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A continuum model for dislocation dynamics incorporating Frank–Read sources and Hall–Petch relation in two dimensions

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ABSTRACT

One of the main targets in the development of dislocation based continuum crystal plasticity theories is to establish continuum constitutive relations which approximately summarize the underlying discrete dislocation dynamics (DDD). However, rigorously transiting from discrete to continuum in describing the evolution of dislocation system is extremely challenging for complex networks of curved dislocations and their interactions at multiple length scales. To address this difficulty, a coarse-grained disregistry function (CGDF) was proposed to represent the continuous distributions of curved dislocations. In this paper, we present a dislocation based continuum model for crystal plasticity incorporating the Frank–Read sources, which serves as a crucial step towards systematically building a three-dimensional dislocation based continuum plasticity theory. The continuum model is derived accurately from the DDD model, and is validated by comparisons of the results with theoretical predictions and DDD simulations conducted under the same conditions. Furthermore by considering dislocation loop pileups within a rectangular grain, we derive analytical formulas which generalize the traditional Hall–Petch relation into two dimensions without any adjustable parameters. It is shown that the yield stress of a rectangular grain depends not only on the grain size, but also on the grain aspect ratio whose exact form is associated with the harmonic mean of the length and width of the rectangle. The derived formulas of the yield stress are shown in excellent agreement with the results by our continuum model and DDD simulations.

1. Introduction

Developing dislocation based plasticity theories has been an active research area along with the development of dislocation theory, and is quite challenging due to the multiscale nature resulting from the discreteness and inhomogeneity of distributions and dynamics of dislocations (Hirth and Lothe, 1982; Argon, 2008). A large number of models proposed to understand the elastic–plastic behaviors of crystals are under the framework of continuum mechanics. In the classical continuum plasticity theories, the deformation process is described based on the (multiplicative) decomposition of the total deformation gradient into an elastic part and an inelastic part, while the microstructural changes are implicitly described by the evolution equations of a set of internal state variables. These phenomenological theories lack the ability to include some important effects such as the size-dependent effect, which has been observed experimentally and are believed to be

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crucial in materials designed for the needs arising in advanced applications. Although improvements have been proposed such as the gradient plasticity theories to describe the size-dependent effect (e.g. Fleck and Solids, 1993; Nix and Gao, 1998; Gurtin, 2002; Svendsen, 2002; Aifantis and Ngan, 2007; Counts et al., 2008; Polizzotto, 2009), these models do not incorporate much information of the underlying dislocation mechanisms that govern the plastic deformation process.

The discrete dislocation plasticity theories, on the other hand, focus on the dynamics of individual dislocations, which are considered as line singularities embedded into an elastic medium. Theories in this group are generally based on the discrete dislocation dynamics (DDD) simulations where the evolving dislocations are represented by a set of transporting line segments. The long-range elastic interaction between dislocation segments can then be numerically calculated by using the Peach–Koehler force formula, and nonlinear short-range interactions are included by assigning respective rules for micromechanisms such as dislocation annihilation, reaction, glide, climb, and cross-slip (e.g. Kubin et al., 1992; Moulin et al., 1997; Zbib et al., 1998; Fivel et al., 1998; Faradjian et al., 1999; Ghoniem et al., 2000; Gómez-García et al., 2000; von Blanckenhagen et al., 2001; Weygand et al., 2002; Xiang et al., 2003; Han et al., 2003; Benzerga et al., 2004; Xiang and Srolovitz, 2006; Arsenlis et al., 2007; Benzerga, 2008; Shishvan et al., 2008; Mordehai et al., 2008; Gao et al., 2011; Zhao et al., 2012; Fitzgerald et al., 2012; Zhou and LeSar, 2012; Keralavarma et al., 2012; Zhu et al., 2013; Chu et al., 2013; Huang et al., 2014). Although DDD simulations serve to reflect the underlying physics on the length scale of dislocation networks during plastic straining, their applications are still confined to materials of small size, due to heavy computational intensities.

Therefore, theories with a good trade-off between resolution (i.e. microstructural information is properly accounted for) and efficiency (being applicable to crystals of size larger than the order of 10 μm) across multiple length and time scales are still highly expected in the study of crystal plasticity. One way to address this purpose is to explore the dislocation-based continuum plasticity theory, that is, to study the evolution of dislocation systems at the continuum level (roughly about 1 μm to 100 μm). One of the main targets in such theories is to establish continuum constitutive relations which approximately summarize the underlying discrete dislocation dynamics. Such constitutive relations include appropriate descriptions for the long-range and short range dislocation–dislocation interactions, the plastic flow induced by dislocation motion, multiplication, annihilation, etc. For the simplest case, the collective behaviors of system of straight parallel dislocations have been studied relatively well (e.g. Groma et al., 2003; Voskoboinikov et al., 2007; Kochmann and Le, 2008; Liu et al., 2011; Oztop et al., 2013; Geers et al., 2013; Zhu and Chapman, 2014). There are also continuum dislocation based plasticity models in which a scalar dislocation density is employed for each slip system without considering the orientations of dislocations (e.g. Krasnikov et al., 2011; Basirat et al., 2012; Engels et al., 2012; Babu and Lindgren, 2013; Li et al., 2014). Some multiscale models that couple DDD simulations with continuum models have been proposed (Zbib and de la Rubia, 2002; Liu et al., 2009). The development in systematically building three-dimensional dislocation based continuum theories, however, is still far from satisfactory despite a number of valuable works (e.g. Nye, 1953; Kröner, 1963; Kosevich, 1979; El-Azab, 2000; Acharya, 2001; Arsenlis and Solids, 2002; Sedláček et al., 2003; Sandfeld et al., 2011; Mayeur and McDowell, 2014; Cheng et al., 2014). The main difficulty in establishing such continuum theories lies in the fact that the complex geometries of curved dislocation ensembles and the associated multiscale interactions make it extremely challenging to rigorously summarize for explicit laws consistent with what takes place on the DDD scales.

To overcome this difficulty, the idea of the coarse-grained disregistry function (CGDF) was proposed by Xiang (2009). The exact disregistry functions were used in the Peierls–Nabarro models (Peierls, 1940; Nabarro, 1947; Xu and Argon, 2000; Xiang et al., 2008) to describe the distribution of the Burgers vectors of dislocations in their slip planes, and take the profile of a regularized jump with height of a Burgers vector representing the dislocation core when passing through a dislocation. The CGDF is to approximate the exact disregistry function by a smoothly varying profile without resolving details of the dislocation cores, so that each contour of CGDF with integer value of b – the magnitude of the Burgers vector – describes a dislocation curve. This smooth CGDF is then employed to represent continuous distribution of dislocation ensembles. Advantages in adopting such a way of representation are straightforward: (1) The geometric information of dislocation microstructures necessary for continuum models, such as the dislocation line direction and curvature, are contained in the CGDF and its spatial derivatives; (2) the Nye dislocation density tensor (Nye, 1953; Kröner, 1963) can be reproduced in terms of the CGDF; and (3) the total plastic strain is associated with the integral of this CGDF over the slip plane.

Based on the CGDFs, a continuum model for the Peach–Koehler force on dislocations in a slip plane was derived from the DDD model by asymptotic analysis (Xiang, 2009). The continuum Peach–Koehler force contains both the long-range force and an accurate form of the local force due to the line tension effect of dislocations. It is essential to include the dislocation line tension force accurately in a continuum plasticity theory because it plays crucial roles in many important dislocation processes such as particle strengthening (Orowan, 1948; Friedel, 1956; Argon, 2008). The plastic flow induced by dislocation motion is governed by evolution equations of the CGDFs (Zhu and Xiang, 2010). Such representation of continuous distributions of dislocations by the CGDFs and the accurate continuum Peach–Koehler force provide a basis for further developing a continuum model incorporating the Frank–Read source (Frank and Read, 1950; Hirth and Lothe, 1982), which is one of the major mechanisms for dislocation multiplication in plastic deformation and in which dislocation line tension effect also plays crucial role. This is one objective of this paper.

When a Frank–Read source is activated, a dislocation segment pinned at both ends bows out in response to the applied shear stress, resulting in a series of dislocation loops. The classical theory of the Frank–Read source is based on the line tension approximation of dislocations and the critical stress is determined when the bowing-out dislocation segment has the shape of a half circle (Frank and Read, 1950). Foreman (1967) obtained the critical stress and shape of the Frank–Read source