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A finite element formulation to solve a non-local constitutive model with stresses and strains due to slip gradients

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Abstract

Solving constitutive models that incorporate the effects of plasticity and slip gradients is often complicated by the non-local nature of the models. This work presents a finite element solution to a crystal plasticity constitutive model that includes kinematic and stress effects due to slip gradients. The foundation of the model is a three term multiplicative decomposition of the deformation gradient that results in a second order differential equation in terms of the stress that drives slip. Converting the equation into a weak form results in an integral equation that includes first order derivatives of the stress as well as boundary conditions for the stress and gradients of slip rate for each slip system. Using this weak form, an incremental finite element method is developed to solve the constitutive model within a finite element solution to the equilibrium equation. Results for the compression of a two-dimensional plate show the effects of including slip gradient effects in the constitutive model and indicate the tendency for localization of the slip and dislocation density into narrow bands separating regions of nearly constant dislocation density and long range strain.

Keywords: Finite element; Constitutive behavior; Crystal plasticity; Gradient plasticity

1. Introduction

The actions of dislocations in a crystal lattice are very complex and it is their actions that are often the primary factor in inelastic deformations in metals and other crystalline materials. Capturing the relevant phenomena of the collective behavior of individual dislocations is the aim of constitutive models of crystal plasticity. For simple materials, in the rational mechanics sense, material behavior at a point is determined by the history of deformation at the point. One phenomenon that does not fit into the definition of a simple material is the long range effects of dislocations distributed through the crystal lattice. The reason for this is these effects are related to the spatial distribution of the dislocations and cannot be reduced to pointwise behavior.

In this work we present a finite element solution to a previously developed constitutive model [28] that incorporates the kinematic and kinetic effects of dislocations distributed through the crystal lattice. These long range effects are related to gradients in plastic deformation in which dislocations remain in the lattice to ensure continuity between neighboring regions of varying plastic deformation. Including these effects in the constitutive model results in a deformation rate consistency equation that is a second order differential equation in terms of the elastic stress. Determining the material response then requires a scheme to solve the differential equation along with specification of the appropriate boundary conditions.

There is a diverse array of methods that have been used to incorporate dislocations in general, and specifically gradient effects, into models for the mechanical behavior of crystalline materials. For example, lattice defects have long been described in the language differential geometry and gauge field theory [6,39,41]. Steinmann

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[61] discusses the relationship between differential geometry and the family of Nye dislocation tensors [54] and Lazar [44] has constructed a theory relating the Cartan torsion of the crystal lattice to a moment stress. In closer connection to standard continuum mechanics, but still within the context of differential geometry, Clayton et al. [10] have developed a three term multiplicative decomposition of the deformation gradient in which the additional term is due to defect arrangement and residual stress. The differential geometry of such a formulation is discussed in detail and a constitutive model is presented by Clayton et al. [11]. Micropolar [19] and Cosserat [14] continua have been used to include point rotations as kinematic variables to model rotation gradients that accompany slip gradients. Forest and co-workers [25,26] have been the principal contributors in this area, as well as contributions by Le and Stumpf [45,46]. The elastic theory of a continuous distribution of dislocations, developed in the early works of Kröner [42,43], Mura [49–51] and Willis [65], has been used by a number of authors to relate the stress to dislocation distributions and behaviors. Using this theory as a foundation, Acharya [1–3] has developed a complete theory of continuum plasticity in terms of the dislocation density tensor as the primary variable and developed a closed set of equations, up to specification of the constitutive models for plasticity and dislocation tensor, that define the material behavior. The discrete dislocation model of Van der Giessen and Needleman [63] uses a set of rules for dislocation motion, nucleation and annihilation to predict the set of discrete dislocations then superimposes the deformation field of each dislocation on an elastic continuum. In work more closely related to that presented below, several authors have formulated yield surface and crystal plasticity constitutive models that incorporate gradient effects. Mühlhaus and Aifantis [48] developed a one parameter yield surface that included second and fourth order gradients of the effective plastic strain and required solution of a forth order differential equation for evolution of the yield surface. Fleck and Hutchinson [22,23] and Fleck et al. [24] have developed a model that includes both a plasticity gradient modified yield stress along with a curvature deformation and couple stress theory somewhat analogous to standard yield surface models. The "Mechanism Based Strain Gradient" model [27,37,53,55] uses the ideas of Fleck and Hutchinson and an assumed deformation field on a sub-computational scale to develop the constitutive model. Gurtin [30,31] has developed a single crystal plasticity constitutive model that includes classical macroscopic work conjugate terms as well as microforce terms that do work as a result of plastic slip. Acharya and Basani [4] have developed a crystal plasticity model in which they propose modifying the critical resolved shear stress for a slip system by a functional relationship on a tensor measure of dislocation density. Evers et al. [20] develop a single crystal material model which incorporates geometrically necessary dislocations in the slip systems hardness and also develops a long range stress that acts as a slip system back stress and is derived from ideas similar to those presented below in Section 2.2.

The work to implement these models in solution schemes is limited to relatively simple methods such as assumed deformation field analytical solutions and a limited number of (primarily) two-dimensional, finite element implementations. The reason for this is the non-local nature of the constitutive models do not easily fit within typical frameworks for the numerical solution of solid mechanics problems. Among the solutions, Mühlhaus and Aifantis [48] and Deborst and Mühlhaus [15] present a finite element solution of a reduced form of their model which is accommodated in standard displacement based finite element solution schemes through the addition of the effective plastic strain to the nodal degrees of freedom. In the early development of the Mechanism Based Strain Gradient model [27,55,37] several analytical solutions for assumed deformation fields including bending of a thin film, torsion of a thin wire, and cavity expansion [36] were presented. Since that time the model has been implemented in two and three-dimensional finite element solutions and principally used to investigate the size effect in indentation testing [38,62]. The yield surface models of Fleck and Hutchinson [22,23] and Fleck et al. [24] were used to develop a class of two-dimensional finite elements suitable for use with strain gradient theories [59]. Huang et al. [35] and Xia and Hutchinson [66] have used the Fleck–Hutchinson model to study mode I and mode II fracture using both assumed deformation field solutions and a two-dimensional finite element method. Chen and Fleck [9] have implemented the model in a two-dimensional finite element package and studied the size effects in shear deformation of a metallic foam. Evers et al. [21] demonstrated their model by simulating the uniaxial plane strain deformation of a collection of 12 grains, each of which is separately meshed and shows the gradients effects inherent in the otherwise macroscopically uniform deformation of the polycrystal structure.

There are, as well, some efforts to provide solutions to the models that don't necessarily fit within standard continuum constitutive modeling. Perhaps the most widely used is the discrete dislocation plasticity model of Van der Giessen and Needleman [63] which has been exercised in a number of two-dimensional simulations. For example, Cleveringa et al. [12] have shown the local stress fields around a mode I crack are affected by the long range stresses due to dislocations; Balint et al. [5] have shown the model reproduces the grain size dependence of hardness; Nicola et al. [52] have used the model to analyze the behavior of a thin film bonded to a substrate undergoing thermal straining; and Deshpande et al. [16] have shown the size and Bauschinger effects in the tension and compression of single crystals. The model of Acharya [1–3], based on the elastic theory of a continuous distribution of dislocations, has been implemented by Roy and Acharya [58] in a three-dimensional finite element method and demonstrated the behav-