Journal of the Mechanics and Physics of Solids 95 (2016) 132–146

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Strain hardening in 2D discrete dislocation dynamics simulations: A new '2.5D' algorithm

S.M. Keralavarma [a,b,*], W.A. Curtin [b]

[a] Department of Aerospace Engineering, Indian Institute of Technology Madras, Chennai 600036, India
[b] Institute of Mechanical Engineering, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

ARTICLE INFO

Article history:
Received 17 May 2016
Accepted 20 May 2016
Available online 24 May 2016

Keywords:
Dislocations
Strengthening mechanisms
Crystal plasticity
Constitutive behavior
Numerical algorithms

ABSTRACT

The two-dimensional discrete dislocation dynamics (2D DD) method, consisting of parallel straight edge dislocations gliding on independent slip systems in a plane strain model of a crystal, is often used to study complicated boundary value problems in crystal plasticity. However, the absence of truly three dimensional mechanisms such as junction formation means that forest hardening cannot be modeled, unless additional so-called '2.5D' constitutive rules are prescribed for short-range dislocation interactions. Here, results from three dimensional dislocation dynamics (3D DD) simulations in an FCC material are used to define new constitutive rules for short-range interactions and junction formation between dislocations on intersecting slip systems in 2D. The mutual strengthening effect of junctions on preexisting obstacles, such as precipitates or grain boundaries, is also accounted for in the model. The new '2.5D' DD model, with no arbitrary adjustable parameters beyond those obtained from lower scale simulation methods, is shown to predict athermal hardening rates, differences in flow behavior for single and multiple slip, and latent hardening ratios. All these phenomena are well-established in the plasticity of crystals and quantitative results predicted by the model are in good agreement with experimental observations.

1. Introduction

Dislocations are line defects in a crystal lattice whose properties and interactions with other defects control macroscopic mechanical properties such as strength, work hardening and ductility. Glide of dislocations in response to applied shear stresses cause plastic deformation while the stress required to sustain plastic flow is governed by the properties of obstacles to dislocation glide such as forest dislocations, precipitates, grain boundaries, dislocation cell walls, etc. The flow stress τ is typically inversely related to the obstacle spacing d, i.e. $\tau \propto d^{-n}$, with the exponent n dependent on several factors such as the type, strength and density of the obstacles and with d ranging from 10 nm $< d <$ 10 μm. Continuum models of plasticity embody these strengthening mechanisms implicitly, but are mainly based on experimental observations at macroscopic length scales ($>$ 1 mm). It is now experimentally well-established (Fleck and Hutchinson, 1997; Arzt, 1998; Uchic et al., 2009) that plasticity is size-dependent when specimen dimensions or spatial variations in stress become comparable to or smaller than the microstructural length scales, with increasing strength with reduced sample dimensions or increasing

* Corresponding author at: Department of Aerospace Engineering, Indian Institute of Technology Madras, Chennai 600036, India.
E-mail address: shyam@iitm.ac.in (S.M. Keralavarma).

http://dx.doi.org/10.1016/j.jmps.2016.05.028
0022-5096/

stress or strain gradients. Well known limitations of continuum plasticity theory, such as the mesh dependence of results in strain localization calculations (De Borst et al., 1993) and the inability to predict realistic values for the fracture toughness of ductile materials (Tvergaard and Hutchinson, 1992), are probably related to length scale effects due to the inherently discrete nature of plasticity in such situations.

Modeling size-dependent behavior requires augmenting continuum plasticity models with embedded length scales. Top-down approaches involve the introduction of gradient plasticity models (Fleck et al., 1994; Gao et al., 1999; Chakravarthy and Curtin, 2011b), while bottom-up methods directly model the dislocations and their motion. The main advantage of the latter discrete dislocation (DD) modeling is the absence of constitutive assumptions at the macro scale, which allows for size-dependent behavior to emerge naturally. The DD method treats dislocations as discrete line defects embedded in an elastic continuum, which move and interact with other crystal defects in response to their mutual interaction forces and the applied mechanical fields, and plastic deformation results from the collective motion of the dislocations. Fully three-dimensional models (3D DD) consider a 3D simulation cell containing closed dislocation loops that nucleate from Frank–Read sources and glide and interact with other defects in response to applied loads. Realistic representation of the crystallographic slip systems and the geometry of the dislocation loops on individual slip systems naturally leads to the emergence of forest hardening by mutual entanglement of these loops. However, 3D DD is computationally very expensive, particularly for problems with non-homogeneous loading and explicit interfaces. An alternative approach is thus a two-dimensional method (2D DD) that sacrifices some physical fidelity for computational efficiency. Following early work by Amodeo and Ghoniem (1990), the most commonly used 2D DD model by Van der Giessen and Needleman (1995) considers parallel straight edge dislocations in plane strain, which permits the study of problems involving complex inhomogeneous loading such as the growth of cracks (Deshpande et al., 2001; Chakravarthy and Curtin, 2010b), bi-material fracture (O'Day and Curtin, 2005), micro-void evolution (Segurado and Llorca, 2009), indentation (Widjaja et al., 2007), thin films (Nicola et al., 2006; Chng et al., 2006) and sliding/friction (Deshpande et al., 2004). The 2D DD method captures the long range interactions between dislocations, which enables size and gradient effects to emerge naturally, but truly 3D phenomena like junction formation and forest hardening are missing, so that standard 2D DD models predict elastic/perfectly plastic response under nominally homogeneous loading conditions. The objective of the present paper is to propose a new algorithm for incorporating strain hardening into 2D DD simulations, which improves upon existing approaches in the literature in several important ways.

Since 2D DD lacks the physics of junction formation, constitutive rules need to be prescribed to represent the effects of the corresponding phenomena in 3D. Such efforts are known as '2.5D' DD (Benzerga et al., 2004; Gómez-Garcia et al., 2006). The first such model was proposed by Benzerga et al. (2004), in which dislocations on intersecting slip planes are allowed to form 'junctions' when they approach within a critical interaction distance, which was fixed at six times the magnitude of the Burgers vector. These immobile junctions, which act as obstacles to slip and possibly also anchoring points for new 'dynamic' Frank–Read sources, can be destroyed by sufficiently high resolved shear stresses on the participating dislocations. The resulting evolution of the source and obstacle population was shown to predict strain hardening as well as size effects in micron-sized compression specimens (Benzerga et al., 2004; Guruprasad and Benzerga, 2008). An alternative approach adopted by Gómez-Garcia et al. (2006) considered a single crystal undergoing nominally homogeneous deformation, a cross-section plane of which was analyzed using periodic boundary conditions to simulate bulk behavior. In contrast with the approach of Benzerga et al. (2004), their model accounted for dislocation density multiplication due to the 3D flux of expanding dislocation loops crossing the plane of analysis, as opposed to nucleation of dipoles from fixed sources. These dislocations subsequently formed junctions with dislocations on other slip systems according to a critical distance criterion, where the interaction distance was taken to vary inversely as the square root of the *local* dislocation density, consistent with the observation that the lengths of junction segments in 3D satisfy the above scaling relation. Despite these differences, strain hardening in both these models resulted from the addition of junction obstacles, following a critical interaction distance criterion in the plane of analysis. However, if we view 2.5D DD as a projection of 3D DD onto a 2D plane, then dislocations on intersecting slip planes in 3D can intersect and form junctions at any location in the 2D plane, with consequent strengthening of all dislocations in the vicinity of the junction. This cannot be captured using a critical distance criterion for junction formation in 2D. Moreover, the existing 2.5D DD models introduce several constitutive parameters related to the strength and stability of the junctions that are used as adjustable parameters to obtain a desired hardening rate. Thus, there is some need for a more physically based 2.5D DD model that cleanly represents realistic 3D phenomena with few additional assumptions or inputs.

In this paper, a new 2.5D DD model is proposed based on the ideas that (i) constitutive rules for short range dislocation interactions in 2D must reproduce the *effects* of the corresponding phenomena in 3D on the overall plasticity rather than attempt to reproduce the details of the mechanisms themselves, and (ii) constitutive parameters related to junction formation and other hardening phenomena must be *derived* from 3D DD simulations. We present such a physically motivated 2.5D DD model using information from 3D DD to select key parameters. We then demonstrate that the model produces initial strengthening, due to preexisting glide obstacles, followed by linear hardening due to forest interactions, with hardening rates under single and multiple slip conditions consistent with experimental behavior. This 2.5D DD model thus represents a general method to include multiple strengthening mechanisms, hardening, and multi-axial plastic behavior, into plasticity simulations of problems involving complex loading conditions in materials with realistic deformation behavior.

The remainder of the paper is organized as follows. A brief summary of the standard 2D DD simulation method is provided