International Journal of Plasticity 72 (2015) 44–59

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

A dislocation-based model for deformation and size effect in multi-phase steels

Hao Lyu [a,*], Annie Ruimi [b], Hussein M. Zbib [a]

[a] School of Mechanical and Materials Engineering, Washington State University, Pullman, WA, USA
[b] Department of Mechanical Engineering, Texas A&M University, Doha, Qatar

ARTICLE INFO

Article history:
Received 2 January 2015
Received in revised form 21 March 2015
Available online 16 May 2015

Keywords:
Multiscale modeling
Dislocations
viscoplastic material
B. Crystal plasticity
Numerical algorithms

ABSTRACT

In this work, we investigate the mechanical behavior of multi-phase steels using a continuum dislocation dynamic model (CDD) coupled with a viscoplastic self-consistent (VPSC) model that accounts for both the effect of dislocations evolution inside the grain as well as grain–grain interactions. Because the conventional viscoplasticity theory does not capture the grain size effect, we introduce an intrinsic length scale within the concepts of geometrically necessary dislocations (GND) by means of the Nye's dislocation tensor. The effect of the GND density is implemented into the model for the mean free path of dislocations and is shown to contribute to strain hardening. As a validation of this multiscale model, we investigate the mechanical behavior of various dual phase steels. The stress-strain response obtained from this approach is compared to experimental data found in the literature and reveal good agreement between experimental results and predictions. The model also predicts the evolution of dislocation densities in each phase and suggests the connection between underlying deformation mechanisms and macroscopic material hardening. The relation between flow stress and grain size is also investigated. The model predictions follow the Hall–Petch relation of strength versus grain size for grains larger than one micron meter but deviates from this relation for grains in the order of tens of nanometers.

1. Introduction

Many experiments such as micro-bending (Parasiz et al., 2010; Chen et al., 2010; Wang et al., 2003; Shi et al., 2008), micro-torsion (Liu et al., 2012, 2013; Dunstan et al., 2009; Fleck et al., 1994; Gan et al., 2014), micro-indentation hardness test (Mayo and Nix, 1998; Wei and Hutchinson, 2003; Abu Al-Rub and Voyiadjis, 2004), and test of particle-reinforced metal composites (Rhee and Zbib, 1994; Zhu and Zbib, 1995; Chen and Wang, 2002; Dai et al., 2001; Askari et al., 2013) have shown that the mechanical behavior of a material is size dependent at the micron scale and that a relation exists between the material hardening and the size of the specimen. Similarly, testing of polycrystalline materials have shown that the material's strength increases with decreasing grain diameter (Lim et al., 2011), effect commonly referred as Hall–Petch effect. The underlying mechanism for this behavior is that the dislocations pile up on the grain boundaries that act as obstacles to the dislocation

* Corresponding author.
E-mail addresses: hao.lu2@email.wsu.edu, lh84601288@live.cn (H. Lyu).

http://dx.doi.org/10.1016/j.ijplas.2015.05.005
0749-6419/

motion, resulting in hardening. In addition, in the case of multi-phase steels, a size-dependent mechanical response is observed at the micron and submicron scales. For these materials, the existence of an interface makes the deformation mechanism more complicated than for a single crystal material. Mechanical test coupled with material characterization experiments using transmission electron microscopy (TEM) have shown an increase of dislocation density at the phase boundary (Korzekwa et al., 1984; Calcagnotto et al., 2010; Jacques et al., 2001) resulting in a plastic strain gradient. This plastic strain gradient is mostly attributed to an inhomogeneous deformation process between the 'soft' matrix and 'hard' inclusions and is responsible for the hardening of the material. The classical plasticity theory does not take into account an internal length scale and cannot be used to explain the size effects. To capture the size effect, plasticity theories that include strain gradients have been developed over the last two decades and have been shown to be successful in predicting size effects and mechanical response. Among them, the work by Zbib and Aifantis (1992) which is based on the introduction of higher order strain gradients into the flow stress, the work by Fleck and Hutchinson (1997) who proposed a higher-order gradient theory, or more recently the work of Abu Al-Rub and Voyiadjis (2006) who introduced a gradient dependent hardening modulus to account for the length scale. In these models, material hardening is attributed to two types of dislocations: the statistically stored dislocations (SSDs) and the geometrically necessary dislocations (GNDs). SSDs are dislocations that arise as the result of plastic strain, and GNDs are dislocations associated with plastic strain gradient (Nye, 1953; Ashby, 1970). The word "statistically stored" indicates that the dislocations are randomly trapped and material hardening is due to the resistance to gliding that the (mobile) dislocations may experience during local deformation. In addition to this internal resistance to dislocation motion, another type of resistance exists that arise from the GNDs which form in order to accommodate the lattice curvature during non-uniform plastic deformations. Most of the models incorporate the density of GNDs within higher order gradient theories and include its effect directly into the constitutive equations for the flow stress (e.g. Fleck et al., 1994; Fleck and Hutchinson, 1997) or hardening law (e.g. Acharya and Beaudoin, 2000; Acharya et al., 2003). Another approach, proposed by Ohashi (2004, 2005) and Ohashi et al. (2007), is to incorporate this effect in the definition of the effective dislocation mean free path. In this context, the density of GNDs is incorporated into the mean free path of moving dislocations within a multi-scale modeling approach that couples dislocation dynamics with continuum finite element crystal plasticity, and shows a clear scale-dependent yield stress.

Most of the current strain gradient models are phenomenological and simply relate the size-effect to strain gradients. Moreover, when implemented into finite element methods one can simulate only a small number of grains due to the intensity of computation involved in such formulations. In this work, we construct a multi-scale modeling framework to investigate the size effect in single phase, dual phase (DP) or even multiphase materials. The approach we take uses a combination of models that include a discrete dislocation dynamic (DDD) model, a continuum dislocation dynamic (CDD) theory and a viscoplasticity self-consistent (VPSC) model. The VPSC model has been advocated by Lebensohn and Tome in the early nineties (1993, 1994) and has the advantage of possessing a robust self-consistent homogenization method for heterogeneous materials in addition to allowing for more grains and grain interactions in the simulations. On the other hand, the VPSC model does not account for the size effect. As a remedy to this, we introduce the Nye's dislocation tensor into the crystal plasticity formulation. More details about the Nye's dislocation tensor can be found in the works of Shizawa and Zbib (1999) and Hardin et al. (2013). Briefly, it uses the strain gradient in each grain on a periodic grid and appears into the mean free dislocation path as a GND density. The multi-scale theory and methodology is outlined in Section 2. Then, in Section 3, the developed multiscale model is used to investigate the mechanical behavior of dual phase (ferrite phase and martensite phase) steels subjected to tensile loading.

2. Theory and methodology

2.1. Two-phase viscoplasticity at mesoscale

Here, we illustrate how we applied the VPSC model to capture the special features of two-phase materials at mesoscale. This model is based on finite deformation theory combined to a homogenization scheme that yields average quantities of a representative volume element (RVE) that includes many grains. The polycrystal is represented by grains with orientations and weight density (volume fractions of grains in the same orientation). Each grain is considered as an ellipsoidal viscoplastic inclusion embedded into an effective anisotropic viscoplastic medium. In the grain domain, it is assumed that the stress and strain fields are homogeneous and that two kinds of phase are under homogenized shear stress. The velocity gradient of a two-phase material with *A*- and *B*-phase can be expressed as (Houtte, 1978; Kalidindi, 1998).

$$L^P = (1-f)\sum_{\alpha=1}^{N^A} \dot{\gamma}^{\alpha} \mathbf{s}^{\alpha} \otimes n^{\alpha} + f \sum_{\beta=1}^{N^B} \dot{\gamma}^{\beta} s^{\beta} \otimes n^{\beta} \quad (1)$$

where f is the volume fraction of *B*-phase, and the N^A and N^B stand for the number of active slip systems in *A*- and *B*-phase, respectively. The symbols $\boldsymbol{s}^{\alpha}$ and $\boldsymbol{n}^{\alpha}$ represent the unit vector in the slip direction and normal to the slip system α, *respectively*. In passing we note that the effect of twinning can also be included in Equation (1) (see, e.g. Askari et al., 2014), but it is not considered in this work. Instead of using the more common phenomenological power law for the shearing rate $\dot{\gamma}^{\alpha}$, we introduce the Orowan relation (Orowan, 1940) i.e.