sigma_{\text{coating}}$ to the single arm dislocation source model to consider the dislocation pinning and pile-up effect. However, the value of $\Delta\sigma_{\text{coating}}$ was directly calculated from the experimental sample strength and its evolution was not provided. Thus, it was difficult to be used to predict the mechanical response for the other samples. On the other hand, some researchers try to correlate the high flow stress with the total dislocation density in the coated pillar based on Taylor hardening theory (Ng and Ngan, 2009; Jennings et al., 2012). For large coated pillar, a good correlation was obtained (Gu and Ngan, 2012). However, for small coated pillar ($\sim < 1$ μm), Taylor relation failed. Generally, Taylor relation worked well when the forest dislocation hardening prevailed. Nevertheless, the previous studies (Gu and Ngan, 2012) indicated that the coating could not effectively store the forest dislocations in small sample. The internal mobile dislocations were scarce and most dislocations were trapped at the interface. Hence, in order to develop an appropriate theoretical model for the coated pillar, it is necessary to distinguish the mobile and trapped dislocation densities and establish their relations with flow stress, respectively.

On the other hand, within the realm of continuum mechanics, the gradient crystal plasticity theory is often applied to investigate confined plasticity at microscale. In the strain gradient theory, the expression of geometrically necessary dislocation (GND) and its influence on strain hardening behavior have been extensively studied (Bayley et al., 2006). One typical work is the higher-order crystal plasticity theory developed by Gurtin (2002), in which the back stress associated with the 'trapped dislocations' are incorporated. The back stress is derived from a defect energy term, which is the quadratic function of GND. This model can capture the size effect successfully in several constraint plastic flow problems (Bittencourt et al., 2003; Nicola et al., 2005; Gurtin et al., 2007). However, the physical meaning of defect energy and the length parameters in the theory still needs further exploration. For the coated pillar during plastic deformation, the coating actually introduces a deformation gradient since the coating and micropillar have different mechanical properties. Therefore, the trapped dislocation can be considered as GND, which is automatically maintained to ensure the deformation compatibility (Ohno and Okumura, 2007). In addition, it is always expected that GND are also concentrated near the interface (Cleveringa et al., 1997; Evers et al., 2004). Accordingly, if the evolution of GND and back stress can be obtained by lower scale discrete dislocation simulation, it can be directly used to develop the strain gradient plasticity theory.

Building on the previous studies above, the present work is aimed at gaining further insight into the microscopic deformation mechanisms in coated pillars, especially focusing on the evolution of dislocation density and flow stress. The numerical simulations, which couple the three-dimensional DDD and finite element method (FEM), are performed to simulate the compression of coated Ni pillars. This coupling method is briefly introduced in Section 2 and has been proved to be a powerful approach for studying the underlying dislocation mechanism of submicron plasticity (Van der Giessen and Needleman, 1995; Zbib and Diaz de la Rubia, 2002). According to the simulations, the dislocation mechanism for high flow stress in the coated pillar is further illuminated, and the evolution of the mobile and trapped dislocation density are preliminarily studied in Section 3, respectively. Moreover, some attempts are made in Section 4 to tentatively find the relation between the phenomenological strain gradient theory and the discrete dislocation simulation results. Based on the physical insight, a theoretical model is developed in Section 5 to predict the stress–strain curve in the coated micropillar. Finally, a brief summary is provided in Section 6.

2. Simulation methods

2.1. DDD–FEM coupling method

The DDD–FEM coupling method used in this study has been described in detail in our previous papers (Liu et al., 2009; Gao et al., 2010). In the DDD part, assuming the dislocation motion is in the over-damped regime, the velocity of a dislocation segment can be determined by the total force acting on it divided by the viscous drag coefficient B. Here, the total force includes the Peach–Koehler (PK) force by applied stress and the other defects, line tension, as well as image stress.

The coupling approach is based on eigenstrain theory, and mainly contains the following information-transferring