Journal of the Mechanics and Physics of Solids 61 (2013) 2659–2679

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

# Grain boundary interface mechanics in strain gradient crystal plasticity

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ARTICLE INFO

*Article history:*
Received 25 October 2012
Received in revised form
19 March 2013
Accepted 15 August 2013
Available online 2 September 2013

*Keywords:*
Grain boundary
Crystal plasticity
Strain gradients
Interface model

ABSTRACT

Interactions between dislocations and grain boundaries play an important role in the plastic deformation of polycrystalline metals. Capturing accurately the behaviour of these internal interfaces is particularly important for applications where the relative grain boundary fraction is significant, such as ultra fine-grained metals, thin films and micro-devices. Incorporating these micro-scale interactions (which are sensitive to a number of dislocation, interface and crystallographic parameters) within a macro-scale crystal plasticity model poses a challenge. The innovative features in the present paper include (i) the formulation of a thermodynamically consistent grain boundary interface model within a microstructurally motivated strain gradient crystal plasticity framework, (ii) the presence of intra-grain slip system coupling through a microstructurally derived internal stress, (iii) the incorporation of inter-grain slip system coupling via an interface energy accounting for both the magnitude and direction of contributions to the residual defect from all slip systems in the two neighbouring grains, and (iv) the numerical implementation of the grain boundary model to directly investigate the influence of the interface constitutive parameters on plastic deformation. The model problem of a bicrystal deforming in plane strain is analysed. The influence of dissipative and energetic interface hardening, grain misorientation, asymmetry in the grain orientations and the grain size are systematically investigated. In each case, the crystal response is compared with reference calculations with grain boundaries that are either 'microhard' (impenetrable to dislocations) or 'microfree' (an infinite dislocation sink).



## 1. Introduction

Internal interfaces (such as grain and phase boundaries) play an important role in the plastic deformation of polycrystalline metals. They provide obstacles to dislocation glide, with a resistance that depends on a number of material and crystallographical parameters. As a consequence, they constrain the plastic deformation of adjacent grains, whose different crystallographic orientations and preferential slip directions result in complex intra-granular strain fields. The high local stresses developing at the tip of a pile-up (Li and Chou, 1970) can influence local plasticity and damage, and are obviously sensitive to the ability of dislocations to transmit through the boundary. The defect structure of a grain boundary can also act as a dislocation source, promoting plastic slip (Venkatesh and Murr, 1978).

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0022-5096/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jmps.2013.08.011

The challenge addressed by the current work is the development of a macroscopic crystal plasticity model which accounts for the fine-scale grain boundary micromechanics. A number of applications motivate this. Metallic thin films and micro-devices can have a grain size comparable with some of the component dimensions, and accurate resolution of interface micromechanics may therefore be important for predicting device performance. For fine-grained and nano-crystalline metals, the large grain boundary area plays a pivotal role in plastic deformation. As outlined in the review by Meyers et al. (2006), a conventional Hall–Petch relationship breaks down for grain sizes below 1 μm, and the mechanisms by which plastic deformation progresses at these small grain sizes remain the subject of continued investigation. Accurate models of grain boundary behaviour during plastic deformation are required in order to capture these phenomena.

Experimental observations and, more recently, numerical simulations at the atomistic and discrete dislocation scales indicate that the micro-scale interactions between dislocations and grain boundaries are complex and diverse. To motivate the model development, we first briefly review these experimental and model observations of the micro- and meso-scale behaviour of grain boundaries. Existing strategies for bridging the length scales to capture the continuum level response are then summarised.

### 1.1. Interactions between dislocations and grain boundaries

Microscopic investigations of dislocation motion in the vicinity of grain boundaries have been used to develop an understanding of the interaction mechanisms and the criteria for the propagation of slip across the interface. Livingston and Chalmers (1957), studying pile-ups at a bicrystal interface, suggest that slip is induced in the adjacent grain in accordance with a resolved shear stress criterion: slip propagates on the slip plane on which the magnitude of the resolved shear stress induced by the pile-up is greatest. Later studies employed transmission electron microscopy (TEM) to track the motion of individual dislocations during interaction with a grain boundary (Lee et al., 1989, 1990; Shen et al., 1986). A number of interaction mechanisms were identified, most common of which is the initiation of slip near the incoming pile-up on the preferentially oriented slip system, leaving a residual Burgers vector at the grain boundary. Three parameters emerge as the most important for determining the slip plane and slip systems on which dislocations are emitted into an adjacent grain: (i) minimising the angle between the projections onto the grain boundary of the incoming and outgoing slip systems, (ii) maximising the resolved shear stress in the slip direction and (iii) minimising the residual defect at the interface, required by conservation of the Burgers vector. These TEM investigations are generally restricted to very local phenomena. Sun et al. (1998, 2000) and Zaefferer et al. (2003) use orientation imaging microscopy (OIM) to measure spatial variations in the densities of geometrically necessary dislocations (GNDs) over a larger area in the vicinity of an interface in a deformed aluminium bicrystal.

Although microscopy can provide insights into governing interaction mechanisms, it is difficult to quantify the resistance to slip posed by an interface. This issue has been addressed using nano-indentation in the vicinity of interfaces. Hardness variations across interfaces in various material and interface combinations have been reported (Lee et al., 1999; Soifer et al., 2002; Wo and Ngan, 2004). While providing a measure of the obstruction to slip provided by the interface, the results appear to be sensitive to experimental conditions, such as indentation force and the orientation of the faces of the indenter tip relative to the interface. A number of authors have also studied 'pop-ins', interpreted as the sudden release of a pile-up through a grain boundary (Soer et al., 2005; Yang and Vehoff, 2005). Although challenging to interpret, these results indicate that grain boundaries pose an obstacle to slip of finite strength, and can be overcome with sufficient applied stress.

More recently, numerical approaches at the micro- and meso-scales have been used to study the interactions between dislocations and grain boundaries. At the atomistic scale, molecular dynamics (MD) has been used to study individual dislocation interactions. The study of de Koning et al. (2002) reveals that transmission of a dislocation loop across a tilt boundary is blocked if the misorientation angle exceeds 20°. Furthermore, de Koning et al. (2003) show that the resistance to transmission is higher for an asymmetric tilt boundary compared to a symmetric interface. The initial interface energy (which is higher in the asymmetric case) appears to play a role. The calculations of Jin et al. (2006) show that the recombination of partial dislocations prior to absorption into a grain boundary (which is influenced by the stacking fault energy) appears to influence the critical applied stress for transmission.

At the meso-scale, discrete dislocation dynamics (DDD) has been used to study the motion of a large number of individual dislocations and their interactions with interfaces, for example Biner and Morris (2002), Lefebvre et al. (2007) and Balint et al. (2008). In these studies, grain boundaries are treated as hard obstacles to the motion of individual dislocations, but stresses local to the head of a pile-up may activate sources in the adjacent grain which reside on favourably oriented slip planes. The propagation of slip therefore depends on the activation strength of dislocation sources, their locations and the elastic stress fields which develop due to slip incompatibility. Recently Li et al. (2009) have introduced penetrable interfaces within a DDD calculation. A criterion is specified by which a dislocation may transmit across a grain boundary, in the form of a threshold shear stress which accounts for the energy balance for the transmission event.

### 1.2. Modelling grain boundary behaviour at the continuum scale

The problem of interest is fundamentally multi-scale in nature: dislocations interacting with interfaces at the micro-scale influence the macroscopic response of the material. This poses a challenge in accounting for the fine-scale behaviour across