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A continuum model for intermittent deformation of single crystal micropillars

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ABSTRACT

Strain bursts are often observed during compression tests of single crystal micropillars. In this work, we formulate a new continuum model that accounts for the strain bursts within the framework of crystal plasticity. The strain bursts are separated from the loading stage (nearly elastic loading) by introducing a dimensionless constant in the continuum model, and are detected by load serrations. The boundary conditions in the context of micropillar compression are studied and they are shown to be changing and unpredictable as plastic deformation proceeds. To evaluate the validity of our model, finite element simulations of the uniaxial compression tests on nickel micropillars are performed. Our simulations produce clearly visible strain bursts during the plastic flow and the produced intermittent flows are comparable with the experimental observations. For the bulk crystal, a series of strain bursts is identified in the course of plastic flow, despite an apparently smooth stress–strain response. We also show that the intermittent flow is intensified in the micrometer-scale due to both increasing numbers of the successive strain bursts and increasing amplitude of the strain burst, when the specimen size decreases. Finally, we show that the occurrences of the strain bursts are always associated with negative values of the second-order work.

1. Introduction

The plastic deformation behavior of bulk single crystals have been successfully described by classical continuum mechanics of plasticity, and have been demonstrated to be associated with a steady rate of work hardening. Many recent compression experiments of single crystal micropillars show that their plastic deformations are characterized by large intrinsic fluctuations (strain bursts) and the yield strength is size-dependent (Greer and Nix, 2006; Uchic et al., 2004). These fluctuations that are usually caused by the collective motion of interacting dislocation, lead to a strongly heterogeneous and intermittent nature of plastic flow on microscopic and mesoscopic scales, whereas in bulk crystals plasticity appears as a smooth and homogeneous process. The strain burst phenomenon is suggested to be universal in plasticity and independent of pillar dimensions (Csikor et al., 2007).

To better understand the crystal plasticity at microscopic level, there have been many studies using three-dimensional (3-D) dislocation dynamics (DD) simulations (3D-DDS) (Csikor et al., 2007; Tang et al., 2008) and multiscale modeling (Akarapu et al., 2010). These simulations show that the strain bursts arise from the continuous operation of one or at most a few dislocation sources (Akarapu et al., 2010; Tang et al., 2008) or the destruction of jammed dislocation configurations (Csikor et al., 2007). In particular, some DD techniques could well reproduce the essential aspects of experimental observations on burst activities (Csikor et al., 2007). In addition, numerical algorithms have also been developed to study such activities (Greer and Nix, 2006; Zaiser and Aifantis, 2006; Zhang and Aifantis, 2011). For example, Greer and Nix (2006) developed a numerical iterative algorithm based on the phenomenological model of dislocation starvation, and captured one single strain burst followed by elastic loading. Zhang and Aifantis (2011) have proposed a strain gradient model from the point of view that plastic deformation occurs through slip zones in the gauge region. These slip zones are divided into elastic and plastic zones and a strain burst occurs when two adjacent zones deform plastically. In such models, the predicted results are in good agreement with the experimental stress–strain curves. Besides such simulation efforts, some statistic models have been proposed to study the characteristics of intermittent flow behavior of small microcrystal (Ng and Ngan, 2008; Ngan and Ng, 2010). Although prior knowledge of survival probability of occurrence for burst events and stress-dependent distributions of burst sizes are required as two inputs to incorporate into these models, the calcu-

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lated results successfully predict other aspects of microcrystal deformation in terms of the intermittent stress–strain response, stress-dependent burst size and power-law behavior of burst events. These results are consistent with the experimental observations. Furthermore, such inputs obtained from one loading condition can also be applied to other loading situations such as creep deformation (Ng and Ngan, 2008; Ngan and Ng, 2010). In addition, statistical theory analysis suggests that the mechanism of the burst activities is related to the continuous activation of a few dislocation sources (Ngan and Ng, 2010).

Alternatively, finite element methods (FEM) using continuum models of plasticity such as crystal plasticity or gradient plasticity are comparatively less used to study intermittent plasticity. Although it has been suggested that strain bursts are associated with deformation patterns in the form of slip lines and slip bands (Csikor et al., 2007; Schwerdtfeger et al., 2010), they are not necessarily or may not always give rise to macroscopic deformation instabilities. As observed in submicron diameter compression tests (Greer and Nix, 2006; Uchic et al., 2004), plastic deformation occurs in a non-localized manner until sufficiently larger strain and the experimental stress–strain curves are relatively smooth. As a result, employment of the continuum crystal plasticity theory to obtain a better understanding of micropillar plasticity may be warranted (Hurtado and Ortiz, 2012; Kuroda, 2013). Additionally, the corresponding boundary-value problems may also be well-posed and thus contribute to the uniqueness and convergence of the solutions in the finite element calculations. In fact, finite element simulations using crystal plasticity theory have been conducted to study the influence of extrinsic effects such as friction and sample geometry, which are involved in micro-compression tests (Choi et al., 2007; Raabe et al., 2007; Shade et al., 2009). Furthermore, several finite element implementations of phenomenological models have recently been employed to investigate the effect of physics on micropillar deformation, such as dislocation nucleation and starvation (Jérusalem et al., 2012), or the self-energy of the dislocations and the energy of dislocation steps at the boundary of the solid (Hurtado and Ortiz, 2012), as well as higher-order gradients arising from geometrically necessary dislocation densities (Kuroda, 2013).

All of the above phenomenological FEM analyses have mainly focused on size effects of the yield strength. However, intermittent deformations have not been reflected in these simulations. This is partly because, conventional continuum theories of plasticity do not reflect the characteristics of strain burst and contain no criteria to judge the stain burst, and hence fail in predicting its occurrence. Besides, there is one problem lying in variability and unpredictability of the microscopic boundary conditions (MBCs) as the plastic flow proceeds. For example, many micro-compression tests are driven by hybrid loading mode (HLM) (El-Awady et al., 2013; Papanikolaou et al., 2012; Uchic et al., 2004), in which a mixture of constant displacement rate and creep-like loading conditions are employed. This method produces a staircase-like stress–strain curve, which is characterized by a nearly constant stress within the strain burst period and a purely elastic strain during the loading stage. Normally, the strain bursts are separated by increments of nearly elastic loading stage during the plastic flow (El-Awady et al., 2013). This phenomenon leads to a change of MBCs during plastic deformations, since the loading system responds differently to the burst slip and the loading stage under the condition of HLM (Uchic and Dimiduk, 2005). This means that the MBCs are time-dependent in the plastic deformation process.

In this paper, we focus on the intermittent flow of micropillars and aim to develop a new continuum model to describe such phenomenon. For this purpose, our continuum model takes into account the following key elements: (i) Separation of the burst slip from loading stage: This is motivated by the difference in features between the burst slip and the loading stage. The burst slip occurs at a high strain rate and is associated with stress relaxation. The loading stage, however, is characterized by a slow strain rate and is associated with continuous increase in load; (ii) A criterion to judge the appearance of the stain burst: This is motivated by the loading system, since it responds differently to the burst slip and loading stage (Uchic and Dimiduk, 2005), resulting in different MBCs for the two cases. Thus, the continuum model should contain a criterion to demarcate the burst slip from the loading stage, similar to the yield stress that demarcates the elastic loading from the plastic flow; (iii) Solution of the problems with time-dependent MBCs: This is motivated by the unpredictability of the MBCs, since the occurrence of the burst slips and their amplitudes are unpredictable. In other words, the MBCs are not predetermined.

This paper is organized as follows: In Section 2, the microscopic boundary conditions in the context of intermittent flow are discussed. In Section 3, the continuum model is proposed in the framework of crystal plasticity (Peirce et al., 1983). To verify our model, Section 4 presents the finite element algorithm of implementing our proposed continuum model, and comparisons are made between our present model and the crystal-plasticity finite element method (CPFEM). In Section 5, the finite element simulations of the uniaxial compression tests on face-centered cubic (FCC) nickel micropillars are described. Finally, the results of Sections 4 and 5 are discussed for further improvements of the proposed model in Sections 6, and the conclusions are presented in Section 7.

2. Problem formulation

The problem considered is graphically represented in Fig. 1(a) and (b). Fig. 1(a) shows the actual displacement vs. time curve obtained from the micro-compression tests on a $\sim$20 μm diameter Ni micropillar under conditions of HLM. Fig. 1(b) shows the schematic plot of the micro-compression test driven by the HLM, which is the simplified and idealized representation of Fig. 1(a). Note that a strain burst is generally characterized by a larger strain increment and a smaller time increment (Dimiduk et al., 2006, 2010), indicating a higher strain rate in a burst slip, compared to that of the loading stage. Thus, the curve portion with positive slope in Fig. 1(b), which has a higher rate than that of constant loading, represents the occurrence of a burst slip. The burst slip is followed by a horizontal line or a line with small positive slope, which indicates a holding stage and it lasts until the actual micropillar displacement reaches the imposed displacement by the nanoindentation system. A loading stage may occur after this, associated with the constant strain-rate loading process. On the basis of these observations, a typical plastic flow expressed in the stress–strain curve normally includes three distinct parts: loading stage ΔE^{l}, burst slip part ΔE^{b} and holding stage ΔE^{h}, where superscripts l, b and h represent the above three processes, respectively (see inset in Fig. 1(b)).

2.1. Loading stage

The loading stage involves the motion of few dislocations, while majority other dislocations are relatively immobile, making little or no contribution to the strain. Thus, many of the nearly elastic zones between strain bursts are frequently observed from the stress–strain curves of micro-compression tests (El-Awady et al., 2013; Papanikolaou et al., 2012; Uchic et al., 2004). Such a stage is induced when the applied load becomes comparable to the internal stress of the micropillar, and the displacement on the top surface of micropillar is kept consistent with the pre-programmed displacement of the indention platen controlled by a feedback control loop (see Fig. 1). As a result, the engineering strain increment ΔE^{l} produced by the imposed displacement Δu^{l}, is only determined by the time increment Δt^{l} due to the applied constant strain rate $\dot{\varepsilon}_0$, and it follows that: