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A stochastic crystal plasticity framework for deformation of micro-scale polycrystalline materials

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ABSTRACT

In this paper we investigate the stochastic behavior in the mechanical response of polycrystalline materials consisting of few grains to hundreds of grains at micron size scales. We study the transition from stochastic (at small scale) to deterministic (at large scale) deformation behavior in polycrystalline samples using both simulation and nanoindentation experiments. Specifically, we develop a stochastic crystal plasticity model combining a Monte Carlo method with a polycrystal continuum dislocation dynamics model in a self-consistent viscoplasticity framework. Using this framework, we numerically calculate the mechanical properties of the polycrystal and gather randomized sampling data of the flow stress. The numerical results are compared to nanoindentation experimental data from three samples with ultra-fine grain structures manufactured via the severe plastic deformation method. The controlling mechanisms of the observed stochastic yield behavior of polycrystals are then discussed using simulations and experimental results. Our results suggest that it is the combination of stochastic plasticity at small scales (where the strength may vary from grain to grain) coupled with the effects of microstructural features such as grain size distribution and crystallite orientations that govern the uncertainty in the mechanical response of the polycrystalline materials. The extent of the uncertainty is correlated to the "effective cell size" in the sampling procedure of the simulations and experiments. The simulations and experimental results demonstrate similar quantitative behavior in terms of coefficient of variation within the same effective cell size.

1. Introduction

Recent studies on nano and micro-scale crystalline samples demonstrate a significant statistical distribution in the mechanical properties of the structures within small length scales. Stochastic yield behavior of single crystals has been the subject of many studies using micropillar compression, thin film loading and nanoindentation tests (Uchic et al., 2004; Huang and Spaepen, 2000; Dimiduk et al., 2005; Akarapu et al., 2010; Yu and Spaepen, 2004; Nix and Gao, 1998; Ngan and Ng, 2010; Ng and Ngan, 2008b,a). However, for polycrystalline materials at micron scales the transition between

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the small stochastic length scales to large deterministic scales is rather unclear. The aim of this study is to explain the mechanisms causing the stochastic response observed in the polycrystals.

Plastic behavior of crystalline materials is controlled by the microstructure and its evolution during plastic flow. Dislocation glide, dislocation nucleation, dislocation–defect and dislocation-grain boundary interactions as well as diffusion processes are amongst the examples of deformation mechanisms (Rhee et al., 1994; Hoagland et al., 2002; Uchic et al., 2004; El-Awady et al., 2011; Abdolrahim et al., 2014). Certain features of the microstructure such as dislocation networks, grain boundaries and grain orientations as well as the loading conditions involved during plastic deformation have a defining role in the activity of these deformation mechanisms. In continuum mechanics the existence and the form of the continuum description of the material depends on the scale of the representative volume element (RVE) and the features that can be addressed inside the RVE scale (Berdichevsky and Dimiduk, 2005). From the thermodynamics basis in terms of the continuum description, three distinct scales including small sub-micron scales, intermediate scales to tens of microns and finally large scales of hundreds of microns to millimeters exhibit different mechanical behaviors (Berdichevsky, 2006). The continuum description at each length scale described above has a different form, if it exists.

At large scales, usually on the order of hundreds of microns or more, the scale of the deformation events are multiple orders of magnitude smaller than the dislocation events (Berdichevsky, 2006; Berdichevsky and Dimiduk, 2005). In this case, usually a large RVE contains a large number of microstructural features that represent the homogeneous response to the plastic deformation. At these scales, characteristics of the microstructure such as properties of the dislocation network and the distribution of grain orientations and size are "statistically equivalent" within samples of the same material. Furthermore, plasticity at these scales can be described as the collective behavior of different mechanisms such as dislocation nucleation, defect structure, dislocation bursts and the interaction of dislocations with defects (Akarapu et al., 2010; Zaiser et al., 2008; Shao et al., 2013; Hiratani and Zbib, 2002). A deterministic definition of the continuum description is viable since a well-defined energy based function can be defined to describe plasticity (Berdichevsky, 2006).

Conversely, at small scales, on the order of tens of microns or less, the scale of the deformation events and microstructural features are comparable to the size of the RVE (Berdichevsky and Dimiduk, 2005) often in the range of single crystal structures. At these scales, aside from the conventional size effect due to the strain gradient involved in the deformation process (Fleck et al., 1994; Ma and Clarke, 1995; Nix and Gao, 1998; Stolken and Evans, 1998), there is another intrinsic size effect arising from various parameters such as the characteristics of dislocation networks, defects and interfaces even in the absence of the so called geometrically necessary dislocations (GNDs) (Uchic et al., 2004; Dimiduk et al., 2005; Akarapu et al., 2010). Hence, the continuum representation changes completely compared to large scales, which may lead to the increased sensitivity of the internal energy with respect to small fluctuations in the microstructure. This effect leads to the situation where a deterministic description of the problem may not be applicable anymore. The total energy in the system demonstrates serious fluctuations depending on the microstructural features of the RVE (Berdichevsky, 2006). These features bring in fundamentally different deformation mechanisms with various activation energies. Their contribution to the plastic response of the structure usually leads to highly stochastic response at these length scales.

For the intermediate scales that demonstrate a transition between the stochastic small scales to deterministic large scales, a definition of the continuum local is still possible. The continuum solution is able to describe the deformation behavior, but with a considerable error that arises from fluctuations in the elastic and plastic fields of the small scales (Berdichevsky and Dimiduk, 2005). At these length scales, local deviation of the microstructure leads to scattered observations in yield behavior from one material point to another due to various reasons including differences in Schmid factor, defect density, etc., leading to different equivalent elastic–plastic modulus (Seok et al., 2014). Also, different dislocation substructures lead to various local yield stresses resulting in stochastic plasticity at the grain level (Shao et al., 2013). Although these mechanisms operate at large scales as well, the number of these events are high enough to show an averaged deterministic response. In this study we demonstrate that a combination of the microstructural effects in the polycrystal and stochastic yielding in the crystals themselves are sources of the scatter at these intermediate scales.

The aim of the present work is to determine the source of stochastic response in the yield behavior of polycrystalline materials at intermediate scales and their sensitivity to length scales. For this purpose, a stochastic crystal plasticity model using a Monte Carlo (MC) method combined with a continuum dislocation dynamics viscoplastic self-consistent (CDD-VPSC) model polycrystal (Askari et al., 2014a) is utilized. The mechanical properties of the polycrystal are sampled using numerical simulations as well as nanoindentation experiments in ultra-fine grain materials to validate the findings from the numerical results. Using a MC based approach to determine plasticity at the crystal level based on previously published data on single crystal copper (Shao et al., 2013), the MC results are expanded to the polycrystalline copper samples using experimental microstructural data. The CDD-VPSC model is then used for simulation of polycrystals containing a small number of grains. The MC simulation for sampling the mechanical properties of the polycrystals requires hundreds of trial runs at various length scales. The use of the CDD-VPSC approach combined with the MC method provides a fast and effective stochastic crystal plasticity framework that includes the effects of microstructural features such as grain orientations, grain size and its distribution (Espinosa et al., 2006; Berbenni et al., 2007; Lawrence et al., 2012; Seok et al., 2014). Also, since the formulation is based on dislocation mechanics, it is straightforward to include the effects of stochastic crystal plasticity. This method calculates the homogenized mechanical response of polycrystals including interactions between grains using Eshelby's method (Eshelby, 1957).

The implementation of the stochastic crystal plasticity in our model is based on the physical representation of the dislocation mechanics and nucleation theory. The distribution functions used in the MC calculations are based on the discrete