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A computational study of a model of single-crystal strain-gradient viscoplasticity with an interactive hardening relation

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ABSTRACT

The behavior of a model of single-crystal strain-gradient viscoplasticity is investigated. The model is an extension of a rate-independent version, and includes a new hardening relation that has recently been proposed in the small-deformation context (Gurtin and Reddy, 2014), and which accounts for slip-system interactions due to self and latent hardening. Energetic and dissipative effects, each with its corresponding length scale, are included. Numerical results are presented for a single crystal with single and multiple slip systems, as well as an ensemble of grains. These results provide a clear illustration of the effects of accounting for slip-system interactions.

1. Introduction

The hardening behavior of a crystalline metal depends on a number of factors such as elastic stiffness, strength, dislocation interaction, etc., as well as on the grain size (see for example Hall, 1951; Petch, 1953). In the context of gradient extended crystal plasticity, which is motivated by the size-dependent effects that predominate at the micron scale, theories have been proposed by various authors. The literature on the subject has increasead significantly in the last decade and more, with representative and important works including those by Fleck and Hutchinson (2001), Gurtin (2000), Nix and Gao (1998) and Shu and Fleck (1999).

Recently, within the small-deformation framework, Gurtin and Reddy (2014) have introduced a rate-independent, thermodynamically consistent, single-crystal plasticity theory which accounts for self- and latent hardening. The behavior of the new hardening relation, and in particular its comparison with other hardening laws that have been in use for some time, have been studied by Povall et al. (2013) for the conventional (that is, non-gradient) theory. These authors show via selected numerical examples that, while the slip resistances as proposed by the different theories vary quite considerably, the overall response of single crystals when subjected to various loading conditions is qualitatively similar for the different models. Other recent contributions that deal with self- and latent hardening include works by Bardella et al. (2013), Bargmann et al. (2011), Conti and Ortiz (2005), Evers et al. (2004), Klusemann et al. (2013a), Levkovitch and Svendsen (2006), Wulfinghoff and Böhlke (2012) and Yalcinkaya et al. (2012).

The Gurtin–Reddy model (Gurtin and Reddy, 2014) has the advantage of simplicity: it is defined as a function of the generalized accumulated slips, while established models such as that due to Peirce et al. (1982) are defined implicitly via a system of differential equations. The purpose of this contribution is essentially to extend the work carried out in Povall et al. (2013), by investigating computationally the behavior of the model of interactive slip resistances, for the strain-gradient theory. This is done in a large-deformation context, and for a viscoplastic extension of the model presented in Gurtin and Reddy (2014).

2. Basic kinematics: Single crystal plasticity

In large-deformation plasticity, the main assumption is the classical multiplicative split of the deformation gradient $\boldsymbol{F}$ into an elastic $\boldsymbol{F}_e$ and a plastic part $\boldsymbol{F}_p$:

$$\boldsymbol{F} = \boldsymbol{F}_e \cdot \boldsymbol{F}_p. \quad (1)$$

The plastic part $\boldsymbol{F}_p$ is assumed to arise due to inelastic slip in the preferred crystallographic planes. The elastic contribution $\boldsymbol{F}_e$ accounts for lattice distortion and rotation. The Green–Lagrange strain and the right Cauchy–Green stretch tensors are defined by

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$$\boldsymbol{E} := \frac{1}{2}[\boldsymbol{F}^t \cdot \boldsymbol{F} - \boldsymbol{I}], \quad \boldsymbol{C} = \boldsymbol{F}^t \cdot \boldsymbol{F} \tag{2}$$

and their elastic counterparts by

$$\boldsymbol{E}_e := \frac{1}{2}[[\boldsymbol{F}_e]^t \cdot \boldsymbol{F}_e - \bar{\boldsymbol{I}}], \quad \boldsymbol{C}_e = \boldsymbol{F}_e^t \cdot \boldsymbol{F}_e, \tag{3}$$

where $\boldsymbol{I}$ and $\bar{\boldsymbol{I}}$ denote the identity tensors in the reference and intermediate configurations respectively.

2.1. Glide system kinematics

As usual, the crystal plasticity model is based on the glide-system geometry described by the glide direction $\boldsymbol{s}_\alpha$ and glide-plane normal $\boldsymbol{n}_\alpha$, both fixed unit vectors in the intermediate configuration $\mathcal{B}_i$. Together with the direction $\boldsymbol{p}_\alpha = \boldsymbol{n}_\alpha \times \boldsymbol{s}_\alpha$ transverse to $\boldsymbol{s}_\alpha$ in the glide plane, they form an orthonormal system. It is well known that often two or more crystallographically equivalent systems contribute to the plastic deformation.

In terms of the glide-system geometry, the evolution of the plastic part $\boldsymbol{F}_p$ of the deformation gradient is given in terms of the glide-system geometry and slip rates v_α by

$$\dot{\boldsymbol{F}}_p = \sum_\alpha v_\alpha \boldsymbol{s}_\alpha \otimes \boldsymbol{F}_p^t \cdot \boldsymbol{n}_\alpha. \tag{4}$$

Thus, the plastic flow $\boldsymbol{L}_p = \dot{\boldsymbol{F}}_p \cdot \boldsymbol{F}_p^{-1}$ is governed by the slip rates v_α. Further, it is convenient to define a generalized slip rate $\boldsymbol{\Gamma}_\alpha$ by

$$\boldsymbol{\Gamma}_\alpha = \begin{pmatrix} v_\alpha \\ l_{d,\alpha} \nabla_{\boldsymbol{X}} v_\alpha \end{pmatrix}, \tag{5}$$

where $l_{d,\alpha}$ is a dissipative length scale associated with slip system α. It is not directly related to microstructural length scales (Gurtin et al., 2007; Voyiadjis and Deliktas, 2009). The idea of introducing more than one internal material length scale within the context of higher-order strain-gradient plasticity has been followed by several authors (see e.g., Anand et al., 2005; Bardella and Giacomini, 2008; Bargmann and Reddy, 2011; Fleck and Hutchinson, 2001; Gurtin and Reddy, 2014; Lele and Anand, 2008; Niordson and Legarth, 2010; Reddy, 2013a).

2.2. Stress measures

Relevant stress measures are the first Piola–Kirchhoff stress

$$\boldsymbol{P} := \det(\boldsymbol{F})\boldsymbol{\sigma} \cdot \boldsymbol{F}^{-t}, \tag{6}$$

and the elastic second Piola–Kirchhoff stress $\boldsymbol{S}_e$ defined by

$$\boldsymbol{S}_e := \det(\boldsymbol{F})\boldsymbol{F}_e^{-1} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{F}_e^{-t} = [\boldsymbol{F}_e]^{-1} \cdot \boldsymbol{P} \cdot [\boldsymbol{F}_p]^t, \tag{7}$$

whereas the Cauchy stress tensor $\boldsymbol{\sigma}$ is a stress measure in the current configuration $\mathcal{B}_t$, the second Piola–Kirchhoff stress $\boldsymbol{S}_e$ is a stress measure in the intermediate configuration.

The resolved shear or Schmid stress τ_α is defined by

$$\tau_\alpha = \boldsymbol{s}_\alpha \cdot \boldsymbol{M}_e \cdot \boldsymbol{n}_\alpha, \tag{8}$$

where $\boldsymbol{M}_e = \boldsymbol{C}_e \cdot \boldsymbol{S}_e$ is the Mandel stress.

2.3. Dislocation densities

During plastic deformation, two types of dislocations are present: statistically stored dislocations (SSDs) which are accumulated by a random trapping process and are responsible for plastic deformation (Arsenlis et al., 2004); and geometrically necessary dislocations (GNDs) which arise due to the locally heterogeneous plastic shear. The first concepts of GNDs were introduced in Nye (1953) and Ashby (1970) to account for modes of plastic deformation, where an internal accumulation of dislocation densities is required to accommodate the gradients of plastic strain induced by the deformation (Needleman and Sevillano, 2003). In this regard, GNDs are necessary to preserve lattice compatibility and represent an additional source of dislocations in the material due to inhomogeneous plastic flow (Gao and Huang, 2003). In a continuum theory there are no discrete dislocations. However, non-uniform slips and slip gradients on the individual glide systems result in quantities that mimic the behavior of microscopic dislocations. The GNDs are usually subdivided into edge and screw dislocations, where edge dislocations are characterized by the fact that the Burgers vector is perpendicular to the dislocation line direction, while for screw dislocations the Burgers vector and one direction are parallel.

The simplest class of models for dislocation evolution is obtained for the case of self-interaction, in which the dislocations on each glide system interact only with themselves.

GNDs do not contribute to the plastic deformation: rather, they act as obstacles to the motion of the SSDs, leading to hardening in the material. The edge and screw dislocation densities are internal state variables defined by (Gurtin et al., 2010, Section 107.4)

$$\dot{\rho}_\alpha^{ge} = -\frac{1}{b}\nabla_{\boldsymbol{X}} v_\alpha \cdot \left[\boldsymbol{F}_p^{-1} \cdot \boldsymbol{s}_\alpha\right], \tag{9}$$

$$\dot{\rho}_\alpha^{gs} = \frac{1}{b}\nabla_{\boldsymbol{X}} v_\alpha \cdot \left[\boldsymbol{F}_p^{-1} \cdot \boldsymbol{p}_\alpha\right], \tag{10}$$

where b is the magnitude of the Burgers vector. The initial conditions are assumed to be $\rho_\alpha^{ge}(\boldsymbol{X}, 0) = 0$ resp. $\rho_\alpha^{gs}(\boldsymbol{X}, 0) = 0$. The dislocation densities may be positive or negative.

Our definition of the GND density differs from that in Gurtin and Reddy (2014) by the use of the length of the Burgers vector b. This is due to the fact that in Gurtin and Reddy (2014) the theory is based strictly on continuum mechanics in which the GND is a quantity measured per unit length. In this work, we follow the approach generally used in material science where the GND represents a quantity measured in dislocations per unit area.

3. The mathematical model

3.1. Force balances

The macroscopic force balance equation is

$$\boldsymbol{0} = \mathrm{Div}\,\boldsymbol{P} + \boldsymbol{f}, \tag{11}$$

where $\boldsymbol{f}(\boldsymbol{x}, t) : \mathcal{B}_0 \times \mathbb{R}_+ \rightarrow \mathbb{R}^{\dim}$ is the body force. Here and henceforth Div refers to the divergence with respect to the reference configuration, i.e., $\mathrm{Div}\{\bullet\} = \nabla_{\boldsymbol{X}} \cdot \{\bullet\}$

On the microlevel, we follow the approach in Gurtin (2000, 2008) and introduce the microforce balance equation [1]

$$0 = \mathrm{Div}\,\xi_{X,\alpha} + \tau_\alpha - \pi_\alpha, \tag{12}$$

where π_α is the scalar internal microforce and $\xi_{X,\alpha}$ is the referential vector-valued microstress power-conjugate to the slip rate gradient $\nabla_{\boldsymbol{X}} v_\alpha$. The microforce balance (12) has to hold for every slip system α. The microstress $\xi_{X,\alpha}$ is split into an elastic and a dissipative contribution (see e.g., Gurtin and Anand, 2005):

$$\xi_{X,\alpha} = \xi_{X,\alpha}^{en} + \xi_{X,\alpha}^{dis}, \tag{13}$$

whereas the internal microforce π_α is purely dissipative in nature.

[1] The existence of the microforce balance (12) is a consequence of the principle of virtual power; cf. Gurtin (2000) for a detailed derivation.