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Insights on slip transmission at grain boundaries from atomistic simulations

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ABSTRACT

To fully understand the plastic deformation of metallic polycrystalline materials, the physical mechanisms by which a dislocation interacts with a grain boundary must be identified. Recent atomistic simulations have focused on the discrete atomic scale motions that lead to either dislocation obstruction, dislocation absorption into the grain boundary with subsequent emission at a different site along the grain boundary, or direct dislocation transmission through the grain boundary into the opposing lattice. These atomistic simulations, coupled with foundational experiments performed to study dislocation pile-ups and slip transfer through a grain boundary, have facilitated the development and refinement of a set of criteria for predicting if dislocation transmission will occur and which slip systems will be activated in the adjacent grain by the stress concentration resulting from the dislocation pile-up. This article provides a concise review of both experimental and atomistic simulation efforts focused on the details of slip transmission at grain boundaries in metallic materials and provides a discussion of outstanding challenges for atomistic simulations to advance this field.

1. Introduction

Grain boundaries are planar defects which accommodate the misorientation between neighboring grains in a polycrystalline material (cf. [1–3]). From a geometric perspective, grain boundaries have five macroscopic and three microscopic degrees of freedom [1]. The five macroscopic degrees of freedom of a grain boundary are commonly specified via a misorientation angle, a misorientation axis vector and the normal vector to the interface plane. The three microscopic degrees of freedom are associated with the mutual translation of the opposing lattice regions parallel and perpendicular to the grain boundary plane. Combined, the specification of both the macroscopic and microscopic degrees of freedom produce the atomic level geometry of a grain boundary associated with unrelaxed atomic arrangements [3]. In real materials, nanoscale movements of individual atoms at the grain boundary occur to minimize the interface energy for a given geometry leading to the presence of structure at the interface. For high-angle tilt grain boundaries in equilibrium, this structure may be described in terms of structural units (cf. [4–7]). However, compatibility between grains in polycrystalline samples can cause disorder leading to nonequilibrium grain boundary structures that deviate from the structural unit model.

The mechanical behavior of metallic polycrystalline materials is strongly influenced by the interaction of dislocations with grain boundaries. In ductile coarse-grained metallic materials, dislocations that are nucleated within the grain interiors by Frank-Read or other sources are impeded by grain boundaries due to slip incompatibility between the neighboring grains. Based on experimental evidence, both Hall [8] and Petch [9] envisioned dislocation pile-ups to occur at grain boundaries and proposed that plastic yield occurred once the stress exerted on the neighboring grain by the dislocation pile-up reached a critical value. This stress concentration may cause: (1) new dislocation nucleation originating from the grain boundary, (2) absorption of the leading dislocation in the pile-up into the grain boundary, (3) direct dislocation transmission through the boundary, or (4) dislocation absorption followed by re-emission of the dislocation at a nearby site along the grain boundary [10]. Focusing on emission and transfer, several authors have proposed models with geometric and/or stress based criteria to predict the activated slip system in the adjacent grain, using static and *in situ* transmission electron microscopy (TEM) experiments for validation. As these models provide motivation to the atomistic simulation community to study dislocation transmission, a concise review of experimentally-validated models for slip system prediction is provided in Section 2 of this article.

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Principally, this article focuses on recent atomistic simulation efforts to study dislocation interactions with grain boundaries and the discrete atomic motions that facilitate dislocation absorption or transmission through grain boundaries in metallic materials. Here, the term "atomistic simulation" is used as an umbrella term referring to either molecular mechanics, where energy minimization is used to solve for a local minimum energy configuration of a set of atoms, or molecular dynamics (MD), where a prescribed set of equations of motion are integrated numerically to solve for the trajectories of a set of atoms. The primary assumption of atomistic simulation is that the interaction between atoms (atomic bonding) can be modeled using an interatomic potential whose mathematical form depends on the material system of interest [11]. By choosing not to model the atomic system with electron-level resolution, a much larger number of atoms can be modeled, compared to direct *ab initio* or density function theory based quantum mechanical simulations. Thus, interatomic potential based atomistic simulations are capable of modeling a sufficient volume of material (number of atoms) necessary to capture the stress and displacement fields characteristic of dislocations and grain boundaries in metallic materials [12]. This article will not provide an overview of atomistic simulation techniques; the interested reader is directed towards texts by Allen and Tildesley [11], Frenkel and Smit [13] and LeSar [14].

2. Predictive models for dislocation transmission

Motivated by both experimental observations and dislocation theory, several authors have proposed criteria to predict which slip system is activated in the neighboring grain due to a dislocation pile-up at a grain boundary [10,15–23]. The following sections provide a brief overview of several proposed prediction criteria for slip system activation and the experimental methods used to validate these criteria. Predominantly, these criteria are motivated by slip system geometry and/or internal stresses and do not consider the discrete atomic interactions between a dislocation and the structure of a grain boundary (with the exception that residual grain boundary dislocation content is considered [18–23]). The goal of most atomistic simulation efforts in this field is to elucidate these discrete interactions to improve the accuracy of slip transmission prediction criteria over a range of metallic materials and grain boundary structures.

2.1. Slip system geometry approach (N criterion)

In seminal work, Livingston and Chalmers [15] considered dislocation activity in bicrystal Al specimens. First, based upon macroscopic plasticity arguments, they showed that additional slip systems must be activated during plastic deformation in bicrystal samples to maintain continuity of the material at the grain boundary. This argument is analogous to that made by Taylor [24] who proved that five independent slip systems must be active in each grain during plastic deformation of a random polycrystalline sample. Second, Livingston and Chalmers proposed a criterion to predict the activated slip system in the neighboring grain due to a dislocation pile-up,

$$N = (e_1 \cdot e_i)(g_1 \cdot g_i) + (e_1 \cdot g_i)(g_1 \cdot e_i) \quad (1)$$

According to this criterion, the slip system that will be activated in the neighboring grain is the one with the largest value of N. In Eq. (1), e_1 and e_i are the unit normal vectors of the pile-up and transmission slip planes, respectively; g_1 and g_i are unit vectors in the slip direction for the pile-up and transmission slip systems, respectively. A schematic of the slip geometry is shown in Fig. 1. The maximum value of N considering all FCC slip system combinations for $\langle 1\,0\,0\rangle$ and $\langle 1\,1\,0\rangle$ symmetric tilt grain boundaries is shown in Fig. 2. Livingston and Chalmers demonstrated the success of this criterion by examining slip lines in Al bicrystals deformed in tension parallel to the grain boundary plane. While this criterion proved successful in the large majority of the cases that they examined, this criterion considers only the relative orientations of the neighboring slip systems and does not consider the orientation of the grain boundary plane relative to either slip system. Thus, this geometric criterion is not expected to be universal.

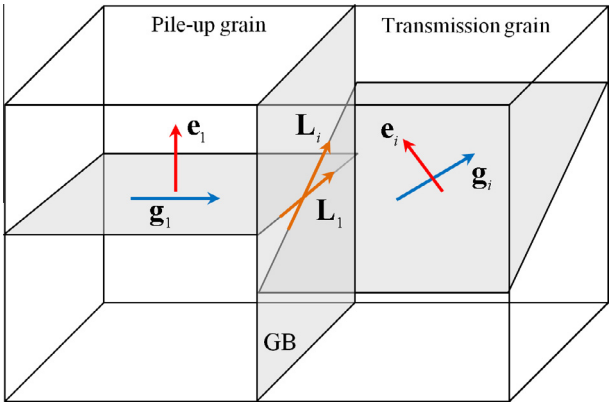

Fig. 1. Schematic of the slip transmission geometry used in Eqs. (1) and (2).

2.2. Combined geometry and stress-based approach (M criterion)

Shen et al. [10,16,17] studied dislocation transmission through grain boundaries in type 304 stainless steel (FCC) and Mo (BCC) using *in situ* TEM. First, based on measured crystallographic and grain boundary data from static TEM and electron diffraction experiments, they computed the anisotropic elastic stress tensor at the intersection of the grain boundary and the dislocation pile-up. This allowed the authors to compute the stress acting on slip systems in the opposing grain and it provided a measure of the obstacle strength of the grain boundary. Then, the authors evaluated four different criteria for predicting slip transmission: (1) the N criterion of Livingston and Chalmers [15], (2) a new criterion which accounts for the relative orientation of the grain boundary plane compared to the slip planes in each lattice region, (3) a maximum force criterion based on the resolved shear stress calculation, and (4) a combination of criteria where the slip plane is determined using geometric arguments and the slip direction within the slip plane is determined from the resolved shear stress. The new criterion that accounts for the orientation of the slip planes relative to the grain boundary plane is specified as,

$$M = (L_1 \cdot L_i)(g_1 \cdot g_i) \quad (2)$$

Analogous to [15], the slip system that will be activated in the neighboring grain due to the dislocation pile-up is the one with the largest absolute value of M. In Eq. (2), L_1 and L_i are unit normal vectors at the intersection of the pile-up and transmission slip planes with the grain boundary, respectively, as shown in Fig. 1. The maximum absolute value of M considering logical FCC slip system combinations for $\langle 1\,0\,0\rangle$ and $\langle 1\,1\,0\rangle$ symmetric tilt grain boundaries is shown in Fig. 3. Grain boundaries in which the pile-up or transmission slip planes are normal to the grain boundary or grain boundaries in which the misorientation axis and the slip directions in each lattice are coincident are not considered. Using *in situ* TEM, the authors showed that criterion (4) provides the best prediction of the activated slip system in the neighboring grain due to a dislocation pile-up in both 304 stainless steel and in Mo. Further, Shen et al. showed that the barrier strength can vary by a factor of four for different grain boundaries [10]. Fundamentally, the barrier