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Finite strain discrete dislocation plasticity in a total Lagrangian setting

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ABSTRACT

We present two total Lagrangian formulations for finite strain discrete dislocation plasticity wherein the discrete dislocations are presumed to be adequately represented by singular linear elastic fields thereby extending the superposition method of Van der Giessen and Needleman (1995) to finite strains. The finite deformation effects accounted for are (i) finite lattice rotations and (ii) shape changes due to slip. The two formulations presented differ in the fact that in the "smeared-slip" formulation the discontinuous displacement field is smeared using finite element shape functions while in the "discrete-slip" formulation the weak form of the equilibrium statement is written to account for the slip displacement discontinuity. Both these total Lagrangian formulations use a hyper-elastic constitutive model for lattice elasticity. This overcomes the issues of using singular dislocation fields in a hypo-elastic constitutive relation as encountered in the updated Lagrangian formulation of Deshpande et al. (2003). Predictions of these formulations are presented for the relatively simple problems of tension and compression of single crystals oriented for single slip. These results show that unlike in small-strain discrete dislocation plasticity, finite strain effects result in a size dependent tension/compression asymmetry. Moreover, both formulations give nearly identical predictions and thus we expect that the "smeared-slip" formulation is likely to be preferred due to its relative computational efficiency and simplicity.

1. Introduction

Over the last 25 years, computational solid mechanics has become an integral part of theoretical materials science. Significant attention has focused on mesoscale continuum mechanics where structural dimensions are important. Such formulations are intermediate between direct atomistic simulations and an unstructured continuum description of deformation processes. A variety of theoretical frameworks are emerging to describe inelastic deformation at the mesoscale: in this study we shall focus on one of these methods viz. discrete dislocation plasticity (DDP). In DDP, the dislocations are treated as line singularities in an elastic solid. A many body interaction problem involving the discrete dislocations needs to be solved together with a complimentary more conventional elasticity boundary value problem.

Following the pioneering work of Van der Giessen and Needleman (1995), the DDP method has been shown to successfully predict numerous observations of plasticity size effects at the micron and sub-micron length scale. These

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observations include size effects in composites (Cleveringa et al., 1997), bending (Cleveringa et al., 1999), indentation (Balint et al., 2006), uniaxial compression (Deshpande et al., 2005), 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., 2002). Numerical methods to extend the framework to three-dimensional (3D) problems (Zbib et al., 1998; Weygand et al., 2002) and quasi-3D or the so-called 2.5D (Benzerga et al., 2003) have also been developed in order to capture essential features of plasticity. Furthermore similar to the work of Van der Giessen and Needleman (1995), Yasin et al. (2001) and Vattré et al. (2014) have presented a framework coupling continuum elasticity with three-dimensional discrete dislocation dynamics. The 3D framework has now been used to investigate a range of problems including the analysis of micro-cracks behaviour in high-cycle fatigue conditions (Prasad Reddy et al., 2013), size effects in bending (Motz et al., 2008) and the behaviour of micro-pillars under uniaxial compression (Senger et al., 2008). The 3D framework has also been applied in more complex settings such as the modelling of poly-crystalline materials (Šiška et al., 2009), indentation (Fivel et al., 1998), radiation hardening (Khraishi et al., 2002), fatigue crack propagation (Déprés et al., 2014) and to investigate the effects of geometrically necessary dislocations on precipitation hardening (Chang et al., 2012). All these studies have been conducted in a “small-strain” context wherein finite deformation effects such as lattice rotations and changes in the geometries of the body are not accounted for.

There have been limited studies which account for finite deformation effects in conjunction with dislocation plasticity. Acharya (2004) developed a finite deformation field theory for continuously distributed dislocations while El-Azab (2006) has developed a finite deformation statistical mechanics formalism for dislocation plasticity. Zbib et al. (2002) have presented a formulation where volume average plastic strain rates and plastic rotation rates, obtained from small deformation discrete dislocation plasticity, are used in a conventional continuum finite deformation visco-plastic constitutive description, so that the finite deformation effects are decoupled from the discrete dislocation dynamics. By contrast, Deshpande et al. (2003) presented a fully coupled framework for carrying out finite deformation discrete dislocation plasticity analyses in an updated Lagrangian setting.

The formulation of Deshpande et al. (2003) accounted for the effect of lattice rotations and finite geometry changes due to the motion of the discrete dislocations. They assumed that the stress and deformation fields associated with individual dislocations are accurately described, outside of the dislocation core region, by linear elasticity and extended the superposition framework of Van der Giessen and Needleman (1995) to finite deformations using an updated Lagrangian setting. However, we shall show that the hypo-elastic relation they implemented does not correctly account for lattice rotations. The main aim of this paper is to present total Lagrangian formulations for finite strain discrete dislocation plasticity which employ a hyper-elastic constitutive model that circumvents the issues of the Deshpande et al. (2003) formulation.

1.1. Scope of study

We present two total Lagrangian formulations for the solution of boundary value problems using finite strain discrete dislocation plasticity. Similar to Deshpande et al. (2003) the finite strain effects that we account for are lattice rotations and finite geometry changes due to the motion of the discrete dislocations with linear elasticity being assumed to accurately describe the dislocations displacements, outside of the dislocation core region. Thus, unlike in conventional crystal plasticity, the displacement field in this continuum is only piecewise continuous. Slip induced by dislocation motion gives rise to a jump in the displacement field; see Figs. 1(a) and (b). Two total Lagrangian formulations are presented to solve the finite strain DDP boundary value problems:

(i) *The smeared-slip formulation*: Here, similar to the numerical results presented by Deshpande et al. (2003), we smear the dislocation slip field using the finite element (FE) shape functions. Thus, geometry change is represented by a continuous displacement field, which is obtained by averaging slip over a finite element as sketched in Fig. 1(c).
(ii) *The discrete-slip formulation*: In this formulation the discontinuous nature of the displacement field is accounted for in

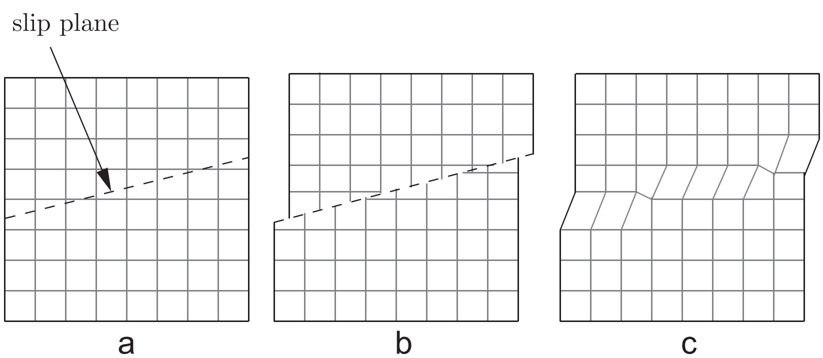

Fig. 1. (a) Undeformed lattice with one active slip plane. (b) Schematic showing the geometry change due to a slip discontinuity across the active slip plane. (c) Effect of smearing the slip on a finite element mesh with bilinear elements.