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A finite element framework for distortion gradient plasticity with applications to bending of thin foils

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ABSTRACT

A novel general purpose Finite Element framework is presented to study small-scale metal plasticity. A distinct feature of the adopted *distortion* gradient plasticity formulation, with respect to *strain* gradient plasticity theories, is the constitutive inclusion of the plastic spin, as proposed by Gurtin (2004) through the prescription of a free energy dependent on Nye's dislocation density tensor. The proposed numerical scheme is developed by following and extending the mathematical principles established by Fleck and Willis (2009). The modeling of thin metallic foils under bending reveals a significant influence of the plastic shear strain and spin due to a mechanism associated with the higher-order boundary conditions allowing dislocations to exit the body. This mechanism leads to an unexpected mechanical response in terms of bending moment versus curvature, dependent on the foil length, if either viscoplasticity or isotropic hardening are included in the model. In order to study the effect of dissipative higher-order stresses, the mechanical response under non-proportional loading is also investigated.

1. Introduction

Experiments have shown that metallic materials display strong size effects at both micron and sub-micron scales (Fleck et al., 1994; Nix and Gao, 1998; Stölken and Evans, 1998; Moreau et al., 2005). Much research has been devoted to modeling the experimentally observed change in the material response with diminishing size (Fleck and Hutchinson, 1997; Qu et al., 2006; Klusemann et al., 2013) in addition to studies of size effects in void growth (Liu et al., 2005; Niordson, 2007), fiber reinforced materials (Bittencourt et al., 2003; Niordson, 2003; Legarth and Niordson, 2010), and fracture problems (Martínez-Pañeda and Betegón, 2015; Martínez-Pañeda and Niordson, 2016). Most attempts to model size effects in metals have been based on higher-order continuum modeling, and different theories, both phenomenological (Fleck and Hutchinson, 2001; Gudmundson, 2004; Gurtin, 2004; Gurtin and Anand, 2005) and mechanism-based (Gao et al., 1999) have been developed. All these theories aim at predicting size effects in polycrystalline metals in an average sense, without explicitly accounting for the crystal lattice, nor for the behavior of internal grain boundaries.

While higher-order energetic and dissipative contributions are a common feature among the majority of the most advanced phenomenological Strain Gradient Plasticity (SGP) theories (see, e.g., Gudmundson, 2004; Gurtin and Anand, 2005; 2009; Fleck and Willis, 2009b), the need to constitutively account for the plastic spin, as proposed about ten years ago by Gurtin (2004), to properly describe the plastic flow incompatibility and associated dislocation densities, has been mostly neglected in favor of simpler models. However, the use of phenomenological higher-order formulations that involve the whole plastic distortion (here referred to as *Distortion Gradient Plasticity*, DGP) has attracted increasing attention in recent years due to its superior modeling capabilities. The studies of Bardella and Giacomini (2008) and Bardella (2009; 2010) have shown that, even for small strains, the contribution of the plastic spin plays a fundamental role in order to provide a description closer to the mechanical response prediction of strain gradient *crystal* plasticity. This has been further assessed by Poh and Peerlings (2016), who, by comparing to a reference crystal plasticity solution obtained with the theory by Gurtin and Needleman (2005), showed that the plastic rotation must be incorporated to capture the essential features of crystal plasticity. Moreover, Poh and Peerlings (2016) numerically elucidated that the localization phenomenon taking place in the Bittencourt et al. (2003) composite unit cell benchmark problem can only be reproduced by DGP. Gurtin (2004) theory has also been employed by Poh and

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co-workers (Poh, 2013; Poh and Phan, 2016) through a novel homogenization formulation to describe the behavior of each grain in a polycrystal where grain boundaries are modeled to describe effects of dislocation blockage or transmittal.

However, despite the superior modeling capability of DGP with respect to SGP, the literature is scarce on the development of a general purpose Finite Element (FE) framework for DGP. Particularly, the use of higher-order dissipative terms - associated with strengthening mechanisms - is generally avoided due to the related computational complexities. This is the case of the very recent FE implementation of Poh and Peerlings (2016) and the earlier work by Ostien and Garikipati (2008), who implemented Gurtin (2004) theory within a Discontinuous Galerkin framework. Energetic and dissipative contributions are both accounted for in the recent *ad hoc* FE formulation for the torsion problem by Bardella and Panteghini (2015), also showing that, contrary to higher-order SGP theories, Gurtin (2004) DGP can predict some energetic strengthening even with a quadratic defect energy.

In this work, a general purpose FE framework for DGP is developed on the basis of an extension of the minimum principles proposed by Fleck and Willis (2009b). The numerical scheme includes both energetic and dissipative higher-order stresses and the effect of the latter under non-proportional loading is investigated. The novel FE framework is particularized to the plane strain case and applied to the bending of thin foils, of particular interest to the study of size effects in metals (see, e.g., Yefimov et al., 2004; Yefimov and Giessen, 2005; Engelen et al., 2006; Evans and Hutchinson, 2009; Idiart et al., 2009; Polizzotto, 2011) since the experiments of Stölken and Evans (1998) (see also Moreau et al., 2005). Computations reveal a dependence of the results on the foil length if either rate-dependent plasticity or isotropic hardening are included in the model. This is a consequence of the definition of the energetic higher-order contribution as a function of Nye's dislocation density tensor (Nye, 1953; Fleck and Hutchinson, 1997; Arsenlis and Parks, 1999), that is intrinsic to Gurtin (2004) theory. This unexpected effect, absent in conventional theories and in many GP theories, is accompanied with the development of plastic shear and plastic spin, which turn out to influence the overall mechanical response in bending. Such a behavior is triggered by the interaction between the conventional and the higher-order boundary conditions, the latter allowing dislocations to exit the foil at the free boundaries. The foil length dependence of the mechanical response is emphasized by the presence of the plastic spin in Gurtin (2004) DGP, but it also characterizes the Gurtin and Anand (2005) SGP theory, still involving Nye's tensor restricted to the assumption of irrotational plastic flow (that is, vanishing plastic spin). Hence, one of the results of the present investigation concerns with the usefulness of two-dimensional analyses with appropriate boundary conditions to model micro-bending phenomenologically.

Outline of the paper. The DGP theory of Gurtin (2004) is presented in Section 2, together with the novel minimum principles governing it. The FE formulation and its validation are described in Section 3. Results concerning bending of thin foils are presented and discussed in Section 4. Some concluding remarks are offered in Section 5.

Notation. We use lightface letters for scalars. Bold face is used for first-, second-, and third-order tensors, in most cases respectively represented by small Latin, small Greek, and capital Latin letters. When we make use of indices they refer to a Cartesian coordinate system. The symbol " · " represents the inner product of vectors and tensors (e.g., $a = \boldsymbol{b} \cdot \boldsymbol{u} \equiv b_i u_i$, $b = \boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon} \equiv \sigma_{ij}\varepsilon_{ij}$, $c = \boldsymbol{T} \cdot \boldsymbol{S} \equiv T_{ijk}S_{ijk}$). For any tensor, say $\boldsymbol{\rho}$, the inner product by itself is $|\boldsymbol{\rho}|^2 \equiv \boldsymbol{\rho} \cdot \boldsymbol{\rho}$. The symbol " × " is adopted for the vector product: $\boldsymbol{t} = \boldsymbol{m} \times \boldsymbol{n} \equiv e_{ijk} m_j n_k = t_i$, with e_{ijk} denoting the alternating symbol (one of the exceptions, as it is a third-order tensor represented by a small Latin letter), and, for $\boldsymbol{\zeta}$ a second-order tensor: $\boldsymbol{\zeta} \times \boldsymbol{n} \equiv e_{jlk}\zeta_{il}n_k$. For the products of tensors of different order the lower-order tensor is on the right and all its indices are saturated, e.g.: for $\boldsymbol{\sigma}$ a second-order tensor and $\boldsymbol{n}$ a vector, $\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n} \equiv \sigma_{ij}n_j = t_i$; for $\boldsymbol{T}$ a third-order tensor and $\boldsymbol{n}$ a vector, $\boldsymbol{T}\boldsymbol{n} \equiv T_{ijk}n_k$; for $\mathbb{L}$ a fourth-order tensor and $\boldsymbol{\varepsilon}$ a second-order tensor, $\boldsymbol{\sigma} = \mathbb{L}\boldsymbol{\varepsilon} \equiv L_{ijkl}\varepsilon_{kl} = \sigma_{ij}$. Moreover, $(\nabla \boldsymbol{u})_{ij} \equiv \partial u_i/\partial x_j \equiv u_{i,j}$, $(\operatorname{div}\boldsymbol{\sigma})_i \equiv \sigma_{ij,j}$, and $(\operatorname{curl}\boldsymbol{\gamma})_{ij} \equiv e_{jkl}\gamma_{il,k}$ designate, respectively, the gradient of the vector field $\boldsymbol{u}$, the divergence of the second-order tensor $\boldsymbol{\sigma}$, and the curl of the second-order tensor $\boldsymbol{\gamma}$, whereas $(\operatorname{dev}\boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} - \delta_{ij}\varsigma_{kk}/3)$ (with δ_{ij} the Kronecker symbol), $(\operatorname{sym}\boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} + \varsigma_{ji})/2$, and $(\operatorname{skw}\boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} - \varsigma_{ji})/2$ denote, respectively, the deviatoric, symmetric, and skew-symmetric parts of the second-order tensor $\boldsymbol{\varsigma}$.

2. The flow theory of distortion gradient plasticity and the new stationarity principles

The theory presented in this section refers to the mechanical response of a body occupying a space region Ω, whose external surface S, of outward normal $\mathbf{n}$, consists of two couples of *complementary* parts: the first couple consists of S_t, where the conventional tractions $\mathbf{t}^0$ are known, and S_u, where the displacement $\mathbf{u}^0$ is known, whereas the second couple consists of S_t^{dis}, where *dislocations are free to exit the body*, and S_u^{dis}, where *dislocations are blocked and may pile-up*: $S = S_t \cup S_u = S_t^{\text{dis}} \cup S_u^{\text{dis}}$.

This section is devoted to the presentation of compatibility, balance, and constitutive equations. For their derivation and for more insight on their mechanical meaning, the reader is referred to Gurtin (2004) and Bardella (2010). Furthermore, we will also provide two minimum principles extending those formulated by Fleck and Willis (2009b) for a higher-order SGP, to Gurtin (2004) DGP. On the basis of these minimum principles we will develop the new FE framework in Section 3.

2.1. Kinematic and static field equations

2.1.1. Compatibility equations

In the small strains and rotations regime, the plastic distortion $\boldsymbol{\gamma}$, that is the plastic part of the displacement gradient, is related to the displacement $\mathbf{u}$ by

$$\nabla \mathbf{u} = (\nabla \mathbf{u})_{\text{el}} + \boldsymbol{\gamma} \quad \text{in} \quad \Omega \tag{1}$$

in which $(\nabla \mathbf{u})_{\text{el}}$ is the elastic part of the displacement gradient. The displacement field $\mathbf{u}$ is assumed to be sufficiently smooth, such that $\operatorname{curl}\nabla\mathbf{u} = \mathbf{0}$ in Ω, and the plastic deformation is assumed to be isochoric, so that $\operatorname{tr}\boldsymbol{\gamma} = 0$. The total strain, Nye's dislocation density tensor (Nye, 1953; Fleck and Hutchinson, 1997; Arsenlis and Parks, 1999), the plastic strain, and the plastic spin are, respectively, defined as:

$$\boldsymbol{\varepsilon} = \operatorname{sym}\nabla\mathbf{u}, \quad \boldsymbol{\alpha} = \operatorname{curl}\boldsymbol{\gamma}, \quad \boldsymbol{\varepsilon}^p = \operatorname{sym}\boldsymbol{\gamma}, \quad \boldsymbol{\vartheta}^p = \operatorname{skw}\boldsymbol{\gamma} \quad \text{in} \quad \Omega \tag{2}$$

2.1.2. Balance equations

For the whole body free from standard body forces, the conventional balance equation reads

$$\operatorname{div}\boldsymbol{\sigma} = \mathbf{0} \quad \text{in} \quad \Omega \tag{3}$$

with $\boldsymbol{\sigma}$ denoting the standard symmetric Cauchy stress.