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Polycrystal deformation in a discrete dislocation dynamics framework

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Abstract

Grain boundaries (GBs) typically play an important role in obstructing the glide of dislocations in polycrystalline materials, giving rise to the classic Hall–Petch effect. Molecular dynamics simulations of the deformation of nanocrystalline materials demonstrate that GBs do much more. We extend the now classical discrete dislocation dynamics (DDD) simulation approach to account for GB sliding and the absorption, emission and transmission of lattice dislocations at GBs. This is done in a framework in which GB dislocations are nucleated and migrate along the GB in a manner that is an extension of the DDD formalism. We demonstrate that incorporation of a dislocation picture of GB dynamics allows all of these effects to competitively relax localized stress fields (such as from dislocation pileups) and act synergistically to modify the mechanical response of polycrystals—well beyond GBs simply blocking dislocation slip.

Keywords: Discrete dislocation dynamics; Polycrystals; Grain boundary sliding

1. Introduction

Grain boundaries (GBs) play major roles in the deformation of polycrystalline materials, the most widely recognized of which is to obstruct the motion of dislocations. This results in dislocation pileups against the GB, which in turn contributes to the hardening of the material. This gives rise to the classical, phenomenological Hall–Petch relationship [1,2], which suggests that the yield strength of the material increases with decreasing grain size in proportion to $1/d^{1/2}$. GBs, however, can play additional roles in accommodating deformation in polycrystalline materials. For example, GBs can be interfaces along which grains slide against each other; they can act as both sources and sinks for dislocations; and/or they can transmit dislocations from one grain to another. In fact, these processes often operate (in varying degrees) simultaneously, and also play important roles in accommodating deformation in a polycrystalline material. The relative contribution of each of these GB phenomena to the overall deformation response depends on several factors including material system, microstructure, grain morphology, grain size, sample size, etc. The main goal of the work described herein is a proposal for an approach that is capable of describing all of these phenomena simultaneously and on an equal footing.

An example of the importance of the roles played by GBs in accommodating deformation can be found in recent studies of the deformation of nanocrystalline (polycrystalline with nanoscale grains) materials. Both experiments [3] and molecular dynamics (MD) simulations [4–7] show that when the grain size is on the tens of nanometers or smaller scale, there is a deviation from the Hall–Petch relation and, in fact, in this regime, smaller often becomes weaker. It is now widely believed that in this nanocrystalline regime, GB sliding, and dislocation generation and absorption at the GB dominate the deformation response of the material.

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This is especially clear in large-scale MD simulations [6,7] which show that most of the plastic deformation that occurs is either by GB sliding or by the emission/absorption of dislocations at GBs. In fact, recent MD simulations have shown [7] that even the dislocation emission events are associated with GB sliding and accommodation of plastic deformation occurs at the GB long before any intragranular slip occurs.

Discrete dislocation dynamics (DDD) models have been widely applied to model the plastic deformation of materials. They have shown excellent qualitative and, with appropriate fitting, quantitative agreement with experimental deformation tests [8]. When used in modeling polycrystalline materials, many earlier models treat GBs as obstacles to dislocation motion [9–13]. This leads to dislocation pileups and, as the grain size is reduced, the Hall–Petch relation is recovered. More recently, dislocation dynamics methods have been extended to incorporate dislocation transmission across GBs, but were limited to the case of low-angle GBs [14,15]. Ahmed and Hartmaier [16] also incorporated dislocation absorption at GBs in a model in which a dislocation approaching a GB is blocked, transmitted or absorbed. Absorption occurs by splitting the incoming dislocation into two dislocations: one with a Burgers vector parallel to the GB and the other with a Burgers vector normal to the GB. The dislocation with a Burgers vector parallel to the GB will glide along the GB leading to GB sliding, while the climb of the dislocations with a Burgers vector normal to the GB is a result of the diffusion of vacancies along the GB. A requirement for any dislocation reaction at the GB is that the total Burgers vector at the GB is conserved. While an important advance, the complex deformation mechanisms associated with GBs are still not fully described. For example, Ahmed and Hartmaiers' [16] model only accounts for GB sliding when a lattice dislocation interacts with the GB, but GB sliding can in fact occur in the absence of lattice dislocations [6,7]; climb of dislocations with a Burgers vector perpendicular to the GB necessarily leads to grain rotation, which is not yet routinely considered in DDD models; and similarly, GB migration is usually not considered in DDD models except when low-angle GBs are described by arrays of dislocations [17,18].

It is interesting to note that all of the deformation mechanisms operating at GBs discussed above can be described in terms of the motion of dislocations. We therefore choose to describe the deformation of polycrystalline materials, and more particularly the mechanisms that operate at GBs, in a "DDD language". In fact, this idea is not new. For decades, dislocation models have been used to characterize GBs. Taylor [19] first calculated the displacement and stress distribution of an array of edge dislocations that describe a low-angle, symmetric tilt GB. Based on this description, models using DDD to simulate the movement of these low-angle GBs have been carried out [17,18]. In general, GBs can be theoretically described by one or more arrays of dislocations that are not necessarily lattice dislocations. With this understanding and motivation, the goal of this work is therefore to develop a unified DDD framework that incorporates the various deformation accommodation mechanisms at the GB. We recognize that the atomistic structure of the GB can play an important role on the deformation mechanism, but in our current continuum model, the detailed description of the dislocation structure of GBs is not specified. However, in our 2-D DDD model, the activation of different mechanisms can be sensitive to the bicrystallography parameters describing a GB such as tilt and inclination—the two degrees of freedom describing a GB in a 2-D space. We show in this paper that the incorporation of deformation mechanisms associated with the GB can lead to significantly different deformation response to a load. The current 2-D DDD model therefore includes (i) nucleation and slip of dislocations in the grain interior; (ii) transmission of dislocations across GBs; (iii) GB sliding; (iv) dislocation emission from GBs; and (v) dislocation absorption at GBs.

In the next section, we briefly describe a now standard approach to 2-D DDD. As a reference, we show the case where a GB is treated merely as an obstacle to dislocation slip, resulting in the formation of a dislocation pileup. This reference is then compared to the case when transmission is considered. Next, we extend the method to the case where GB sliding can occur, followed by how this same description can lead to a partial absorption of dislocations at the GB. We then study the deformation behavior of a bicrystal and compare between the cases with and without GB sliding. Finally, we discuss some of the underlying assumptions in the current model and where extensions to account for additional physics is desirable.

2. Discrete dislocation dynamics

The 2-D DDD framework was first used to model defect evolution and dislocation pattern formation in single crystals [20–24]. Van der Giessen and Needleman [25] extended and popularized the approach as a means of including the effects of dislocation plasticity in the mechanics of materials. Unlike in a conventional crystal plasticity model governed by a constitutive relationship, in the DDD framework, dislocations are modeled as point (2-D) or line (3-D) singularities that are sources of deformation and are characterized by the Burgers vector, b. We briefly describe the main aspects of the 2-D DDD model here and refer interested readers to the details of the model in the numerous references available (e.g. [8–11,25,26]).

To introduce the concepts and ideas of a DDD framework for a polycrystal, we build an illustrative 2-D model; of course, similar ideas may be extended to 3-D. In this context, we model a simulation cell in 2-D with periodic boundary conditions in two directions (x and y). In a general 2-D DDD model, the dislocations are assumed to be infinitely long, straight and parallel edge dislocations with line directions perpendicular to the 2-D simulation plane.