Available online at www.sciencedirect.com
ScienceDirect
Journal of the Mechanics and Physics of Solids 55 (2007) 1879–1898
JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS
www.elsevier.com/locate/jmps

Higher-order stress and grain size effects due to self-energy of geometrically necessary dislocations

Nobutada Ohno*, Dai Okumura

Department of Mechanical Science and Engineering, Nagoya University, Chikusa-ku, Nagoya 464-8603, Japan

Received 23 October 2006; received in revised form 12 February 2007; accepted 18 February 2007

Abstract

The higher-order stress work-conjugate to slip gradient in single crystals at small strains is derived based on the self-energy of geometrically necessary dislocations (GNDs). It is shown that this higher-order stress changes stepwise as a function of in-plane slip gradient and therefore significantly influences the onset of initial yielding in polycrystals. The higher-order stress based on the self-energy of GNDs is then incorporated into the strain gradient plasticity theory of Gurtin [2002. A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. J. Mech. Phys. Solids 50, 5–32] and applied to single-slip-oriented 2D and 3D model crystal grains of size D. It is thus found that the self-energy of GNDs gives a D^{-1}-dependent term for the averaged resolved shear stress in such a model grain under yielding. Using published experimental data for several polycrystalline metals, it is demonstrated that the D^{-1}-dependent term successfully explains the grain size dependence of initial yield stress and the dislocation cell size dependence of flow stress in the submicron to several-micron range of grain and cell sizes.

Keywords: Dislocations; Strengthening and mechanisms; Crystal plasticity; Elastic–plastic material; Metallic material

1. Introduction

It is well known that the yield stress of polycrystalline metals depends on the grain size. According to the Hall–Petch relation, the yield stress has an inverse square-root

*Corresponding author. Tel.: +81 52 789 4475; fax: +81 52 789 5131.
E-mail address: ohno@mech.nagoya-u.ac.jp (N. Ohno).

0022-5096/$ - see front matter
doi:10.1016/j.jmps.2007.02.007

dependence on the grain size. The Hall–Petch relation is an empirical law that and has been verified experimentally. However, nonlinearity can occur in the Hall–Petch plot if the grain size is smaller than about 10 μm (Kimura, 2002). In fact, fine-grained metals have shown nonlinearity in the Hall–Petch plot of initial yield stress *around grain sizes of one to several microns*, where the initial yield stress had a stronger grain size dependence than the inverse square-root used by the Hall–Petch relation (Lloyd, 1980; Kashyap and Tangri, 1995; Yu et al., 2005). It is noted that fine-grained metals tend to clearly exhibit *initial yield points at stresses that depend markedly on the grain size* (e.g., Thompson and Baskes, 1973; Thompson, 1977; Lloyd, 1980; Kashyap and Tangri, 1995; Tsuji et al., 2002; Yu et al., 2005). Breakdown of the Hall–Petch relation has also occurred for the dependence of flow stress on the dislocation cell size in stage II: by plotting the data obtained in several experiments, it was demonstrated that flow stresses satisfy a unique relation which has inverse proportionality to the dislocation cell size (Staker and Holt, 1972). This size dependence, stronger than the inverse square-root, was observed with respect to dislocation cell sizes ranging from submicron to several microns, and hence seems similar to the grain size dependence of initial yield stress in fine-grained metals mentioned above. It is thus worthwhile to analyze the grain size dependence of initial yield stress in the submicron to several-micron range of grain size.

The size effects mentioned above are good targets to be analyzed using the so-called strain gradient plasticity theories, which have been proposed in a number of studies after the initiatory work of Aifantis (1984). The theories can be classified into two groups, i.e., higher-order and lower-order theories. In the higher-order theories, higher-order stress is defined to be the work-conjugate to strain gradient, leading to the necessity of using higher-order governing equations and additional boundary conditions (e.g., Fleck et al., 1994; Fleck and Hutchinson, 1997, 2001; Gao et al., 1999; Gurtin, 2000, 2002; Huang et al., 2000; Menzel and Steinmann, 2000). In the lower-order theories, on the other hand, no higher-order stress is introduced so that governing equations and boundary conditions need not be complicated (e.g., Acharya and Bassani, 2000; Bassani, 2001; Han et al., 2005). Unified treatments of strain gradient plasticity theories have been studied in recent works (Gudmundson, 2004; Kuroda and Tvergaard, 2006).

Gurtin (2000, 2002) developed a higher-order theory of single crystal plasticity by postulating an extended principle of virtual work. In his theory, the higher-order stress called microstress is defined to be the work-conjugate to the slip gradient on each slip system, and slips and displacements are allowed to vary independently of each other. His theory thus permits the constraint of slips to be explicitly prescribed at grain boundaries. This additional boundary condition, referred to as the microclamped condition, is interpreted as no dislocation passing through a grain boundary. Gurtin and Needleman (2005) proposed to replace the microclamped condition by taking account of the Burgers vector in the additional boundary condition of slips. Okumura et al. (2007) employed the Gurtin theory, along with a homogenization method, in order to simulate the grain size dependence of yield behavior of polycrystalline metals. The microclamped condition at grain boundaries then gave a noticeable influence of grain size on the strain hardening rather than the initial yield stress, while the flow of Burgers' vector across grain boundaries resulted in some influence of grain size on the initial yield behavior rather than the strain hardening. It is thus suggested that some other physical factors need to be considered to