International Journal of Plasticity 57 (2014) 29–51

Contents lists available at ScienceDirect

International Journal of Plasticity

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

A comparison of Gurtin type and micropolar theories of generalized single crystal plasticity

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ARTICLE INFO

Article history:
Received 24 April 2013
Received in final revised form 8 January 2014
Available online 22 February 2014

Keywords:
A. Gradient plasticity
B. Crystal plasticity
A. Geometrically necessary dislocations
B. Microforce balance
C. Finite elements

ABSTRACT

We compare and contrast the governing equations and numerical predictions of two higher-order theories of extended single crystal plasticity, specifically, Gurtin type and micropolar models. The models are presented within a continuum thermodynamic setting, which facilitates identification of equivalent terms and the roles they play in the respective models. Finite element simulations of constrained thin films are used to elucidate the various scale-dependent strengthening mechanisms and their effect of material response. Our analysis shows that the two theories contain many analogous features and qualitatively predict the same trends in mechanical behavior, although they have substantially different points of departure. This is significant since the micropolar theory affords a simpler numerical implementation that is less computationally expensive and potentially more stable.

1. Introduction

Generalized single crystal plasticity theories can be separated into two distinct classes: (i) low-order theories and (ii) higher-order theories, which are differentiated, in part, by the order of the governing differential equations. Higher-order theories are further subdivided into work conjugate and non-work conjugate theories (Kuroda and Tvergaard, 2008), with the distinction that work conjugate theories feature higher-order stress measures (hyperstresses) and nonstandard expressions of deformation power. Higher-order theories have recently gained favor amongst researchers since they admit boundary conditions on slip or alternative supplementary kinematic variables that are necessary for modeling certain classes of problems. In this work, we examine work conjugate higher-order theories of single crystal plasticity. A distinguishing aspect of work conjugate higher-order theories is the separation of gradient strengthening effects into energetic and dissipative contributions. Energetic gradient effects reflect scale-dependent behavior that emerges from the free energy dependence on nonlocal variables, whereas dissipative gradient effects contribute to the scale-dependence of the dissipation rate. It has been argued that both energetic and dissipative gradient behavior must be accounted for in order to capture trends exhibited for certain sets of experimental data.

Gurtin (2000, 2002) developed a work conjugate higher-order single crystal plasticity theory that has been subsequently adopted and advanced by many researchers (cf. Bittencourt et al., 2003, Borg, 2007; Okumura et al., 2007; Gurtin, 2008, 2010; Yalcinkaya et al., 2011; Reddy, 2011). For convenience, we label these as "Gurtin type" (GT) models. Gurtin's approach to generalized single crystal plasticity is a particular, special case of the broader class of continuum dislocation theories (cf. Naghdi and Srinivasa, 1994; Le and Stumpf, 1996; Shizawa and Zbib, 1999; Acharya, 2001; Berdichevsky, 2006; Clayton et al.,

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http://dx.doi.org/10.1016/j.ijplas.2014.01.010
0749-6419/

2006; Le and Günther, 2014) in which the geometrically necessary dislocation (GND) density tensor plays a fundamental kinematic role. The origin of the relationship between deformation incompatibility and the continuum GND density tensor date back to the works of Kondo (1953), Nye (1953), Bilby et al. (1955) and Kröner (1959). According to our definition, the distinguishing feature of a GT model is that it treats the slip system shearing rates as generalized continuum velocities in the work-conjugate sense. This assumption leads to a very specific form of an additional mechanical balance law, the so-called microforce balance, which governs the evolution of the slip system shears and is distinct to the GT theory. Prior works have established the effectiveness of GT theories in capturing certain aspects of 2D discrete dislocation dynamics simulations (Bittencourt et al., 2003; Nicola et al., 2005), and the relationship between different scale-dependent strengthening mechanisms and material response (Gurtin et al., 2007).

Building upon the earlier work of Forest and collaborators (Forest et al., 1997; Forest et al., 2000), we developed a micropolar single crystal plasticity theory (Mayeur et al., 2011) as an alternative approach to work-conjugate higher-order single crystal plasticity. Despite appreciable foundational differences, the micropolar model was demonstrated to predict many of the same trends in scale-dependent behavior as exhibited by GT theories. Furthermore, our micropolar model was shown to compare favorably with 2D discrete dislocation dynamics simulations of pure bending (Mayeur and McDowell, 2011), constrained simple shear (Mayeur and McDowell, 2013), and particle strengthening (Mayeur, 2010). Motivated by these observations and results, we explore the relationship between GT and micropolar models of single crystal plasticity.

GT theories are among the more widely employed generalized single crystal models; therefore, examining alternative models within the context of this framework is useful. Subsequently, we are better equipped to evaluate their relative strengths and weaknesses, which will facilitate the development of next generation models. Prior works have examined the relationship of the GT theory to other classes of models including those due to Kuroda and Tvergaard (2006), Erturk et al. (2009), Svendsen and Bargmann (2010) and Bargmann et al. (2010). However, a detailed comparison of micropolar and GT theories has not been carried out, although Forest and collaborators have certainly addressed some of the key similarities (Forest, 2008; Cordero et al., 2010).

This work presents a detailed comparison of the governing equations and predictive capabilities of GT and micropolar theories of generalized single crystal plasticity. Both modeling frameworks, which belong to the class of work conjugate higher-order theories, feature higher-order stresses that arise due to gradients in GND density and/or lattice torsion-curvature fields. The governing equations of the respective theories are presented within a thermodynamic setting to facilitate the identification of equivalent terms and to ensure that the proposed constitutive equations are thermodynamically consistent. Attendant finite element (FE) simulations of a constrained thin film subjected to simple shear are used to demonstrate the qualitative agreement of several aspects of predicted scale-dependent material behavior. The simulation results also highlight model differences that become apparent when dissipative gradient behavior is considered, which is directly related to underlying distinctions in the structure of the governing equations.

2. Constitutive models

2.1. Gurtin type theory

The GT theory of generalized single crystal plasticity (Gurtin, 2000; Gurtin, 2002) treats the set of slip system shears, $\vec{\gamma} = \{\gamma^1, \gamma^2, \ldots, \gamma^N\}$, as additional scalar micro degrees-of-freedom (dofs). Within the context of this model, the micro dofs are subject to boundary conditions and contribute, along with their gradients, to an enriched, nonclassical expression of deformation power. This contrasts with the classical theory in which the slip system shears are prescribed via constitutive equations and do not admit additional boundary conditions.

2.1.1. Kinematics

The fundamental set of kinematic field quantities in the GT theory include the displacement and the set of slip system shears, i.e., $\mathcal{U} = (\mathbf{u}, \vec{\gamma})$. We restrict the discussion here to linearized kinematics (i.e., small strain assumption). Following standard convention, the distortion tensor (displacement gradient) is additively decomposed into elastic and plastic parts as

$$\mathbf{H} = \mathbf{u}\nabla = \mathbf{H}^{e} + \mathbf{H}^{p} \tag{1}$$

where $\mathbf{H}^{p}$ is defined as the sum over all active glide systems, i.e.,

$$\mathbf{H}^{p} = \sum_{\alpha} \gamma^{\alpha}\mathbf{s}^{\alpha} \otimes \mathbf{n}^{\alpha} \tag{2}$$

Here, $\mathbf{s}^{\alpha}$ is the slip direction and $\mathbf{n}^{\alpha}$ is the slip plane normal. The small strain tensor is the symmetric part of the distortion tensor, i.e.,

$$\boldsymbol{\varepsilon} = \mathrm{sym}(\mathbf{H}) = \underbrace{\boldsymbol{\varepsilon}^{e}}_{\mathrm{sym}(\mathbf{H}^{e})} + \underbrace{\boldsymbol{\varepsilon}^{p}}_{\mathrm{sym}(\mathbf{H}^{p})} \tag{3}$$

The Burgers tensor, which is central to the GT theory, is a measure of the deformation incompatibility and is defined in terms of the curl of the plastic distortion as