International Journal of Plasticity 67 (2015) 1–25

Contents lists available at ScienceDirect

International Journal of Plasticity

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

A new dislocation-density-function dynamics scheme for computational crystal plasticity by explicit consideration of dislocation elastic interactions

H.S. Leung, P.S.S. Leung, B. Cheng, A.H.W. Ngan *

Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, PR China

ARTICLE INFO

Article history:
Received 22 March 2014
Received in final revised form 23 July 2014
Available online 2 October 2014

Keywords:
Crystal plasticity
Dislocations
Dislocation-density functions
Stress–strain behavior
Size effect

ABSTRACT

Current strategies of computational crystal plasticity that focus on individual atoms or dislocations are impractical for real-scale, large-strain problems even with today's computing power. Dislocation-density based approaches are a way forward but a critical issue to address is a realistic description of the interactions between dislocations. In this paper, a new scheme for computational dynamics of dislocation-density functions is proposed, which takes full consideration of the mutual elastic interactions between dislocations based on the Hirth–Lothe formulation. Other features considered include (i) the continuity nature of the movements of dislocation densities, (ii) forest hardening, (iii) generation according to high spatial gradients in dislocation densities, and (iv) annihilation. Numerical implementation by the finite-volume method, which is well suited for flow problems with high gradients, is discussed. Numerical examples performed for a single-crystal aluminum model show typical strength anisotropy behavior comparable to experimental observations. Furthermore, a detailed case study on small-scale crystal plasticity successfully captures a number of key experimental features, including power-law relation between strength and size, low dislocation storage and jerky deformation.

1. Introduction

The concept of crystal dislocations has been coined for over a century, with a huge knowledge base on how single dislocations behave, or how they interact in individual events, gathered for a wide range of crystalline (See above-mentioned references for further information.)materials. On the other hand, although crystal plasticity has to take place in units of dislocations, decades of experience have witnessed the impracticalities involved in computing all the participating dislocations, given that they can quickly multiply to very large quantities during plastic deformation. The introduction of atomistic molecular dynamics (MD) simulation in the 1960s has allowed the cores of dislocations to be studied (Vitek et al., 1970; Vitek, 1974). However, despite computer speeds are faster than ever before, and new rare-event sampling and other computational methodologies have been developed, MD simulations are still limited to nano- space and time scales which are far too small compared to most engineering applications of interest, and it is hard to see how such a bottleneck can be circumvented in the future. In the 1990s, discrete dislocation dynamics (DDD) emerged as a dislocation plasticity simulation technique which deals with the evolution of individual dislocation lines according to their laws of motion (Amodeo and Ghoneim, 1990;

* Corresponding author.
E-mail address: hwngan@hku.hk (A.H.W. Ngan).

http://dx.doi.org/10.1016/j.ijplas.2014.09.009
0749-6419/

Devincre and Condat, 1992; Devincre and Kubin, 1997; Bulatov et al., 1998; Bulatov and Cai, 2006). In this approach, however, each curved dislocation line is discretized into short linear segments and very expensive calculation is performed on each of these to predict their trajectories according to their very complicated line-tension and mutual interaction effects. Therefore, although promising results have been demonstrated for situations with relative small quantities of dislocations, this method is impractical for higher dislocation quantities due to the amount of computation involved. DDD is therefore self-limiting at increasing strains, and is not practical for situations where patterns of dense dislocations develop (Walgraef and Aifantis, 1985; Aifantis, 1986; Hähner, 1996; Ngan, 2005; Pontes et al., 2006), although observations from DDD simulations can be fed into a continuum crystal plasticity model as a multi-scale approach, to predict more realistic behaviors (Devincre et al., 2008).

In stark contrast with these approaches which emphasize on individual atoms or dislocation segments, a number of researchers have advocated the use of a modeling strategy that focuses on dislocation density (Walgraef and Aifantis, 1985; Groma, 1997; Acharya, 2001; Arsenlis et al., 2004; Zhou and Sun, 2004; Evers et al., 2004; Yefimov and Van der Giessen, 2005; Pontes et al., 2006; Ma et al., 2006; Hochrainer et al., 2007; Lee et al., 2010; Watanabe et al., 2010; Alankar et al., 2011; Hirschberger et al., 2011; Bargmann et al., 2011; Liu et al., 2011; Shanthraj and Zikry, 2012; Engels et al., 2012; Aghababaei and Joshi, 2013; Li et al., 2014). Unlike DDD which becomes handicapped at high strains, such a strategy would be well suited for large-strain problems with high quantities of dislocations, since any amount of dislocations can still be represented a dislocation density. The earlier group of dislocation-density models deals with discrete categories of dislocation density, such as mobile vs. immobile, cell-interior vs. cell-wall, and edge vs. screw (Roters et al., 2000; Prasad et al., 2005; Ma et al., 2006; Alankar et al., 2011; Vinogradov et al., 2012), but without considering the field nature of the dislocation densities and the conservative nature of their motion (Walgraef and Aifantis, 1985). A more sophisticated group of approach focuses primarily on the kinematics or dynamics of slip systems (Asaro and Rice, 1977) and their relationships to densities of dislocations. Typically, the shear of slip systems against a critical resolved shear stress governed by certain basic dislocation-level physics, such as Taylor's forest hardening, is considered (Busso et al., 2000; Dunne et al., 2007, 2012; Alankar et al., 2009; Cordero et al., 2012). Other models have focused on dislocation densities as continuous functions of space, with conservation including generation and annihilation duly taken into account (Acharya, 2001; Arsenlis et al., 2004; Zhou and Sun, 2004; Evers et al., 2004; Yefimov and Van der Giessen, 2005; Pontes et al., 2006; Hochrainer et al., 2007; Hirschberger et al., 2011; Bargmann et al., 2011; Puri et al., 2011). These models are based on crystal kinematics rules which govern the relationship between the evolution of geometrically necessary dislocations (GNDs) and the rate of change of the crystal shape (Asaro and Rice, 1977). In doing so, the statistically stored dislocations (SSDs) are modeled much less rigorously, and so the interactions between dislocations and the internal stresses are not completely described.

Still within the framework of crystal kinematics, other models have featured improved descriptions of the internal stresses that resist slip. In the "field dislocation mechanics" (FDM) and "phenomenological mesoscale field dislocation mechanics" (PMFDM) models developed by Acharya and co-workers (Acharya, 2001; Taupin et al., 2008; Puri et al., 2011), the crystal kinematics laws for the GND evolution are modified to include the effects of lattice incompatibility in the plastic and elastic deformation matrices due to the presence of the dislocations themselves. The evolution of the GNDs is coupled to that of SSDs, the motion of which is modeled in terms of a phenomenological back-stress interaction resistance which involves empirical hardening and recovery coefficients (Puri et al., 2011). The models by Yefimov and Van der Giessen (2005) and Hirschberger et al. (2011) also involve a similar empirical back stress resistance, which lacks details of the long-range elastic interactions between dislocations. In the model by Arsenlis et al. (2004), a configurational resistance is also involved which is an empirical back stress pertinent only to elastic interactions in 2-D dislocation arrays (Groma et al., 2003). In the recent approach by Bertin et al. (2013), the coupled evolutions of GNDs and SSDs are also considered, and for the SSDs, a virtual loop concept is involved to sample interactions for different line orientations.

Another line of development to capture realistic dislocation interactions was made by Hochrainer and co-workers (Hochrainer et al., 2007; Zaiser et al., 2007; Sandfeld et al., 2010, 2011). In their continuum dislocation dynamics (CDD) theory, the curvature and line-tension effects of dislocations are emphasized as the main factors contributing to the internal stress, in addition to Taylor's interactions. The inclusion of the dislocation curvature requires its evolution to be modeled as a coupled problem with the evolution of the dislocation density, and this inevitably greatly increases the computational efforts needed (Sandfeld et al., 2011). For this reason, successful numerical implementation has been limited to situations involving crude discretization of the line-direction space (Zaiser et al., 2007), or very simple slip-system configurations (Zaiser et al., 2007; Sandfeld et al., 2010, 2011). While this approach is elegant, efficient numerical implementation algorithms are yet to be developed for problems involving realistic dislocation microstructures. Moreover, this approach highlights the "self" line tension and Taylor hardening as the only internal stresses (Zaiser et al., 2007; Sandfeld et al., 2011), while the long-range elastic interactions between dislocation groups are not modeled.

The above summary points to the fact that an accurate description of the mutual elastic interactions between dislocations has been a critical issue in developing realistic dislocation-density models. In this paper, we propose a new formulation which fully considers such mutual elastic interactions between 3-D dislocation densities, in an exact manner without involving any *ad hoc* back-stress assumption as in some of the previous models. This is made possible by generalizing the elastic interactions between dislocation segments (Hirth and Lothe, 1992) for dislocation densities, and reducing the line-integral formulation involved into an algebraic form comprising only elementary functions which are straightforward enough for efficient numerical implementation. Also, instead of separating the dislocation population into GNDs and SSDs as in the previous crystal-kinematics-based models, we use a fully dynamics approach which is similar to that used in MD and DDD