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# Modelling dislocation transmission across tilt grain boundaries in 2D

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ABSTRACT

A line tension approach is reviewed to model slip transfer across tilt grain boundaries (GBs). It is implemented as a constitutive rule in the already existing two-dimensional discrete dislocation plasticity model of polycrystalline thin films. GBs are treated as obstacles to dislocation motion but with a finite strength. Dislocation transmission across a GB is potentially allowed, provided that three known geometrical criteria are satisfied. If allowed, the motion of the dislocation across the GB is enabled by dynamically creating a GB source near the GB, the stress on which must exceed the boundary strength. To separate transmission effects from other discrete dislocation features of the plastic deformation of thin films, comparisons are carried out by modelling GBs as impenetrable barriers to dislocation motion. It is shown that slip transfer tends to make the film softer if the density of bulk sources is sufficiently low. Since the position of the boundary source lies within the high-stress region of dislocation pile-ups, once activated the transmission process becomes independent of the source strength. In addition, the Bauschinger effect (BE) in thin films has been studied and a decrease of the BE is seen when dislocation transmission across GBs is enabled.



## 1. Introduction

Grain boundaries (GBs) can have a significant effect on the plastic response of polycrystalline metals. While deformation inside the GBs themselves can directly contribute to plasticity in the case of nanocrystalline materials, GBs primarily play a role in their interaction with dislocations when the grain size is in the (sub-)micrometer range. GBs can absorb or emit dislocations [1,2], and, depending on the misorientation between the adjacent crystals, they can act as strong obstacles to dislocation motion and thus inhibit plasticity. In bulk materials, this results in a Hall–Petch [3,4] type relationship for the yield strength as a function of grain size, which is primarily due to the piling-up of dislocations against the GBs [5,6]. In thin films with thicknesses and grain sizes in the micrometer range, the importance of GB–dislocation interaction increases due to the increase in area of GBs per unit grain volume (i.e. the GB density) with decreasing size [7]. Thus, the yield properties of such films are strongly governed by the way dislocations interact with GBs.

Until now, classical crystal plasticity models have treated GBs essentially as planes that separate the slip systems in one grain from those in the adjacent one. There are some modern, nonlocal theories, however, that treat the slip as internal variables for which the GBs can set boundary conditions. Examples are the continuum theories of the type proposed by Gurtin [8] and by Geers and co-workers [9], and discrete dislocation models of crystal plasticity [10]. The typical assumption made in these studies of (sub-)micron grain-sized polycrystals so far has been that GBs block slip; in a continuum model this means that the slip is defined to vanish at the GB, while in discrete dislocation plasticity this translates into treating GBs as impenetrable obstacles. With this assumption, discrete dislocation studies have been able, for instance, to predict the Hall–Petch effect [11] of bulk polycrystals and to obtain quantitative agreement with the size-dependent yield strength of Cu thin films [12]. Despite this success, the issue remained as to what the possible influence of GB–dislocation interactions could be; yet, approaches to incorporate these into discrete dislocation plasticity were lacking. With the advance of computing facilities and atomistic modeling techniques, several efforts have recently been made to understand and quantify these dislocation–GB interactions in materials with micron size grains [13–19].

In this work, we address one of the observed types of dislocation–GB interactions, namely the transmission of a glide dislocation across a GB. A method is developed to handle dislocation transmission across low angle tilt boundaries within a framework of two-dimensional (2D) discrete dislocation plasticity. In this approach, we will borrow the idea from de Koning et al. [13] to treat transmission as the nucleation of a new dislocation from the GB in a way akin to the operation of a Frank-Read source inside the grain. The approach involves the introduction of the strength of a GB source, the value of which can be taken from a line tension model,

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as proposed in [13], or from atomistic simulations. After its formulation, we will adopt the dislocation transmission model to study the effect of transmission on the macroscopic yield properties of thin films, in dependence of bulk source density, grain size, and GB source strength. We start with a brief summary of the 2D approach.

## 2. Two-dimensional discrete dislocation plasticity

### 2.1. Framework and constitutive rules

In two dimensions, plane-strain plastic deformation can be described by the evolution of edge dislocations in an elastic medium. The dislocations are incorporated in the form of dipoles as being the 2D analogue of three-dimensional dislocation loops. The magnitude of the Burgers vector of all dislocations is $b$, and their sign represents the line direction out of the plane of consideration. While their long-range interaction is described by the elastic fields (assuming isotropic elasticity with shear modulus $\mu$ and Poisson ratio $\nu$), the short-range interactions between dislocations are incorporated by constitutive rules. Four rules were proposed by Van der Giessen and Needleman [10] and have been adopted in the majority of applications since. First of all, each dislocation $I$ glides in response to the glide component of the Peach–Koehler force, $f^{(I)}$, according to the linear drag law

$$v^{(I)} = f^{(I)}/B,$$

for its velocity with drag coefficient $B$. This force is calculated from the stress fields of other dislocations in the domain and image fields due to the actual boundary conditions. The second rule is that when dislocations move, they can hit point obstacles at which they are pinned, as long as the Peach–Koehler force does not exceed an obstacle dependent strength $b\tau_{obs}$. Thirdly, dislocations of opposite sign on the same slip plane will annihilate when they are within a distance of $6b$ from each other.

The fourth and final rule in the conventional formulation is concerned with the generation of new dislocations. For this purpose, a 2D source is used that mimics the Frank-Read mechanism as illustrated in Fig. 1a: the resolved shear stress has to be sufficiently high for the initially pinned segment to bow out, to fold around itself, annihilate partly on the backside and to eventually leave a new loop along with a copy of the original segment. This process is characterised by three parameters: (i) the value of the resolved shear stress at which the bowed-out segment becomes unstable (the source strength); (ii) the time it takes for the new loop to be created; and (iii) the size of the loop, all of which depend on the length of the Frank-Read segment. In [10] it was proposed to represent a source in 2D by a point (as a cross-section of a Frank-Read segment) that generates a dipole, as illustrated in Fig. 1b, when the shear stress at the source has exceeded the source strength $\tau_{nuc}$ for a sufficiently long time $t_{nuc}$. For computational reasons, the delivery process of the dipole (as the 2D counterpart of expansion till a full loop) is not simulated; instead, the dipole is inserted instantaneously once the above-mentioned criterion is met, with a size given by

$$L_{nuc} = \frac{\mu b}{2\pi(1-\nu)\tau_{nuc}}. \quad (1)$$

The reason for this is simply that a smaller dipole would collapse under its own self-attraction. At a distance of $L_{nuc}$ according to (1), the attractive force is balanced by the internal stress which is assumed to be close to the value $\tau_{nuc}$ that operates the source. If the actual internal stress is lower, the dipole gets annihilated and the nucleation event was unsuccessful.

In previous studies carried out within this framework, e.g. [7,11,12], GBs were assumed to be impenetrable (implemented through infinitely strong obstacles located at the intersections of slip planes with GBs) by lack of a constitutive rule describing transmission or absorption. In the following we develop a first simple rule for transmission.

### 2.2. New rules for transmission

Initially, Shen et al. [2,20] and, later, Lee et al. [21] have performed several experimental studies of the transmission of dislocations across GBs. On the basis of their findings, the latter authors proposed three criteria for transmission: (a) the slip plane in the outgoing grain is such that the misorientation with the incoming one is minimal; (b) the Burgers vector of the resulting residual Burgers vector at the GB has a minimum length; and (c) the resolved shear stress on the outgoing slip plane is maximal. The above are necessary conditions; whether or not the incoming dislocation actually does transmit depends on the details of the mechanism.

In order to shed more light on this mechanism, several atomistic [13,15,22,23] and hybrid [14,17] studies have been carried out during the last decade. Although much has been learned, a complete picture is not yet available because of the myriad of parameters in the problem: the type of GB, the slip systems on either side of the boundary, as well as external conditions such as the stress state and temperature. Fortunately, for the 2D simulations we are aiming at, the situation is more favourable since the number of possible slip systems is significantly reduced and, more importantly, only tilt boundaries are relevant. Within these realms, the work by de Koning et al. [13] is of great interest, since it is dedicated to the glide of dislocations across tilt GBs. In particular, they

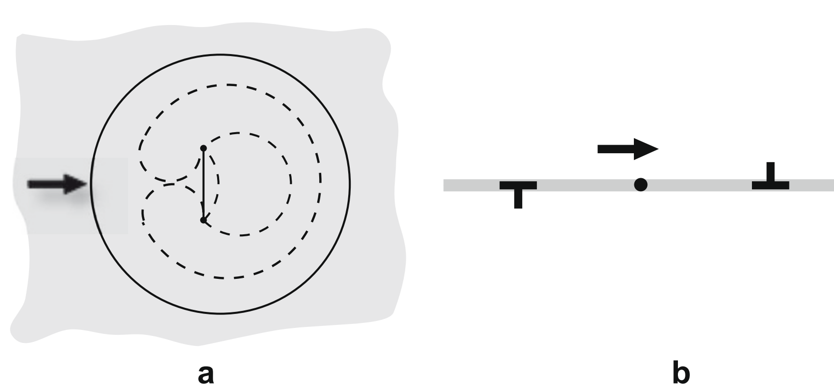


**Fig. 1.** (a) Schematic of various stages in the Frank-Read mechanism to generate a dislocation loop from a segment pinned at two points (•) in top view. (b) Two-dimensional Frank-Read source proposed in [10].