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Augmented Lagrangian method for Eulerian modeling of viscoplastic crystals

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ABSTRACT

A robust numerical algorithm for an Eulerian rigid-viscoplastic crystal model that accounts for high-strain rates, large strains, and large material and lattice rotations, was developed. The viscoplastic law is obtained from Schmid law by using an overstress approach; the numerical instabilities associated to the classical Norton law are thus eliminated.

A time implicit (backward) Euler scheme for time discretization, was used. At each time iteration, a four steps iterative algorithm was proposed. To handle the non-differentiability of the plastic terms an iterative decomposition–coordination formulation coupled with the augmented Lagrangian method was adopted. This formulation was modified to fit to the crystal (non-isotropic) viscoplastic model, for which the stress deviator is not coaxial with the rate of deformation tensor. The proposed algorithm is consistent and permits to solve alternatively, at each iteration, the equations for the velocity field and for the lattice orientation. A mixed finite element-finite volume strategy was adopted: the equation for the velocity field is discretized using the finite element method while a finite volume method, with an upwind choice of the flux, is adopted for the hyperbolic equation related to the lattice orientation.

Several two-dimensional boundary value problems are selected to analyze the robustness of the numerical algorithm. The influence of the mesh and of the time step on simulation of the in-plane flow of a fcc crystal in an equal channel angular die extruder was investigated. The transitional flow of a grain embedded in a parent crystal was computed. The grains interaction during channel die compression of a multi-crystal was analyzed using an ALE description.

1. Introduction

The description of plastic flow by crystallographic slip in metals with cubic crystals structure dates back to the pioneering work of Taylor and Elam [34,35] and Taylor [36,37] that established the experimental laws that are the foundation of crystal mechanics. A general kinematics of the finite deformation of elastic–plastic single crystals that includes lattice distortion was first given by Rice [27] and may be found in equivalent forms in [15,2] (see also the overviews [3,14,31,7,41]).

In some processes, such as metal cutting, extrusion, penetration, etc., large deformations, high pressures, and high-strain rates may occur. Thus, for computational purposes, an Eulerian description seems to be most suitable. In current rate-dependent models a FE Lagrangean description is generally adopted (e.g. [21,29]); hence the large lattice rotations that occur in dynamic flow regime may not be accurately captured. As concerns the flow rule, a Norton-type power-law is generally used. This law, adequate for the description of low strain rate behavior, is very stiff and predicts unrealistic slip rates (see for example [24,4]). There have been a lot of efforts in order to overcome the severe numerical instabilities that arise in the integration of the Norton-type power-law model (see reviews of the computational strategies in [8,19]).

An Eulerian rate-dependent single crystal model that accounts for high-strain rates, large strains and rotations was developed in [5]. The viscoplastic law, as well as the evolution equations for the lattice, are written in terms of vectorial and tensorial quantities associated with the current configuration. The viscoplastic law is obtained from Schmid law using an overstress approach. The expression of this viscoplastic law is motivated by the microdynamics of crystal defects (see [38]). By adopting such a law, the numerical instabilities that arise in the integration of the classical Norton law are eliminated.

The main goal of this paper is to develop a robust Eulerian numerical algorithm for the rigid-viscoplastic single crystal model proposed in [5]. We will use a time implicit (backward) Euler scheme for time discretization, which gives a coupled system of nonlinear equations for the velocities and lattice orientation fields. At each time iteration, an iterative algorithm is developed to solve these nonlinear equations. Specifically, a mixed finite element and

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finite volume strategy is proposed. The equations for the velocity field are discretized using the finite element method, while a finite volume method, with an upwind choice of the flux, is adopted to solve the hyperbolic equations that describe the evolution of the lattice orientation.

To handle the non-differentiability of the plastic terms an iterative decomposition–coordination formulation coupled with the augmented Lagrangian method (see [13,9]) is adapted. Since in crystal (anisotropic) plasticity there is non co-axiality between the stress deviator and the rate of deformation, the original method, developed for the Bingham model [13,9], cannot be used. We have to find firstly the decomposition of the strain rate into the slip rates of the crystal, to introduce the slip rate multipliers and to work with the decomposition–coordination formulation at the level of each slip system. It is worth noting that this type of algorithm permits also to solve alternatively, at each iteration, the equations for the unit vectors that define the lattice orientation. If the Eulerian domain has time variations then the above algorithm could also be adapted to an ALE (Arbitrary Eulerian–Lagrangien) description of the crystal evolution.

Let us outline the content of the paper. In Section 2 the boundary value problem is stated and in Section 3 we describe the numerical strategy. After the time discretization (Section 3.1) we present in Section 3.2, the four steps of the proposed iterative algorithm. We prove that the iterative algorithm is consistent (i.e. it provides a solution if the convergence is achieved). In Section 4 we reformulate the rigid-viscoplastic constitutive equations for the in-plane deformation. The resulting boundary value problem has a more simpler form: only one differential equation, involving the orientation of one composite in-plane slip system, is necessary to describe the lattice evolution. Several two-dimensional boundary value problems are selected to analyze the robustness of the numerical algorithm and the predictive capabilities of the mechanical model. In Section 5 we simulate the in-plane flow of a fcc crystal in an equal channel angular extruder. The influence of the mesh and of the time step are investigated. Both the stationary flow of single crystal and the flow of a grain embedded in a parent crystal are further analyzed. From a numerical point of view, the presence of grains means that the initial condition contains discontinuities (shocks) which propagate in the parent crystal. Section 6 concerns the ALE computations for the channel die compression of a fcc crystal. Here, we investigate the grains interaction by analyzing the compression of a bi-crystal and of a sixteen grains multicrystal.

2. Statement of the boundary value problem

We begin by presenting the equations governing the motion in a domain $\mathscr{D} = \mathscr{D}(t)$ of an incompressible rigid-viscoplastic crystal. The momentum balance law in the Eulerian coordinates reads

$$\rho(\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}) - \mathbf{div}\, \boldsymbol{\tau} + \nabla p = \rho \boldsymbol{f} \quad \text{in } \mathscr{D}, \qquad (1)$$

where the velocity $\boldsymbol{v} : [0,T] \times \mathscr{D} \to \mathbb{R}^3$, the deviator of the Cauchy stress tensor $\boldsymbol{\tau} : [0,T] \times \mathscr{D} \to \mathbb{R}^{3\times 3}_S$ and the pressure (mean stress) $p : [0,T] \times \mathscr{D} \to \mathbb{R}(\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I}$ is the Cauchy stress tensor) are the unknowns fields, while the mass density $\rho > 0$ and the body forces $\boldsymbol{f}$ are considered known.

The gradient of the velocity field $\nabla \boldsymbol{v}$ is decomposed into its symmetric part (rate of deformation) $\mathbf{D}(\boldsymbol{v})$ and its antisymmetric part (spin tensor) $\mathbf{W}(\boldsymbol{v})$ through

$$\boldsymbol{D}(\boldsymbol{v}) = \frac{1}{2}(\nabla \boldsymbol{v} + \nabla^t \boldsymbol{v}), \quad \mathbf{W}(\boldsymbol{v}) = \frac{1}{2}\left(\nabla \boldsymbol{v} - \nabla^T \boldsymbol{v}\right).$$

The incompressibility condition (mass balance law) reads

$$\mathrm{div}\boldsymbol{v} = 0 \quad \text{in } \mathscr{D}. \qquad (2)$$

The lattice orientation of the crystal is modeled through the slip direction distribution $\mathbf{b}_s : [0,T] \times \mathscr{D} \to \mathbb{R}^3$ and the slip plane normal distribution $\mathbf{m}_s : [0,T] \times \mathscr{D} \to \mathbb{R}^3$. We denote by $\boldsymbol{M}_s, \boldsymbol{R}_s$ the symmetric and the skew part of their tensorial product:

$$\boldsymbol{M}_s = \frac{1}{2}(\boldsymbol{b}_s \otimes \boldsymbol{m}_s + \boldsymbol{m}_s \otimes \boldsymbol{b}_s), \quad \boldsymbol{R}_s = \frac{1}{2}(\boldsymbol{b}_s \otimes \boldsymbol{m}_s - \boldsymbol{m}_s \otimes \boldsymbol{b}_s). \qquad (3)$$

In Fig. 1 are represented the twelve crystallographic systems $\{(\boldsymbol{b}_s, \boldsymbol{M}_s)\}_{s=1}^N$(i.e. 12 pairs of glide directions and glide plane normals) for a fcc. crystal in the crystal basis $\{\mathbf{c_1}, \mathbf{c_2}, \mathbf{c_3}\}$. Note that the crystal basis orientation could vary with respect to time t or with the Eulerian position $x \in \mathscr{D}$.

In applications involving large deformations and high-strain rates, the elastic component of the deformation is small with respect to the inelastic one. That is why it can be neglected it here and a rigid-viscoplastic approach adopted (e.g. [16,20,18]). Since the viscoplastic deformation is due to slip only, the rate of deformation $\boldsymbol{D}$ can be decomposed into the N slip systems ([27,38]) as

$$\boldsymbol{D}(\boldsymbol{v}) = \sum_{s=1}^{N} \dot{\gamma}_s \boldsymbol{M}_s, \qquad (4)$$

where $\dot{\gamma}_s$ is the slip rate on the system s.

Concerning the inelastic flow, a Perzyna-like viscoplastic law, which relates the slip rate $\dot{\gamma}_s$ to the resolved stress $\tau_s = \boldsymbol{\tau} : \boldsymbol{M}_s$, is considered (see [5]):

$$\dot{\gamma}_s = \frac{1}{\eta_s}[|\ \tau_s\ | - \tau_{cs}]_+ \mathrm{sign}(\tau_s), \qquad (5)$$

where τ_{cs} is the slip resistance (also called critical resolved shear stress or CRSS), η_s is the viscosity and $[x]_+ = (x + |x|)/2$ is the positive part of x. One can use (4) and the viscoplastic law (5) for each slip system s, to relate the rate of deformation tensor $\boldsymbol{D}(\boldsymbol{v})$ to the deviator $\boldsymbol{\tau}$ of the Cauchy stress tensor

$$\boldsymbol{D}(\boldsymbol{v}) = \sum_{s=1}^{N} \frac{1}{\eta_s}\left[1 - \frac{\tau_{cs}}{|\ \boldsymbol{\tau} : \boldsymbol{M}_s\ |}\right]_+ (\boldsymbol{\tau} : \boldsymbol{M}_s)\boldsymbol{M}_s. \qquad (6)$$

It is worth noting that since the resolved shear stresses τ_s are not independent, the shear rates $\dot{\gamma}_s$ given by the viscoplastic flow rule (5) are not independent; they have to satisfy the kinematic constraint (4). Given the rate of deformation $\boldsymbol{D}$, the shear rates $\dot{\gamma}_s$ are determined by minimizing the internal power

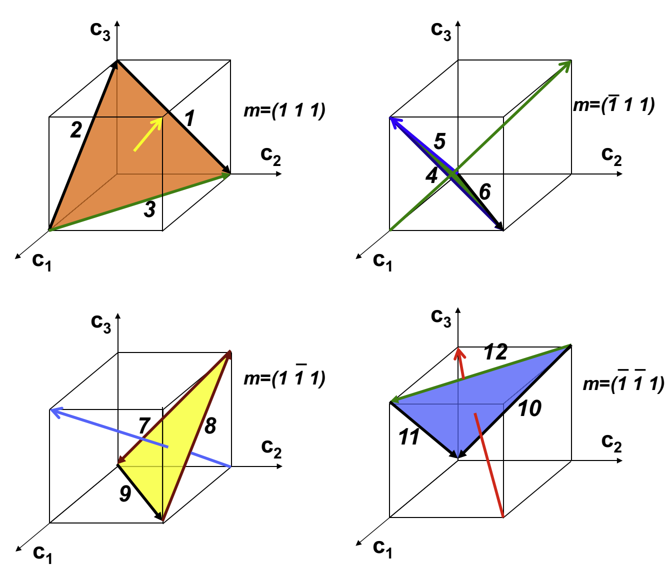

Fig. 1. The 12 pairs $\{(\boldsymbol{b}_s, \boldsymbol{M}_s)\}_{s=1}^{12}$ of slip directions and slip plane normals for a fcc crystal.