Mechanics of Materials 88 (2015) 30–43

Contents lists available at ScienceDirect

Mechanics of Materials

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

Interface modeling in continuum dislocation transport

M.M.W. Dogge [a,b], R.H.J. Peerlings [b,*], M.G.D. Geers [b]

[a] Materials innovation institute M2i, P.O. Box 5008, 2600 GA Delft, The Netherlands
[b] Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

ARTICLE INFO

Article history:
Received 12 August 2014
Received in revised form 12 March 2015
Available online 23 April 2015

Keywords:
Crystal plasticity
Interfaces
Dislocation transport
Finite element method

ABSTRACT

Predictive microstructural models of poly-crystalline materials require a correct description of the mechanical behavior of internal boundaries, e.g. grain, phase and twin boundaries. Dislocations are the carriers of plastic deformation and the presence of internal boundaries restricts their motion. Interactions between dislocations and the resistance to their motion caused by the interfaces give rise to hardening and size effects, which should therefore be considered. In this paper, a continuum dislocation transport model in single slip is used to model a two-phase laminated microstructure containing (plastically) hard and soft phases. The phase boundary constitutes an interface in the model. The transport equations require continuity of the dislocation flux throughout the domain. Expressions for the dislocation flux in the bulk as a function of the dislocation densities and their gradients are readily available in the literature. However, the interface requires an additional constitutive model for the dislocation flux passing through it. Such a model is derived here from the interactions of infinite dislocation walls on both sides of the parallel boundary. A qualitative analysis is performed to reveal the effect of interface, material and geometrical parameters on the overall response of a two-phase laminate. The presence of the interface in the two-phase laminate gives rise to the observed characteristic hardening of dual-phase materials as well as to size effects.

1. Introduction

The mechanics of materials on smaller length scales becomes increasingly important as a result of the intrinsic microstructural size effects result from the ratio of different microstructural length scales, e.g. Hall–Petch, Friedel and Orowan effects (Sevillano et al., 2001; Geers et al., 2006). In this case, classical continuum models describing the material behavior fail to capture relevant mechanics governing plastic behavior. Another aspect is that by altering the microstructure of materials their properties may be influenced. Therefore, in order to derive predictive models for these materials, relevant mechanics on the microstructural level should be included.

On the microstructural scale, the behavior of (collections of) dislocations dictates plastic behavior. The understanding and correct description of the dislocations, including their interactions with interfaces, is therefore key for predicting the resulting engineering properties (Shen et al., 1988). When the motion of dislocations is restricted, the material is unable to deform plastically, thereby enhancing the strength of the material. Grain, phase and twin boundaries are examples of interfaces where dislocation motion is partially impeded. The presence of such interfaces explains experimentally observed size effects (Lasalmonie and Strudel, 1986; Arzt, 1998; Aldazabal and Sevillano, 2004; Hansen, 2004). They are often induced by strain gradients due to the pile-up of dislocations against boundaries (Smyshlyaev and Fleck, 1996;

* Corresponding author.
E-mail addresses: m.dogge@m2i.nl (M.M.W. Dogge), r.h.j.peerlings@tue.nl (R.H.J. Peerlings).

http://dx.doi.org/10.1016/j.mechmat.2015.04.007
0167-6636/

Fleck and Hutchinson, 1997). Internal boundaries act as barriers to dislocation motion, because a mismatch in glide plane orientation or differences in the underlying crystal lattices locally increase the stress required to transport dislocations through the lattice. As more dislocations accumulate near such a boundary, the repulsive stress exerted by them increases, resulting in a pile-up against the boundary (Roy et al., 2008). Depending on the accumulated stress field, dislocations can interact with a boundary in a number of ways, e.g. transmission, absorption, nucleation or stagnation. They can further act as barriers to dislocation motion, assist in overcoming the resistance of the boundary, as well as activate sources in the neighboring grain. When the interface spacing decreases, the effects of these interactions are becoming more pronounced.

The objective of this article is to develop an interface model that describes and captures the effect of interfaces on dislocation transport, including relevant interaction mechanisms between dislocations and interfaces, to improve the predictive capabilities of crystal plasticity models.

In lower-scale models like Molecular Dynamics (Zhang and Wang, 1996; de Koning et al., 2003; Li et al., 1998) and Discrete Dislocation Dynamics (Balint et al., 2008; Li et al., 2009), the interaction of dislocations can be modeled in an accurate way, because each individual dislocation (or atom) is resolved. However, in a continuum description the resolution is limited to the level of densities of dislocations and the effect of dislocation motion and interactions with other dislocations and interfaces must be incorporated at this level. Many continuum frameworks have been proposed which include dislocation and boundary mechanics, see Cermelli and Gurtin (2002), Gudmundson (2004), Ma et al. (2006), Gurtin (2008), Roters et al. (2010) and van Beers et al. (2013).

However, the majority of these models do not explicitly take into account the transport of dislocations, but solve for the (plastic) incompatibility due to plastic slip, and relate the gradients in plastic slip to the presence of Geometrically Necessary Dislocations (GNDs). Nonetheless, there are continuum models available considering the plastic deformation as the result of dislocation motion (Groma et al., 2003; Kratochvíl and Sedlaček, 2008; Sedlček et al., 2007; Hochrainer et al., 2007). Based thereon, a continuum dislocation transport model (Groma et al., 2003; Yefimov et al., 2004) is adopted here, modeling the transport of dislocations on their glide planes both in the bulk and across the boundary. In Dogge et al. (submitted for publication-a) a Finite Element Method (FEM) framework was developed to solve the resulting transport equations in single slip, including an extended description of the relevant short-range dislocation–dislocation interactions. This model was used to study the effect of dislocation transport, and especially the dislocation interactions, on the response of a two-phase laminate in Dogge et al. (submitted for publication-b). The microstructure considered consisted of a soft and a hard phase with identical elastic properties, but different plastic properties, i.e. a different resistance to dislocation motion. However, in this two-phase microstructure the boundary between the two phases was considered transparent, i.e. dislocations are transmitted from one phase to the other without penalty. In spite of this obvious simplification, size effects could still be observed due to the dislocation–dislocation interactions near the interface, as dislocation motion was more restricted in the harder of the two phases.

In this paper, the continuum dislocation transport framework is extended by treating the interface as an additional barrier to dislocation motion, which is physically more relevant. An interface element is developed for this purpose and the dislocation transport through this interface is governed by an additional constitutive relation for the dislocation flux in this interface element. The transmitted interface flux depends on the difference in dislocation density at both sides of the interface. To derive an expression for this dependence, an idealized configuration of infinite edge dislocation walls is used, where the negative walls are shifted with respect to the positive walls by half of the internal wall spacing. This approach is inspired by the methods presented by Dogge et al. (submitted for publication-a), where interactions in the bulk material were investigated. Using regularized dislocation stress fields (Cai et al., 2006), and adopting continuous densities in order to characterize the horizontal spacing of the walls, an expression for the interaction stress at the interface is derived. This stress drives the dislocation flux against a resistance, which is assumed to be purely viscous and linear in the dislocation velocity.

The resulting contribution of this interface model is first examined in a single-phase material with a single interface between two identical phases, i.e. a 'grain boundary'. The extended model is then used to model the dislocation transport in an idealized two-phase laminate in which, unlike in Dogge et al. (submitted for publication-b), the phases are now separated by a discrete phase boundary which presents additional resistance against dislocation motion. In addition to the bulk properties, the influence of interfacial properties on the macroscopic material response is investigated.

The outline of this paper is as follows. In Section 2 the microstructural configuration, the used continuum model for dislocation transport and the novel interface model are discussed. In Section 3 the role of the interface resistance is investigated for identical phases separated by a boundary. In Section 4 the influence of the interface on the response of an idealized two-phase laminate is investigated, along with a parameter study of the interfacial, bulk and geometrical effects. Finally, in Section 5 the conclusions are presented.

2. Interface modeling in continuum dislocation transport

2.1. Microstructural model

An idealized representation of a two-phase microstructure is used as the starting point in the analysis of the interface model (Cordero et al., 2010). The idealized two-phase configuration used is shown in Fig. 1. A unit cell of length L is deformed at a constant shear rate $\dot{\Gamma}$, resulting in vertical displacements $u(x)$ in the material. On the