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Crystal plasticity modeling and simulation considering the behavior of the dislocation source of ultrafine-grained metal

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Ultrafine-grained metals (UFGMs) produced by warm- or cold-rolling under severe plastic deformation have attracted interest as high-strength structural materials. UFGMs with a grain size less than 1 μm exhibits remarkable material and mechanical properties, and a computational model predicting these properties is desired in the field of materials science and engineering. In order to clarify the utility of UFGM numerically, it is important to investigate the size effects of metallic materials that depend on initial grain size. It is assumed that such unusual mechanical properties originate in grain size and the enormous volume fraction of the grain boundary. When grains are of the submicron order, dislocation loops are hardly generated from Frank–Read sources smaller than the grain size. Grain boundaries play an important role in dislocation dynamics. In this study, we develop a crystal plasticity model considering the effect of the grain boundary and dislocation source. In order to predict variation of critical resolved shear stress (CRSS) due to grain boundaries or dislocation sources, information on dislocation source and grain boundary is introduced into a hardening law of crystal plasticity. In addition, FE simulation for FCC polycrystal is used to analyze stress–strain responses such as increased yield stress and yield point drop, from the viewpoint of grain size and dislocation density. We thoroughly investigate the effect of dislocation behavior on the material properties of UFGMs.

1. Introduction

Ultrafine-grained metals (UFGMs) produced by warm- or cold-rolling under severe plastic deformation have attracted interest as high-strength structural materials (Tsuji et al., 2002; Cho et al., 2004; Kim et al., 2005; Miyajima et al., 2010). UFGMs with a grain size less than 1 μm exhibit remarkable material and mechanical properties (e.g., increased yield stress, decreased hardening ratio, yield point drop of FCC metal (Segal et al., 2006), temperature dependency (Duckham et al., 2003), tension–compression asymmetry (Cheng et al., 2003), and increased strain-rate sensitivity (Sabirov et al., 2009)). A computational model predicting these properties is desired in the field of materials science and engineering. It is assumed that such unusual mechanical properties originate from grain size and the enormous volume fraction of the grain boundary. When grains are of submicron order, few dislocation loops are generated from Frank–Read sources smaller than the grain size. Grain boundaries play important roles in dislocation dynamics. Yang et al. (2009) proposed a model based on the absorption of dislocation pile-up by the grain boundary to explain work softening. Sauvage et al. (2012) demonstrated that grain boundaries of UFGMs differ from regular grain boundaries in atomic structure and stress field.

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In order to clarify the utility of UFGM numerically, it is important to investigate the size effects of metallic materials that depend on initial grain size. Multiscale crystal plasticity models expressing a size effect on grain size have been proposed by introducing information on grain size as a material parameter (Ohashi et al., 2007; Ohno and Okumura, 2007). However, conventional theory cannot express the effect of the grain boundary precisely and directly. Recently, the effect of the grain boundary has attracted the attention of many researchers as an important factor determining the mechanical properties of UFGM. Lim et al. (2011) developed a two-scale method to predict the interactions of dislocations with grain boundaries. Duhamel et al. (2010) investigated the activation volume of UFGMs based on the Cottrell–Stokes law. Gürses and Sayed (2011) proposed a viscoplastic constitutive model based on competing grain boundary and grain interior deformation mechanisms. The mechanical properties of UFGMs are modeled within the framework of the multiparameter microstructural work-hardening model developed by Nes et al. (2005). In addition, studies on a multiscale crystal plasticity model with a hardening law dependent on dislocation density have been conducted by many researchers. A hybrid multiscale calculation method considering dislocation field and deformation field was developed by coupling discrete dislocation dynamics with crystal plasticity theory (Liu et al., 2009; Gao et al., 2010). Groh et al. (2009) constructed a progressive multiscale model bridging three scales: a nanoscale calculated by molecular dynamics simulation, a microscale described by discrete dislocation dynamics, and a mesoscale represented by a crystal plasticity model. Lee et al. (2010) investigated the accuracy of a multiscale crystal plasticity model, comparing precisely the results for single crystals obtained from crystal plasticity simulations based on dislocation density with those from a widely used phenomenological crystal plasticity model. Liu et al. (2011) developed a higher-order crystal plasticity model based on both geometrically necessary (GN) dislocation density and statistically stored (SS) dislocation density in order to predict the crystal plasticity of thin films. A crystal plasticity model considering dislocation based on an intrinsic length scale was proposed by Watanabe et al. (2010) and applied to peculiar yielding characteristics of metals (e.g., yield point elongation). The authors propose a reaction–diffusion system expressing dislocation patterning in order to reproduce the fine graining caused by severe plastic deformation (Aoyagi et al., 2013). In order to investigate the mechanical properties of UFGM from the viewpoint of dislocation behavior, dislocation dynamics whose order is less than submicron and macroscopic deformation should be bridged by multiscale modeling.

In this study, we develop a crystal plasticity model considering the effects of grain boundaries and dislocation sources. In order to predict variation of critical resolved shear stress (CRSS) due to grain boundaries or dislocation sources, information on grain boundaries as dislocation sources is introduced into a hardening law of crystal plasticity. In addition, carrying out FE simulation for FCC polycrystal, stress–strain responses such as increased yield stress are discussed from the viewpoint of grain size and dislocation density. We thoroughly investigate the effect of dislocation characteristics on the material properties of UFGMs.

2. Multiscale crystal plasticity model

2.1. CRSS model considering the effects of grain boundaries and dislocation sources

CRSS approaches the ideal shear strength of a perfect crystal in a region where dislocation density is extremely low because there is no dislocation source or mobile dislocation in the region. In such metals, dislocations should first be generated from grain boundaries. The generated dislocations form new dislocation sources in the grain, and the value of CRSS becomes that of ordinary metal. CRSS is determined by the number of dislocation sources, the existence of grain boundaries, and the dislocation density when the dislocation density is low. In this study, we define the flow stress of crystal plasticity as in Aoyagi et al. (2012) considering information on dislocations and grain boundaries as dislocation sources.

$$g^{(\alpha)} = \tau_d^{(\alpha)} + \min\{\tau_s^{(\alpha)},\ \tau_m^{(\alpha)},\ \tau_g^{(\alpha)}\} \tag{1}$$

Here, $g^{(\alpha)}$ is the flow stress on slip system α, $\tau_d^{(\alpha)}$ is the deformation resistance originating in accumulated dislocations, $\tau_s^{(\alpha)}$ is that originating in the initial dislocation sources, $\tau_m^{(\alpha)}$ is that originating in mobile dislocations, and $\tau_g^{(\alpha)}$ is that originating in grain boundaries. Eq. (1) indicates that plastic deformation is caused by activation of a dislocation source that is most easily activated. Usually, $\tau_d^{(\alpha)}$ is given by the extended Bailey–Hirsch equation (Aoyagi and Shizawa, 2007).

$$\tau_d^{(\alpha)} = \tau_0^{(\alpha)} + \sum_\beta \Omega^{(\alpha\beta)} a\mu\tilde{b}\sqrt{\rho_d^{(\beta)}} \tag{2}$$

Here, $\tau_0^{(\alpha)}$ is the reference resolved shear stress that is the CRSS of single crystal when the dislocation density is zero, $\Omega^{(\alpha\beta)}$ is the dislocation interaction matrix (Ohashi, 1997), a is a numerical factor whose order is 0.1, μ is the elastic shear modulus, $\tilde{b}$ is the magnitude of the Burgers vector, and $\rho_d^{(\beta)}$ is the dislocation density. The reference resolved shear stress $\tau_0^{(\alpha)}$ can be substituted for $\min\{\tau_s^{(\alpha)},\ \tau_m^{(\alpha)},\ \tau_g^{(\alpha)}\}$. However, if $\min\{\tau_s^{(\alpha)},\ \tau_m^{(\alpha)},\ \tau_g^{(\alpha)}\}$ is used instead of $\tau_0^{(\alpha)}$, $g^{(\alpha)}$ approaches zero in the special situation that $\min\{\tau_s^{(\alpha)},\ \tau_m^{(\alpha)},\ \tau_g^{(\alpha)}\}$ is very small. Since the calculation is unstable when $g^{(\alpha)}$ is extremely low, we leave $\tau_0^{(\alpha)}$ in our model. In order to express activation of dislocation due to dislocation sources, $\tau_s^{(\alpha)}$ is modeled as

$$\tau_s^{(\alpha)} = -\frac{1}{2}(\tau_P - \tau_{FR})\tanh\left\{\frac{c}{\rho_{sr}}(\rho_s^{(\alpha)} - \rho_{sr})\right\} + \frac{1}{2}(\tau_P + \tau_{FR}), \tag{3}$$