Journal of the Mechanics and Physics of Solids 84 (2015) 230–253

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

A continuum model for dislocation dynamics in three dimensions using the dislocation density potential functions and its application to micro-pillars

Yichao Zhu, Yang Xiang*

Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

ARTICLE INFO

Article history:
Received 22 September 2014
Received in revised form
14 July 2015
Accepted 27 July 2015
Available online 29 July 2015

Keywords:
Dislocation density
Crystal plasticity
Continuum model
Size effect
Micro-pillars
Finite elements

ABSTRACT

In this paper, we present a dislocation-density-based three-dimensional continuum model, where the dislocation substructures are represented by pairs of dislocation density potential functions (DDPFs), denoted by ϕ and ψ. The slip plane distribution is characterized by the contour surfaces of ψ, while the distribution of dislocation curves on each slip plane is identified by the contour curves of ϕ which represents the plastic slip on the slip plane. By using DDPFs, we can explicitly write down an evolution equation system, which is shown consistent with the underlying discrete dislocation dynamics. The system includes (i) a constitutive stress rule, which describes how the total stress field is determined in the presence of dislocation networks and applied loads; (ii) a plastic flow rule, which describes how dislocation ensembles evolve. The proposed continuum model is validated through comparisons with discrete dislocation dynamics simulation results and experimental data. As an application of the proposed model, the "smaller-being-stronger" size effect observed in single-crystal micro-pillars is studied. A scaling law for the pillar flow stress σ_{flow} against its (non-dimensionalized) size D is derived to be $\sigma_{\text{flow}} \sim \log(D)/D$.

1. Introduction

It is widely agreed that plasticity theories that properly integrate the accumulated knowledge in small-scale physics can facilitate the design of high-end materials. The continuum crystal plasticity (CCP) theories (e.g. Rice, 1971; Peirce et al., 1983; Fleck and Hutchinson, 1993; Nix and Gao, 1998; Gurtin, 2002) have shown their values in understanding the elasto-plastic behavior of crystals, but they are still phenomenological. On the other hand, the (three-dimensional) discrete dislocation dynamical (DDD) models take the dislocation microstructural evolution into account based on the fact that plastic deformation of crystals is carried out by the motion of a large number of dislocations (e.g. Kubin et al., 1992; Zbib et al., 1998; Fivel et al., 1998; Ghoniem et al., 2000; von Blanckenhagen et al., 2001; Weygand et al., 2002; Xiang et al., 2003; Benzerga et al., 2004; Quek et al., 2006; Arsenlis et al., 2007; Rao et al., 2007; El-Awady et al., 2008; Tang et al., 2008; Senger et al., 2008; El-Awady et al., 2009; Chen et al., 2010; Zhao et al., 2012; Zhou and LeSar, 2012; Ryu et al., 2013; Zhu et al., 2013; Zhu and Chapman, 2014b; Wang et al., 2014). In DDD models, dislocations are treated as line singularities embedded into an elastic medium. The kinematics of individual dislocations is governed by a collection of laws for dislocation gliding, climb,

* Corresponding author.
E-mail address: maxiang@ust.hk (Y. Xiang).

http://dx.doi.org/10.1016/j.jmps.2015.07.015
0022-5096/

multiplication, annihilation, reaction, etc., and the microstructural changes within crystals are then captured by the evolution of dislocation curves. DDD models have been well applied to provide insights in understanding many plastic deformation processes observed in micro- or nano-crystalline structures, such as in thin films and interfaces (e.g. von Blanckenhagen et al., 2001; Weygand et al., 2002; Quek et al., 2006; Zhou and LeSar, 2012; Wang et al., 2014) and in micropillars (e.g. Rao et al., 2007; El-Awady et al., 2008; Tang et al., 2008; Senger et al., 2008; El-Awady et al., 2009; Ryu et al., 2013). However, three-dimensional DDD models become too computationally intensive when the specimen size exceeds the order of several microns.

Therefore, a successful dislocation-density-based theory of plasticity (DDBTP) whose associated length scale lies between CCP's and DDD's is still highly expected. The development of DDBTP dates back to the works of Nye (1953), where a dislocation network is represented by a continuously distributed second-order tensor, known as the Nye dislocation tensor. Nowadays with more knowledge in physics taking place on smaller scales, a successful DDBTP should be constituted by laws that are consistent with the underlying discrete dislocation dynamics from the following two aspects: (i) a constitutive stress rule to determine the stress field in the presence of a continuous dislocation density distribution and applied loads; (ii) a plastic flow rule to capture the motion of dislocation ensembles (in response to the calculated stress field), which results in plastic flows in crystals.

As the simplest dislocation configuration, systems of straight and mutually parallel dislocations have been analyzed relatively well at the continuum level (e.g. Groma et al., 2003; Berdichevsky, 2006; Voskoboinikov et al., 2007; Kochmann and Le, 2008; Hall, 2011; Oztop et al., 2013; Geers et al., 2013; Le and Guenther, 2014; Schulz et al., 2014; Zhu and Chapman, 2014a; Le and Guenther, 2015). In this case, each dislocation can be treated as a point singularity in a plane that is perpendicular to all dislocations. As a result, the Nye dislocation density tensor is reduced to several scalar dislocation density functions. The geometric complexity of the dislocation networks is dramatically reduced in this case. However, the development of three-dimensional DDBTP is still far from satisfactory despite a number of valuable works (e.g. Nye, 1953; Kroener, 1963; Kosevich, 1979; Nelson and Toner, 1981; Mura, 1987; Head et al., 1993; El-Azab, 2000; Acharya, 2001; Svendsen, 2002; Arsenlis and Parks, 2002; Sedláček et al., 2003; Alankar et al., 2011; Sandfeld et al., 2011; Engels et al., 2012; Hochrainer et al., 2014; Li et al., 2014; Cheng et al., 2014). One of the main barriers in establishing a successful three-dimensional theory is due to the fact that the complex networks of curved dislocation substructures make the upscaling of discrete dislocation dynamics extremely difficult.

To overcome such difficulties, Xiang (2009) introduced the idea of a coarse-grained disregistry function (CGDF), which is defined to approximate the exact disregistry function (plastic slip) used in the Peierls–Nabarro models (Peierls, 1940; Nabarro, 1947; Xiang et al., 2008), by a smoothly varying profile without resolving details of dislocation cores. By this way, the density distribution of a discrete curved dislocation network in a single slip plane (after local homogenization) can be simply represented by the scalar CGDF (more precisely, the spatial derivatives of CGDF), and dislocation dynamics on the slip plane at the continuum level is explicitly formulated in terms of the evolution of the CGDF (Zhu and Xiang, 2010). Using this representation of CGDF for dislocation density distribution, connectivity condition of dislocations is automatically satisfied. The underlying topological changes of dislocations are automatically handled by the evolution equation of the CGDF, and no law for dislocation annihilation needs to be further imposed. The dynamics of dislocations in the continuum model is derived from the DDD model, and the dislocation velocity in the continuum model depends on a continuum version of the Peach–Koehler force on dislocations. It has been rigorously shown by Xiang (2009) that in the continuum model, the Peach–Koehler force due to the resolved shear stress of a family of curved dislocations can be decomposed into a long-range dislocation interaction force and a short-range self-line tension force, and they can both be expressed in terms of the spatial derivatives of CGDFs. The Frank–Read source, which is one of the major mechanisms for dislocation multiplication, is also well incorporated into this continuum framework (Zhu et al., 2014). As one application of this continuum model using CGDFs, a two-dimensional Hall–Petch law, which relates the flow stress of a polycrystal not only to the physical dimension of its constituent grains, but also to the grain aspect ratio, is derived without any adjustable parameters (Zhu et al., 2014).

In this paper, we generalize our previous single-slip-plane model to that for dislocation ensembles in three-dimensions, where the density distribution of dislocations is locally co-determined by an in-plane dislocation density distribution and a slip plane distribution. To take into account the spatial variation from these two aspects, we define a pair of *dislocation density potential functions* (DDPFs) for each active slip system. One DDPF ψ is employed to describe the slip plane distribution (after local homogenization) by its contour surfaces, and the other DDPF ϕ is defined such that ϕ restricted on each slip plane describes the plastic slip across the slip plane and identifies the density distribution of dislocation curves (after local homogenization) on that plane. Here we name ϕ and ψ by density potential functions, because the Nye dislocation density tensor is represented in terms of the spatial derivatives of these two functions. As our previous continuum model in a single slip plane (Xiang, 2009), the major advantage of this three-dimensional continuum model lies in its simple representation of distributions of curved dislocations (after local homogenization) using two scalar DDPFs, which automatically satisfies the connectivity condition of dislocations.

To derive the constitutive stress rule in the continuum framework with the DDPFs, we sequentially express the Nye dislocation density tensor, the plastic distortion and the elastic strain tensor in terms of the DDPFs. As in our previous continuum model in a single slip plane (Xiang, 2009), the continuum Peach–Koehler force due to the resolved shear stress consists of a long-range dislocation interaction force and a short-range self-line tension force. The long-range stress field is determined by the derived constitutive stress rule and the equilibrium equations along with boundary conditions, and a finite element (FE) formulation is proposed to compute this long-range stress field. The local self-line tension effect can be