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Climb-enabled discrete dislocation plasticity

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ABSTRACT

A small strain two-dimensional discrete dislocation plasticity framework coupled to vacancy diffusion is developed wherein the motion of edge dislocations is by a combination of glide and climb. The dislocations are modelled as line defects in a linear elastic medium and the mechanical boundary value problem is solved by the superposition of the infinite medium elastic fields of the dislocations and a complimentary non-singular solution that enforces the boundary conditions. Similarly, the climbing dislocations are modelled as line sources/sinks of vacancies and the vacancy diffusion boundary value problem is also solved by a superposition of the fields of the line sources/sinks in an infinite medium and a complementary non-singular solution that enforces the boundary conditions. The vacancy concentration field along with the stress field provides the climb rate of the dislocations. Other short-range interactions of the dislocations are incorporated via a set of constitutive rules. We first employ this formulation to investigate the climb of a single edge dislocation in an infinite medium and illustrate the existence of diffusion-limited and sink-limited climb regimes. Next, results are presented for the pure bending and uniaxial tension of single crystals oriented for single slip. These calculations show that plasticity size effects are reduced when dislocation climb is permitted. Finally, we contrast predictions of this coupled framework with an ad hoc model in which dislocation climb is modelled by a drag-type relation based on a quasi steady-state solution.

1. Introduction

Plastic deformation in crystalline metals is a consequence of the motion of large numbers of dislocations, and much is known about the collective behaviour of dislocations. Investigations of dislocation pattern formation in macroscopically deformed solids have been carried out where the individual dislocations are described as line singularities in an elastic solid; see for example Gulluoglu et al. (1989), Kubin et al. (1992), Amodeo and Ghoniem (1990), and Lubarda et al. (1993). The pioneering work of Van der Giessen and Needleman (1995) extended this methodology to solve boundary value problems by using superposition of the infinite body elastic fields of the dislocations with a complimentary non-singular solution that enforces the boundary conditions. This ability to solve boundary value problems, in essence, created a new plasticity theory in which a range of material length scales were inherently in-built. We shall refer to this technique as discrete dislocation plasticity (DDP).

The DDP method has been shown to successfully predict numerous observations of plasticity size effects at the micrometer and sub-micrometer length scale. These include size effects in composites (Cleveringa et al., 1997), bending

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(Cleveringa et al., 1999), indentation (Balint et al., 2006), uniaxial compression (Deshpande et al., 2005), in thin films (Nicola et al., 2003; Ayas and Van der Giessen, 2008) and under constrained shear (Danas et al., 2010). The framework has also been used to investigate crack growth under monotonic (Cleveringa et al., 2000) and fatigue loading (Deshpande et al., 2003b). Numerical methods to extend the framework to three-dimensional (3D) problems (Fivel and Canova, 1999) and quasi-3D or the so-called 2.5D approaches (Benzerga et al., 2004) have also been developed in order to capture essential features of plasticity including strain hardening under tensile loading. In keeping with the idea of developing a plasticity framework capable of solving boundary value problems, Deshpande et al. (2003a) extended the methodology of Van der Giessen and Needleman (1995) to account for finite strains.

In all the studies mentioned above, the motion of dislocations is restricted to glide-only along specific slip planes which is appropriate for deformations at temperatures significantly less than about $0.3T_m$, where T_m is the absolute melting temperature of the metal. Diffusion is a significant mechanism of deformation at the temperatures encountered in many applications including for example the manufacture of semiconductor devices (Ayas and Van der Giessen, 2009) and the deformation of superalloys used in turbine blades; see a recent study by Zhu et al. (2012) into the mechanisms of creep in nickel-based single crystal superalloys.

Diffusion of vacancies permits dislocations to climb out of their slip planes and this is a potent relaxation mechanism: with the aid of small amounts of climb, dislocations can surmount small obstacles and thereby prevent the build-up of large pile-ups (Artz, 1998; Zhu et al., 2012). In fact, recent experimental measurements of the uniaxial compressive response of indium micro-pillars at room temperature (room temperature is above $0.3T_m$ for Indium) by Lee et al. (2011) revealed significantly smaller size effects compared with corresponding measurements for Gold (Greer et al., 2005), Ni and Ni_3Al (Uchic et al., 2004) single crystals at room temperature. Moreover, a reduced indentation hardness size effect too has recently been reported by Franke et al. (2010) in copper as the temperature is increased from ambient to 200 °C. It is thus of considerable interest to extend the DDP framework to higher temperatures, where diffusion of vacancies results in plastic deformation due to dislocation climb.

Mordehai et al. (2008) have reported three-dimensional discrete dislocation calculations wherein climb motion of the dislocations is included in the form of a drag-type relation. This early study demonstrated the effect of climb in an infinite FCC crystal by investigating the activation of Bardeen–Herring sources. Other notable contributions which have incorporated climb into a discrete dislocation studies include the work by Xiang and Srolovitz (2006), Bako et al. (2006) and Raabe (1998) who outlined a formulation for including climb in discrete dislocation calculations and then employed this idea to model creep of Nickel superalloys in Haghighat et al. (2013). These studies however did not solve boundary value problems. More recently, a number of studies have attempted to extend the DDP framework to include glide and climb of dislocations; see for example Ayas et al. (2012), Danas and Deshpande (2013), Davoudi et al. (2012) and Buehler et al. (2004). However, all these studies have used some version of a drag-type relation based on the quasi steady-state solution of Hirth and Lothe (1968). Keralavarma et al. (2012) augmented these approaches by solving a “discretized” subsidiary diffusion problem by assuming that dislocations within an arbitrary volume element climb by a drag-type relation and diffusion governs the flow of vacancies between these discrete volume elements. On the other hand, Ahmed and Hartmaier (2011) modelled creep of ultra-fine grained materials by accounting for the climb of dislocations at grain boundaries. Here we present a methodology to solve the fully coupled mechanical equilibrium and vacancy diffusion boundary value problems wherein a drag-type relation for dislocation climb is not assumed *a priori* and dislocation climb is a direct outcome of the coupled problem solution.

1.1. Outline and scope of study

We consider a two-dimensional (2D) plane strain crystalline solid with plastic deformation taking place by both glide and climb of edge dislocations along a specified set of crystallographic directions. Attention is confined to quasi-static deformation and body forces are assumed to be absent. The basic assumptions are: (i) a combination of dislocation glide and climb is the mechanism of plastic deformation; (ii) elastic properties are assumed to be unaffected by dislocation motion and the vacancies within the crystal; (iii) outside the dislocation cores, the dislocation stress, strain and displacement fields are accurately described by linear elasticity; (iv) vacancies are modelled as smeared-out entities as represented by their concentration (i.e. not discretely like the dislocations); and (v) the contribution of the vacancies to the stress and strain fields is ignored. Throughout, we adopt Cartesian tensor notation and $\dot{(\,)}$ denotes $\partial(\,)/\partial t$.

The problem essentially comprises of three parts:

(i) A mechanical boundary value problem that is largely along the lines of that first described by Van der Giessen and Needleman (1995): this is discussed in Section 4.1 along with the necessary modifications to the Van der Giessen and Needleman (1995) formulation.
(ii) A subsidiary vacancy diffusion problem that provides the climb rate of the dislocations.
(iii) Calculation of short-range dislocation interactions through a set of constitutive rules.

We first begin by describing the climb of edge dislocations and the associated vacancy diffusion problem. Next, we discuss the climb of a single edge dislocation in an infinite medium subjected to remote tensile loading. Third, we describe the