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Micromorphic approach to single crystal plasticity and damage

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A B S T R A C T

Eringen's micromorphic approach for materials with microstructure is applied to the plasticity and damage of single crystals. A plastic microdeformation variable and its rotational part are introduced in a standard crystal plasticity model in order to predict size effects in the overall stress response of crystalline solids. In the case of an ideal laminate microstructure including a purely elastic layer and a plastic layer undergoing single slip, the model, called *microcurl*, is shown to produce a kinematic hardening component that depends on the size of the layers. In a second part of the paper, a microdamage variable is introduced that accounts for cleavage or plasticity induced pseudo-cleavage phenomena in single crystals. The formulation accounts for straight crack paths but also allows for crack branching and bifurcation.

1. Introduction

The links between the micromorphic continuum and the plasticity of crystalline materials have been recognized very early by Eringen himself (Claus & Eringen, 1969; Eringen & Claus, 1970). Lattice directions in a single crystal can be regarded as directors that rotate and deform as they do in a micromorphic continuum. The fact that lattice directions can be rotated and stretched in a different way than material lines connecting individual atoms, especially in the presence of static or moving dislocations, illustrates the independence between directors and material lines in a micromorphic continuum, even though their deformations can be related at the constitutive level.

The identification of a micromorphic continuum from the discrete atomic single crystal model is possible based on suitable averaging relations proposed in Chen et al. (2003). These works contain virial formula for the higher order stress tensors arising in the micromorphic theory. This atomistic-based approach can be used to predict phonon dispersion relations (see also Claus & Eringen, 1971 for the study of dispersion of waves in a dislocated crystal).

Analytical solutions have been provided that give the generalized stress fields around individual screw or edge dislocations embedded in an elastic generalized continuum medium, like the micromorphic medium. The physical meaning of such a calculation is the account of non-local elasticity at the core of dislocations that may suppress or limit the singularity of the stress fields. For instance, non-singular force and couple stress were determined by Lazar and Maugin (2004) for a screw dislocation embedded in a gradient micropolar medium that combines the first strain gradient with independent rotational degrees of freedom. The unphysical singularities at the core of straight screw and edge dislocations are also removed when the second gradient of strain is introduced in the theory, while the first strain gradient is not sufficient (see Lazar, Maugin, & Aifantis, 2006).

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The next step is to consider the collective behavior of dislocations in a single crystal by means of the continuum theory of dislocations. The material volume element is now assumed to contain a large enough number of dislocations for the continuum theory of dislocation to be applicable. Non-homogeneous plastic deformations induce material and lattice incompatibilities that are resolved by a suitable distribution of the dislocation density tensor field which is a second rank statistical mean for a population of arbitrary dislocations inside a material volume element (Kröner, 1969). Nye's fundamental relation linearly connects the dislocation density tensor to the lattice curvature field of the crystal. This fact has prompted many authors to treat a continuously dislocated crystal as a Cosserat continuum (Forest, Barbe, & Cailletaud, 2000; Günther, 1958; Kröner, 1963). The Cosserat approach records only the lattice curvature of the crystal but neglects the effect of the rotational part of the elastic strain tensor, which is a part of the total dislocation density tensor (Cordero et al., 2010). Full account of plastic incompatibilities is taken in strain gradient plasticity theories, starting from the original work by Aifantis (1984) up to recent progress by Gurtin (2002) and Acharya (2004). Formulation of crystal plasticity within the micromorphic framework is more recent and was suggested in Clayton, Bamman, and McDowell (2005) for a large spectrum of crystal defects, including point defects and disclinations. Limiting the discussion to dislocation density tensor effects, also called geometrically necessary dislocation (GND) effects, it is shown in Cordero et al. (2010), within a small deformation setting, how the micromorphic model can be used to predict grain and precipitate size effects in laminate crystalline materials. These models represent extensions of the conventional crystal plasticity theory (see for instance Teodosiu & Sidoroff, 1976), that accounts for single crystal hardening and lattice rotation but does not incorporate the effect of the dislocation density tensor.

The objective of the present work is, first, to formulate a finite deformation micromorphic extension of conventional crystal plasticity to account for GND effects in single crystals, and, second, to show that the micromorphic approach can also be used to introduce cleavage induced damage in a single crystal model. The first part, see Section 2, represents an extension to finite deformation of the model proposed by Cordero et al. (2010). It also provides new analytical predictions of size effects on the hardening of laminate microstructures. The theory is called the *microcurl* model because the evaluation of the curl of the microdeformation, instead of its full gradient, is sufficient to account for the effect of the dislocation density tensor. The second part, see Section 3, reports on a crystallographic model of damage in ductile single crystals, assuming that cracking occurs on specific crystallographic planes. The micromorphic approach is used here to obtain finite size damage zones and mesh-independent simulations of crack growth. In that way, the model is able to predict crack branching and bifurcation which are frequently observed in single crystals. It represents an extension to finite deformation and full coupling between plasticity and damage of the work initiated in Aslan and Forest (2009) and Aslan, Quilici, and Forest (2011).

The models proposed in this work for single crystals fall in the class of anisotropic elastoviscoplastic micromorphic media for which constitutive frameworks at finite deformations exist (Forest & Sievert, 2003; Lee & Chen, 2003; Regueiro, 2010; Sansour, Skatulla, & Zbib, 2010). The introduction of damage variables was performed in Grammenoudis, Tsakmakis, and Hofer (2009). In fact, the micromorphic approach can be applied not only to the total deformation by introducing the microdeformation field, but can also be restricted to plastic deformation, for specific application to size effects in plasticity, or to damage variables for application to regularized simulation of crack propagation, as proposed in Forest (2009) and Hirschberger and Steinmann (2009).

Vectors and second rank tensors are denoted by $\underline{\boldsymbol{a}}, \underset{\sim}{\boldsymbol{a}}$, respectively. The theories are formulated within the general finite deformation framework essentially following Eringen's choice of strain measures (Eringen, 1999). The initial and current positions of the material point are denoted by $\underline{\boldsymbol{X}}$ and $\underline{\boldsymbol{x}}$, respectively. Throughout this work, the initial configuration of the body is V_0 whereas V denotes the current one. The associated smooth boundaries are ∂V_0 and ∂V with normal vector $\underline{\boldsymbol{N}}$ and $\underline{\boldsymbol{n}}$. The gradient operators with respect to initial and current coordinates are called ∇_X and ∇_x, respectively. Similarly, the divergence and curl operators are Div, div and Curl, curl whether they are computed with respect to initial or current positions, respectively. Intrinsic notation is used in general but it is sometimes complemented or replaced by the index notation for clarity. A Cartesian coordinate system is used throughout with respect to the orthonormal basis ($\underline{\boldsymbol{e}}_1, \underline{\boldsymbol{e}}_2, \underline{\boldsymbol{e}}_3$). The notations for double contraction and gradient operations are

$$\underset{\sim}{\boldsymbol{A}} : \underset{\sim}{\boldsymbol{B}} = A_{ij}B_{ij}, \quad \underline{\boldsymbol{u}} \otimes \nabla_X = \frac{\partial u_i}{\partial X_j} \underline{\boldsymbol{e}}_i \otimes \underline{\boldsymbol{e}}_j \tag{1}$$

2. The *microcurl* model for crystal plasticity

2.1. Balance equations

The degrees of freedom of the proposed theory are the displacement vector $\underline{\boldsymbol{u}}$ and the microdeformation variable $\hat{\underset{\sim}{\boldsymbol{\chi}}}^p$, a generally non-symmetric second rank tensor. The field $\hat{\underset{\sim}{\boldsymbol{\chi}}}^p(\underline{\boldsymbol{X}})$ is generally not compatible, meaning that it does not derive from a vector field. The exponent ^{p} indicates, in advance, that this variable will eventually be constitutively related to plastic deformation occurring at the material point. In particular, the microdeformation $\hat{\underset{\sim}{\boldsymbol{\chi}}}^p$ is treated as an invariant quantity with respect to rigid body motion. The constitutive model will eventually ensure this invariance property. A first gradient theory is considered with respect to the degrees of freedom. However, the influence of the microdeformation gradient is limited to its curl part because of the aimed relation to the dislocation density tensor associated with the curl of plastic distortion. The following sets of degrees of freedom and of their gradients are therefore defined:

$$DOF = \left\{ \underline{\boldsymbol{u}}, \hat{\underset{\sim}{\boldsymbol{\chi}}}^p \right\}, \quad GRAD = \left\{ \underset{\sim}{\boldsymbol{F}} := \underset{\sim}{\boldsymbol{1}} + \underline{\boldsymbol{u}} \otimes \nabla_X, \underset{\sim}{\boldsymbol{K}} := \mathrm{Curl}\, \hat{\underset{\sim}{\boldsymbol{\chi}}}^p \right\} \tag{2}$$