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ScienceDirect
International Journal of Plasticity 23 (2007) 897–914
INTERNATIONAL JOURNAL OF Plasticity
www.elsevier.com/locate/ijplas

A multiscale approach for modeling scale-dependent yield stress in polycrystalline metals

Tetsuya Ohashi [a,*], Masato Kawamukai [a], Hussein Zbib [b]

[a] *Kitami Institute of Technology, Koencho 165, Kitami, Hokkaido 090-8507, Japan*
[b] *School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164-2920, USA*

Received 18 March 2006; received in final revised form 12 August 2006
Available online 28 November 2006

Abstract

Modeling of scale-dependent characteristics of mechanical properties of metal polycrystals is studied using both discrete dislocation dynamics and continuum crystal plasticity. The initial movements of dislocation arc emitted from a Frank-Read type dislocation source and bounded by surrounding grain boundaries are examined by dislocation dynamics analyses system and we find the minimum resolved shear stress for the FR source to emit at least one closed loop. When the grain size is large enough compared to the size of FR source, the minimum resolved shear stress levels off to a certain value, but when the grain size is close to the size of the FR source, the minimum resolved shear stress shows a sharp increase. These results are modeled into the expression of the critical resolved shear stress of slip systems and continuum mechanics based crystal plasticity analyses of six-grained polycrystal models are made. Results of the crystal plasticity analyses show a distinct increase of macro- and microscopic yield stress for specimens with smaller mean grain diameter. Scale-dependent characteristics of the yield stress and its relation to some control parameters are discussed.

Keywords: A. Dislocations; B. Crystal plasticity; B. Polycrystalline material; B. Constitutive behavior; B. Scale dependency

* Corresponding author. Tel./fax: +81 157 26 9227.
E-mail addresses: ohashi@newton.mech.kitami-it.ac.jp (T. Ohashi), zbib@wsu.edu (H. Zbib).

0749-6419/$ - see front matter
doi:10.1016/j.ijplas.2006.10.002

1. Introduction

Scale-dependent characteristics of mechanical properties of metal polycrystals are well known and are summarized in the form of a Hall–Petch type relation,

$$\sigma = \sigma_0 + k\bar{d}^{-1/2}, \tag{1}$$

where σ denotes strength-related physical quantity such as yield stress, plastic flow stress, tensile strength, and $\bar{d}$ denotes the average grain diameter of the polycrystal or another length scale. In recent years, there have been many efforts to model such effects into the theory of continuum mechanics, and among them, introduction of the concept of plastic strain gradient, or more directly the concept of geometrically necessary dislocations (GNDs), into the framework of the theory induced a wide range of discussion. Density of GNDs has been incorporated in the expression of flow stress (Fleck et al., 1994; Gao et al., 1999; Shu and Fleck, 1999), strain hardening (Acharya and Beaudoin, 2000; Acharya et al., 2003; Ohashi, 2004a, 2005; Akasheh et al., in press), or free energy (Shizawa and Zbib, 1999; Gurtin, 2002; Mesarovic, 2005). Among them, Ohashi (2004a) introduced a new model of crystal plasticity analysis where not only the statistically stored dislocations (SSDs) but also GNDs contributed to the mean free path of moving dislocations, and we successfully reproduced the Hall–Petch type relation of plastic flow stress level. However, scale-dependent characteristics of yield stresses are not yet fully understood in terms of mechanics and there are a lot of points to be studied (for example, Fredriksson and Gudmundson, 2005; Cheong et al., 2005; Khan et al., 2006; Berbenni et al., 2007).

Let us consider the first step of slip deformation in a crystal grain. There should be a variety of defects, including pinned dislocations. Among them, a certain dislocation segment may act as a multiplication source of dislocations when the resolved shear stress on it reaches a critical value. When the grain size is infinite and the lattice friction stress for dislocation movement is zero, a Frank-Read type dislocation source (abbreviated hereafter as FR source) with size λ starts to emit dislocation loops when the resolved shear stress reaches the value (for example, Hull and Bacon, 2001)

$$\tau_\infty = \frac{\mu\tilde{b}}{\lambda}, \tag{2}$$

where μ and $\tilde{b}$ denote the elastic shear modulus and the magnitude of Burgers vector, respectively. The larger the source size λ is the smaller is the critical resolved shear stress. If the size of the crystal grain is finite, the dislocation source length cannot be larger than the grain size, and this fact brings about a strong size effect of yield stress and strain hardening in single crystals (Uchic et al., 2004; Benzerga and Shaver, 2006). Similar and even more complex phenomena are thought to take place in crystal grains in polycrystals (Ohashi and Kawamukai, 2005). As dislocations are emitted from a dislocation source situated inside a grain, they will propagate outwards from the source until they hit grain boundaries which cause resistance to the further movement of dislocations and subsequent emission from the source.

In this paper, we first focus on the initial movement of a dislocation arc that expands from a FR source and its interaction with grain boundaries. To simulate such a process, we use a dislocation dynamics software code and find the minimum resolved shear stress for the FR source to emit at least one closed loop. Results of the dislocation dynamics simulations are then modeled into the expression of critical resolved shear stress of slip