Acta Materialia 128 (2017) 428–439

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

A continuum model for dislocation pile-up problems

Xiaohan Zhang

Department of Mechanical Engineering, Stanford University, CA, United States

ARTICLE INFO

Article history:
Received 26 November 2016
Received in revised form
26 January 2017
Accepted 27 January 2017
Available online 4 February 2017

Keywords:
Dislocation pile-ups
Bi-metallic interface
Anisotropy
Stacking fault energy

ABSTRACT

A 2-d dislocation pile-up model is developed to solve problems with arrays of edge dislocations on one or multiple slip planes. The model developed in this work has four unique features: 1) As a continuum mechanics model, it captures the discrete behaviors of dislocations including the region near pile-up boundaries. 2) It allows for a general distribution of dislocations and applied boundary conditions. 3) The computational complexity does not quadratically scale with increased number of dislocations. 4) The effect of anisotropy and stacking fault energy can be naturally modeled. Pile-ups against a lock under shear load are extensively investigated, which shows the dependence of near-lock piles distribution on the total number of dislocations. The stacking fault energy effect is found to be positively correlated to the length of an equilibrated pile-up. The stress intensity near a bi-metallic interface is studied for both isotropic material and anisotropic materials. The model is validated by reproducing the solutions of problems for which analytical solutions are available. More complicated phenomena such as interlacing and randomly distributed dislocations are also simulated.

1. Introduction

The prediction of plastic deformation of metals has been an important research topic for decades, which primarily reduces to the question of properly understanding the motions of dislocations as the major cause of plastic flows in metals. A modern plasticity theory, Field Dislocation Mechanics (FDM), has been developed to predict the time-dependent mechanical response of bodies containing a distribution of dislocations mathematically represented by the dislocation density tensor. FDM has been completed, generalized, and understood as a rigorous, continuum thermomechanical model of dislocation dynamics and its collective behaviors (Acharya [3–5]; Acharya and Roy [1], Acharya [6,7]). The theory has been majorly applied to modeling some physically interesting phenomenological plasticity problems, for instance, size effects and back-stress development (Roy and Acharya [34]; Puri et al. [29–31]). Although these works take into account the dislocation generation and motion statistically based on the dislocation density tensor, the discrete nature of dislocation evolution, which becomes very important when the characteristic length of internal deformation fields or external sample size is at micron/submicron scale (Berdichevsky and Dimiduk [10]), has not been fully captured. Therefore, one of the objectives of this work is to demonstrate the capability of FDM in modeling and predicting the motions of dislocation microstructures. A well-known benchmark problem that serves such a purpose is the study of dislocation pile-ups, which, in addition to providing a key mechanism for size effects (Mesarovic et al. [24]), also plays an important role in other phenomena such as work-hardening, yielding, and cleavage.

The solution to the dislocation pile-up problem was first attempted by Eshelby, Frank and Nabarro Eshelby et al. [14]; who framed the question as follows: considering an array of identical straight dislocations on the same slip plane forced against an impenetrable wall, what are the equilibrated positions/distribution of the dislocations and their corresponding stress fields? It should be clearly noted that the problem stated as such is mathematically simplified by the assumption of long, straight slip bands despite the fact that such slip bands are rarely observed experimentally. The impenetrable walls are also mathematically abstracted from various physical objects in general, such as grain boundaries and bimetallic interfaces (Pacheco and Mura [27]). However, despite such simplifications, solving pile-up problems is difficult in the sense that the equilibrium state of each dislocation is determined by the combination of mutually repulsive/attractive dislocation interactions and the externally applied loads. From a numerical point of view, the computational cost of handling interactions between pairs of dislocations scales quadratically with the number of dislocations, which is known as the major bottleneck for Discrete Dislocation Methodologies in simulating strain hardening. Our

E-mail address: xzhang11@stanford.edu.

http://dx.doi.org/10.1016/j.actamat.2017.01.057
1359-6454/

model does not have this constraint but requires a good quality of mesh refinement near dislocation cores. Therefore the computational cost scales with the number of grid points.

As a brief review, we list some classical methods that have been developed specifically for solving dislocation pile-up problems.

i The first model developed by Eshelby et al. [14] is based on the balance of Peach Kohler forces on each dislocation, i.e.,

$$\sum_{i=1, i\neq j}^{n} \frac{A}{x_j - x_i} + P(x_j) = 0,\ j = 1, 2, \ldots n. \tag{1}$$

where $x_{i,j}$ are the i, jth dislocation positions to be solved; n is the total number of dislocations; $P(x_j)$ is the applied stress at the jth dislocation; A is a constant depending on the dislocation type with $A = \mu b / 2\pi(1-\nu)$ for edge dislocations. Eq. (1) is solved by introducing a polynomial,

$$f(x) = \prod_{i=1}^{n} (x - x_i) \tag{2}$$

such that one can equivalently convert it to the following ordinary differential equation,

$$f''(x) + 2P(x)f'(x) + q(n,x)f(x) = 0 \tag{3}$$

Eq. (3) is solvable provided that $q(n,x)$ is chosen in a way such that the equation has a n^{th} degree polynomial solution whose roots are real and distinct; thus x_j can be determined as the roots of a set of orthogonal polynomials subjected to certain constraints. However, this immediately sets a limitation to the method since finding proper $q(n,x)$ becomes mathematically difficult for arbitrary loading/boundary conditions.

ii Head [19] considered solving double pile-ups and interlacing problems by numerically exploring Eshelby‘s method. Here *double pile-ups* refers to a group of positive dislocations next to a negative group while both groups are forced to glide in opposite directions and form pile-ups on two sides. *Interlacing* refers to two groups of dislocations with opposite signs that lie on adjacent slip planes. The leading dislocations of adjacent planes may interlace and set the whole system equilibrium. Head‘s method requires applied stresses large enough so that dislocations cannot annihilate in double pile-ups. Also, the interlacing of more than three pairs of dislocations is reported to be intractable.

iii Leibfried (1951) [46] shows that one can obtain approximate solutions by treating discrete dislocations with continuously distributed dislocation density that can be determined from an integral transform. This methodology is applied in recent works, e.g., Akarapu and Hirth [8] and Ockendon et al. [26]; to study pile-ups and double pile-ups. However, it has been demonstrated that neglecting short range interaction effects leads to inaccurate results Roy et al. [35]. A semi-continuum version has to be developed Hall [17] in an attempt to improve the appropriateness of Leibfried's model in approximating discrete microstructure near the pile-up head with continuous functions.

iv Voskoboinikov et al. [39] proposes a methodology that accommodates the near-lock behavior of pile-ups by discretely representing dislocations in the near-lock field and matching the discrete stress field with the far field stress (where dislocations are still continuously represented with dislocation density). The method is applied in solving pile-ups against bimetallic interface Voskoboinikov et al. [40] and Voskoboinikov et al. [41]. However, the method is only valid for constant shear load and infinite isotropic domain. Some upscaling methods for dynamics of dislocation walls by means of Γ convergence on the space of probability measures have been recently developed (van Meurs and Muntean [38], Scardia et al. [36]). Those methods only deal with dislocation walls (pile-ups on n slip planes with $n \to \infty$) despite the non-physical assumption that dislocations move in the form of walls. Rezaei Mianroodi et al. [32] applied Peierls-Nabarro model to solve such problems and report qualitative agreement with discreteness based methods.

The methodology proposed in this work stems from the 2-d FDM framework developed in Acharya and Zhang [2]; Zhang et al. [45], where the motion of dislocations is governed by a kinematical rule of the plastic strain implying the conservation law of the Nye tensor (The detailed proof of this geometrical argument can be traced back to Acharya [7]). The whole system is governed by a set of partial differential equations and therefore the computational cost does not explicitly depend on the number of dislocations. This differentiates our model from all discrete-based methodologies. In the 2-d FDM approach, modeling dislocation microstructures is made possible by building multi-well non-convex inelastic energy and dislocation core energy into the system dissipation, which has the advantage in terms of capturing discreteness behaviors, compared to the continuum and semi-continuum approaches derived from Leibfried‘s model. This inelastic energy can be analogous to the stacking fault energy accounted for in phase-field (Shen and Wang [37]; Wang et al. [43]; Wang and Li [42]) and Peierls-Nabarro (PN)-based (Hu et al. [20], Xiang et al. [44]; Mianroodi et al. [25]) dislocation models. We should point out that those continuum models also have potential to model equilibrated discrete dislocations and their interactions. However, none of the models have yet solved the problems presented in this paper, i.e., explicitly modeling discrete dislocations (up to 500) with nonlocal stress field in the 2-d domain.

It should be pointed out that both stacking fault energy and dislocation core energy are physical quantities and that can be fitted from finer scale calculations. Therefore, our model serves as a multiscale modeling tool that connects the mesoscale phenomena of dislocation pile-ups to the finer scale of atomic information.

In this paper, we validate our model by first solving a few classical problems for which analytical solutions exist. Some more complicated phenomena such as interlacing are thereafter modeled. Specifically, the problem of dislocations piled-up against a bi-metallic interface is investigated for both isotropic and anisotropic materials. It is shown that behaviors of individual dislocations are well captured, including in the near-interface region. We are able to establish the relationship between the applied stress and the dislocation spacings near the head of the dislocation pile-up. The capability of modeling a quite general distribution of many dislocations is shown by simulating a body with randomly distributed dislocations, for which the stress-strain response is examined. The problem of dislocations pile-up against a lock under shear load is addressed in details. We show that the near-lock distribution of dislocations depends on the number of dislocations (up to 100). The pile-up length at equilibrium is shown to be negatively correlated to the generalized stacking fault energy. Note that a recent study (Pan et al. [28]) of pile-up effect in micro-pillars using statistic model suggests that low stacking fault energy exhibits more obvious plie-up effect (a longer pile-up length). Our findings support their conclusions from the microscopic point of view.

The rest of the paper is organized as follows, in section 2 the formulations of the model are described; section 3 presents