may be entirely replaced after thermomechanical treatment, and the metalworking allows a certain control of the average grain size and crystalline orientation in the new microstructure. While extensively researched, several aspects of this microstructure evolution are still not fully understood or quantified. Questions remain regarding such issues as the exact conditions that favor recovery over recrystallization, or the relationship between the static and dynamic grain boundary properties.

Several approaches have been proposed to model the microstructure evolution that is produced by thermomechanical processing. In this work, a monolithic continuum approach is adopted. The particularity of the proposed framework is that it (i) treats the crystalline orientation as a degree of freedom, (ii) the energy associated with lattice curvature is explicitly taken into account, as well as (iii) the production and annihilation of dislocations in an averaged sense. The main aim is to predict qualitatively the microstructure evolution. This is achieved by combining a crystal plasticity model formulated for a Cosserat continuum and a phase-field method[1]. The Cosserat framework provides the microrotational degrees of freedom which are constrained to follow the crystal orientation of the grains. Unlike a classic crystal plasticity approach, the grain boundaries are diffuse and mobile due to the inclusion of the phase-field dynamics. The phase-field parameter is an order parameter that is sensitive to crystal lattice curvature. Simulations for single crystals and small polycrystals have demonstrated that the proposed approach can predict subgrain boundary formation, dislocation driven grain boundary migration, and possibly grain nucleation [2].

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Size-dependent elastoplasticity relying on Eulerian rates of elastic incompatibilities

Lorenzo Bardella

(joint work with M.B. Rubin)

1. Summary

The notion of elastic incompatibilities considers elastic deformations from one configuration to another. In this contribution elastically anisotropic materials are discussed within the context of a large deformation Eulerian formulation that is free from arbitrary choices of reference and intermediate configurations as well as total and plastic deformation measures. An elastic deformation is defined from an arbitrary initial configuration that can have a state with elastic incompatibilities. Necessary and sufficient conditions are obtained for additional elastic incompatibilities developing from this initial configuration. Moreover, a second-order Eulerian tensor R_{ij} is proposed, based on the current curl of the rate of plastic deformation tensor, which measures the current rate of elastic incompatibilities related to developing edge and screw dislocations. R_{ij} can in fact be seen as an extension of the elastic counterpart of the rate of the Nye-Kröner dislocation density tensor, as originally defined for small strains and rotations. This allows the study of the size-effect ensuing from a hardening law dependent on R_{ij}. In order to unveil the features of the proposed theory, the torsion of a cylinder is studied under both monotonic and cyclic loading paths.

2. A Lagrangian formulation of total deformation incompatibility

Finite deformation total strains are purely kinematic variables that measure deformation from a specified reference configuration to the current configuration. For example, a material point located by $\mathbf{X}$ in the reference configuration is deformed to its location $\mathbf{x}$ in the current configuration at time t by a one-to-one mapping

$$\mathbf{x} = \mathbf{X}(\mathbf{X}, t)\,, \tag{1}$$

and the associated deformation gradient $\mathbf{F}$ is defined by

$$\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}\,.$$

By definition, this mapping and the associated deformation gradient characterize a compatible deformation field from the reference configuration to the present configuration.

One question of compatibility arises when $\mathbf{F}$ is a specified function of $(\mathbf{X}, t)$ and it is not known if an associated compatible deformation field with a mapping of the form (1) exits. Yavari [1] discussed the history of this problem for nonlinear elasticity and generalized the solution for multiply connected regions. Here, attention is confined to simply connected regions for which the necessary and sufficient condition for a compatible mapping (1) to exist is that

$$\oint_C \mathbf{F}\mathrm{d}\mathbf{X} = \int_S \mathrm{Curl}(\mathbf{F})\mathbf{N}\mathrm{d}A = \mathbf{0}$$

for all closed paths C in the body, where Stoke's theorem has been used to convert the line integral to an integral over the enclosed surface. Moreover, Curl( ) is the curl operator with respect to $\mathbf{X}$, $\mathbf{N}$ is the unit normal to the surface S, right-handed relative to the direction of integration on C, and $\mathrm{d}A$ is the reference area element on the surface S. Assuming sufficient continuity, it follows that

$$\mathrm{Curl}(\mathbf{F}) = \mathbf{0}$$

at every point in the body.

3. An Eulerian formulation of elastic deformation for elastoplastic materials

Eckart [2] seems to be the first to propose an Eulerian formulation of constitutive equations for elastically isotropic elastoplastic response of solids. A similar formulation for polymeric liquids was formulated in [3]. These formulations are Eulerian in the sense that they are free from arbitrary specification of reference or intermediate configurations as well as total or plastic deformation measures [4]. An Eulerian formulation of constitutive equations for elastoplastic response of elastically anisotropic materials was developed in [5]. This formulation introduces evolution equations for a right-handed triad $\mathbf{m}_i$ of linearly independent microstructural vectors of the forms

$$\dot{\mathbf{m}}_i = (\mathbf{L} - \mathbf{L}_p)\mathbf{m}_i \,, \tag{2}$$

where $\dot{(\;)}$ denotes the material time derivative, $\mathbf{L}$ is the total velocity gradient, and $\mathbf{L}_p$ is a general second-order tensor characterizing plastic rate, which requires a constitutive equation. The microstructural vectors $\mathbf{m}_i$ characterize elastic deformations and orientation changes of anisotropic directions in the material relative to a zero-stress state. They also determine the Cauchy stress $\mathbf{T}$ in the current state. These microstructural vectors $\mathbf{m}_i$ are internal state variables, as defined by Onat [6], which are assumed to be measurable in the current state.

4. A Lagrangian formulation of elastic incompatibility for elastoplastic materials

The notion of elastic compatibility is Lagrangian in the sense that it requires a definition of elastic deformation between two configurations. Consequently, it is convenient to define the values $\mathbf{M}_i$ of $\mathbf{m}_i$ in the initial configuration at $t = 0$ and the reciprocal vectors $\mathbf{M}^i$ at $t = 0$. Then, the elastic deformation $\mathbf{F}_m$ from this initial configuration to the current configuration at time t is defined by

$$\mathbf{F}_m(t) = \mathbf{m}_s(t) \otimes \mathbf{M}^s \,, \quad \mathbf{F}_m(0) = \mathbf{I} \,,$$

where $\otimes$ denotes the tensor product, the usual summation convention applies to repeated indices, and $\mathbf{I}$ is the identity tensor. This tensor $\mathbf{F}_m$ remains a measure of elastic deformation from the initial configuration even for a general initial configuration in a state with residual stresses. Then, a Nye-Kröner-like tensor $\boldsymbol{\alpha}_e$ [7, 8], which measures elastic incompatibilities from the initial configuration, can be defined by

$$\boldsymbol{\alpha}_e = \mathrm{Curl}(\mathbf{F}_m) \,, \tag{3}$$

where the Curl operator is relative to the initial configuration. If $\boldsymbol{\alpha}_e = \mathbf{0}$ the deformation, as described by $\mathbf{F}_m$ through the evolution of the microstructural vectors $\mathbf{m}_i(t)$, is compatible.

5. Eulerian rates of elastic incompatibilities for elastoplastic materials

By taking the material derivative of (3) and evaluating the result in the current configuration, it can be shown that Eulerian rates of elastic incompatibility can be defined by

$$R_{ij} = -\mathrm{curl}(\mathbf{L}_p) \cdot (\mathbf{m}'_i \otimes \mathbf{m}'_j)\,, \tag{4}$$

where the curl operator is defined relative to the current configuration, the distortional microstructural vectors $\mathbf{m}'_i$ are defined by

$$\mathbf{m}'_i = J_e^{-1/3}\mathbf{m}_i \quad \text{with} \quad J_e = \mathbf{m}_1 \times \mathbf{m}_2 \cdot \mathbf{m}_3 > 0\,,$$

and $\cdot$ and $\times$ denote, respectively, the inner and vector products. If restricted to small strains and rotations, R_{ij} is the opposite of the rate of the Nye-Kröner dislocation density tensor [7, 8]. Therefore, its off-diagonal and diagonal components, respectively, correspond to edge and screw dislocation density rates.

It is emphasized that the rates R_{ij} are Eulerian as they depend only on the current configuration and rate of deformation. Moreover, they are not pure kinematic measures, being also dependent on the constitutive prescription for $\mathbf{L}_p$. Also, the definition (4) of R_{ij} ensures its invariance under superposed rigid body motion, such as each of its components can be used to introduce size-dependent hardening in the modeling. This approach is an alternative to that followed in [9], which is an Eulerian extension of the higher-order strain gradient plasticity theory of Gurtin [10].

6. The torsion problem

Consider an isotropic cylinder of circular cross-section experiencing cyclic torsional loading governed by the applied twist $\kappa(t)$. The cylindrical polar base vectors $(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_z)$ are defined relative to the fixed orthonormal triad of vectors $\mathbf{e}_i$ by the expressions

$$\begin{aligned} \mathbf{e}_r &= \cos(\hat{\theta})\mathbf{e}_1 + \sin(\hat{\theta})\mathbf{e}_2\,, \quad & \mathbf{e}_\theta &= -\sin(\hat{\theta})\mathbf{e}_1 + \cos(\hat{\theta})\mathbf{e}_2\,, \\ \mathbf{e}_z &= \mathbf{e}_3\,, & \hat{\theta} &= \theta + \kappa z\,. \end{aligned}$$

Also, the current location of a material point $\mathbf{x}$ is given by

$$\mathbf{x} = r\mathbf{e}_r + z\mathbf{e}_z\,,$$

such as the total velocity gradient reads

$$\mathbf{L} = z\dot{\kappa}(\mathbf{e}_\theta \otimes \mathbf{e}_r - \mathbf{e}_r \otimes \mathbf{e}_\theta) + r\dot{\kappa}\mathbf{e}_\theta \otimes \mathbf{e}_z\,.$$

This kinematic assumption may for instance be adequate to model severe plastic deformation in higher-pressure torsion [11]. Equilibrium can be satisfied by a radial body force equal to $-\partial T_{rr}/\partial r - (T_{rr} - T_{\theta\theta})/r$. Under these circumstances, the non-vanishing components of R_{ij} are

$$
\begin{aligned}
R_{11} &= \frac{L_{p\theta z}}{r} m_{1r}^2 \,, \\
R_{22} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta}^2 - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2\theta} m_{2z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2\theta} m_{2z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z}^2 \,, \\
R_{33} &= \frac{\partial L_{p\theta z}}{\partial r} m_{3\theta}^2 - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{3\theta} m_{3z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{3\theta} m_{3z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{3z}^2 \,, \\
R_{23} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta} m_{3\theta} - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2\theta} m_{3z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2z} m_{3\theta} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z} m_{3z} \,, \\
R_{32} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta} m_{3\theta} - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2z} m_{3\theta} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2\theta} m_{3z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z} m_{3z} \,,
\end{aligned} \tag{5}
$$

where m_{1r}, $m_{2\theta}$, m_{2z}, $m_{3\theta}$, and m_{3z} are the five non-vanishing components of the microstructural vectors $\mathbf{m}_i$. In the framework of small strains and rotations, $L_{prr} = L_{p\theta\theta} = L_{pzz} = 0$, $m_{2z} = m_{3\theta} = 0$, and $R_{23} = R_{32} = 0$ [12].

Given that $\mathbf{L}_p$ depends on $\mathbf{m}_i$, in a complex nonlinear way also involving the plastic spin rate [13], it turns out that the solution of this torsion problem is obtained by integrating five nonlinear differential equations for m_{1r}, $m_{2\theta}$, m_{2z}, $m_{3\theta}$, and m_{3z}, which are functions of r and $\kappa(t)$, to be coupled, in a system, with the evolution equations for the adopted hardening laws. This system of equations automatically satisfies the condition of isochoric total deformation, $J_e = 1$.

This contribution aims at studying the effect on the torsional response of a hardening law dependent on the rates of incompatibilities (5). A similar study has already been carried out in [14] by neglecting finite deformations and the plastic spin. Here, a conventional hardening law is enhanced by adding a dependence on R_{ij} using the smooth transition model proposed in [15, 16]. Among several aspects, this investigation highlights the crucial role of the influence of the material parameter controlling the plastic spin rate, thus confirming and enriching the findings of [12] in the context of higher-order small-strain gradient plasticity.

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Elasto-viscoplastic FFT-based method for mesoscale field dislocation mechanics with defect energy

Stéphane Berbenni

(joint work with Vincent Taupin, Ricardo A. Lebensohn)

A crystal plasticity elasto-viscoplastic FFT (Fast Fourier Transform) formulation with a mesoscale continuum field dislocation mechanics model is presented. The present approach accounts for plastic flow, hardening and densities of geometrically necessary dislocations (GND), in addition to statistically stored dislocations (SSD). Here, the model incorporates a defect energy density that depends on GND densities and an associated internal length scale. This allows to thermodynamically derive internal length scale dependent intra-crystalline backstress (energetic-type hardening) and Peach-Koehler force acting on GND densities. The model considers GND density evolution through a filtered numerical spectral approach [1], which is coupled with stress equilibrium through the elasto-viscoplastic FFT algorithm using Augmented Lagrangian (AL) algorithm. The discrete Fourier transform method together with finite difference schemes [2, 3], is applied to solve both the GND lattice incompatibility problem and the Lippmann-Schwinger equation.