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Fluid Model of Crystal Plasticity: Numerical Simulations of 2-turn Equal Channel Angular Extrusion

P. Minakowski

Considering severe plastic deformation experiments as a motivation, the plastic behaviour of crystalline solids is treated as a flow of a highly viscous, compressible material. Starting from classical single crystal hypothesis we present a purely Eulerian set of equations describing flow of a plastic material. Moreover, we provide a thermodynamic justification of the evolution of the Cauchy stress based on the Gibbs potential. Numerical simulations for a 2-turn equal channel angular extrusion are reported.

Introduction

Recent experimental studies show that severe plastic deformations of certain materials can achieve exceptionally high strength accompanied by relatively good ductility. It is shown that simple shear is a good deformation method for structure and texture formation in metal-working. Several metal forming processes achieving severe plastic deformations are now available. We chose the equal channel angular extrusion (ECAE) because it has proven highly suitable for experimental and theoretical studies since in was first developed by Segal (Segal et al., 1981; Segal, 1995, 1999). A work piece is extruded several times through a die in the shape of curved channel with a $90°-$angle turn. Each pass introduces additional strain. The main advantages of using ECAE in comparison to alternative experiments (e.g. rolling, forging) are minor changes in the cross-section of the billet and that one can look at various amounts of strain in a specimen.

In the presented approach the plastic behaviour of crystalline solids is treated as a highly viscous material flow through an adjustable crystal lattice (Kratochvíl et al., 2009). Looking at severe plastic deformation experiments, it seems that crystalline materials at yield behave as a special kind of anisotropic, compressible, highly viscous fluid.

In early references, such as Hill and Rice (1972); Peirce et al. (1982, 1983); Asaro and Needleman (1985), the authors postulate that the Jaumann rate of the Kirchhoff stress is related to the elastic rate of stretching by the usual elastic moduli tensor. In this approach, the constitutive equation is stated phenomenologically. Moreover, it can not be derived from a Helmholtz potential. To the author's knowledge the only description of this phenomena, which is thermodynamically admissible, uses the Helmholtz potential and does not lead to a rate type model, see Srinivasa and Srinivasan (2009).

Following the paper by Rajagopal and Srinivasa (2011), we employ the Gibbs potential to derive an equation, which describes the evolution of the Cauchy stress. For detailed discussion on models of a rate type,

$$f(\dot{\boldsymbol{T}}, \boldsymbol{T}, \boldsymbol{L}) = 0, \tag{1}$$

where the constitutive relation contains the Cauchy stress $\boldsymbol{T}$, the rate of stress $\dot{\boldsymbol{T}}$, and the velocity gradient $\boldsymbol{L}$, we refer to Rajagopal and Srinivasa (2000, 2011).

The paper is structured as follows. In Section 1 we introduce all necessary assumptions and derive the Eulerian model of crystal plasticity, including compressible elastic stretches. Section 2 consists of the formulation of an initial boundary value problem, the description of the finite element approach, and the results of numerical simulations.

1 Crystal Plasticity Model

1.1 Kinematics

Let Ω denote the reference configuration of the body and let Ω_t denote the current configuration at time t. The point, which was at the position $X \in \Omega$ in the reference configuration, is in the current configuration at time t in the position

$$x = \chi(X,t) \text{ for } X \in \Omega,\ x \in \Omega_t. \tag{2}$$

The mapping $\chi(X,t)$ is continuously differentiable with respect to the position. The deformation gradient $\boldsymbol{F}$ is defined through $\frac{\partial \chi(X,t)}{\partial X}$ and we assume its multiplicative decomposition, see Kröner (1961),

$$\boldsymbol{F} = \frac{\partial \chi(X,t)}{\partial X} = \boldsymbol{F_e}\boldsymbol{F_p}, \tag{3}$$

where $\boldsymbol{F_e}$ stands for the elastic distortion (stretches and rotations of the lattice) and $\boldsymbol{F_p}$ for the plastic distortion (the distortion of the lattice due to the motion of dislocations). Moreover, the deformation gradient is non-singular and all the volumetric changes are assumed to result from the elastic stretches in the lattice,

$$\det \boldsymbol{F} > 0, \quad \det \boldsymbol{F_p} = 1, \quad \det \boldsymbol{F} = \det \boldsymbol{F_e}. \tag{4}$$

Since the velocity field is defined as $\boldsymbol{v}(X,t) = \frac{\partial \chi(X,t)}{\partial t}$, equation (3) leads to the additive decomposition of the velocity gradient

$$\nabla \boldsymbol{v} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} = \dot{\boldsymbol{F}}_{\boldsymbol{e}}(\boldsymbol{F_e})^{-1} + \boldsymbol{F_e}(\dot{\boldsymbol{F}}_{\boldsymbol{p}}(\boldsymbol{F_p})^{-1})(\boldsymbol{F_e})^{-1} = \boldsymbol{L_e} + \boldsymbol{F_e}\boldsymbol{L_p}(\boldsymbol{F_e})^{-1}, \tag{5}$$

where the superposed dot denotes the material time derivative ($\dot{a} = \frac{\partial a}{\partial t} + \boldsymbol{v}\nabla a$).

The evolution of the state of the body is subject to the balance of mass, momentum, angular momentum, and total energy per unit mass, which in the Eulerian coordinates take the form

$$\dot{\varrho} + \varrho \operatorname{div} \boldsymbol{v} = 0, \tag{6}$$

$$\varrho \dot{\boldsymbol{v}} - \operatorname{div} \boldsymbol{T} = \boldsymbol{f}, \quad \boldsymbol{T} = \boldsymbol{T}^T, \tag{7}$$

$$\varrho \dot{\varepsilon} = \varrho r - \operatorname{div} \boldsymbol{q} + \boldsymbol{T} : \boldsymbol{D}, \tag{8}$$

where $\varrho(x,t)$ stands for the density, $\boldsymbol{T}(x,t)$ is the Cauchy stress tensor, $\boldsymbol{D}$ is the symmetric part of the velocity gradient, $\boldsymbol{f}$ is the external force, r is the heat source per unit mass, ε is the specific internal energy and $\boldsymbol{q}$ is the heat flux vector.

1.2 Evolution of the Cauchy Stress

We aim to give thermodynamic justification for the constitutive equation for the rate of stress (1). The starting point of any thermodynamical analysis is the introduction of convenient state variables. We introduce the thermodynamic variables, which depend on the temperature θ and the Kirchhoff stress $\boldsymbol{S}$

$\varepsilon(\boldsymbol{S},\theta)$ - specific internal energy,

$\Psi(\boldsymbol{S},\theta)$ - specific Helmholtz potential,

$\eta(\boldsymbol{S},\theta)$ - specific entropy.

The Kirchhoff stress $\boldsymbol{S}$ is related to the Cauchy stress $\boldsymbol{T}$ by $\boldsymbol{S} = \boldsymbol{T}/\varrho$ or $\boldsymbol{S} = \boldsymbol{T} \det \boldsymbol{F}/\varrho_0$. Remembering that the determinant of the deformation gradient is the Jacobian of the mapping χ ($\varrho(x,0)\mathrm{dX} = \varrho(x,t) \det \boldsymbol{F}\, \mathrm{dx}$), it represents the ratio of the current volume to the reference volume.

Usually the stress is defined as the derivative of a Helmholtz potential with respect to a proper strain measure. In our case we would like to avoid any dependency on the strain. To this aim we transform the Helmholtz potential into the Gibbs potential $G(\boldsymbol{S},\theta)$. The relation is given by the Legendre transformation

$$\Psi(\boldsymbol{S},\theta) = G(\boldsymbol{S},\theta) - \frac{\partial G(\boldsymbol{S},\theta)}{\partial \boldsymbol{S}} : \boldsymbol{S}. \tag{9}$$

Knowing that the entropy is given by $\eta(\boldsymbol{S},\theta) = -\frac{\partial G(\boldsymbol{S},\theta)}{\partial \theta}$ and that the thermodynamic variables are related by $\varepsilon = \Psi + \theta\eta$ we substitute (9) into (8),

$$\varrho\left(\overline{G - \frac{\partial G}{\partial \boldsymbol{S}} : \boldsymbol{S} - \frac{\partial G}{\partial \theta}\theta}^{\cdot}\right) = \varrho r - \operatorname{div}\boldsymbol{q} + \boldsymbol{T} : \boldsymbol{D}$$

$$-\varrho\theta\overline{\frac{\partial G}{\partial \theta}}^{\cdot} + \varrho\left(\frac{\partial G}{\partial \boldsymbol{S}} : \dot{\boldsymbol{S}} - \frac{\partial G}{\partial \boldsymbol{S}} : \dot{\boldsymbol{S}} - \overline{\frac{\partial G}{\partial \boldsymbol{S}}}^{\cdot} : \boldsymbol{S}\right) = \varrho r - \operatorname{div}\boldsymbol{q} + \boldsymbol{T} : \boldsymbol{D}$$

$$\varrho\theta\dot{\eta} - \varrho\frac{\partial^2 G}{\partial \boldsymbol{S}^2}\dot{\boldsymbol{S}} : \boldsymbol{S} = \varrho r - \operatorname{div}\boldsymbol{q} + \boldsymbol{T} : \boldsymbol{D}$$

$$\varrho\theta\dot{\eta} = \varrho r - \operatorname{div}\boldsymbol{q} + \varrho\left(\boldsymbol{S} : \left(\boldsymbol{D} + \frac{\partial^2 G}{\partial \boldsymbol{S}^2}\dot{\boldsymbol{S}}\right)\right).$$

The second law of thermodynamics involving the specific entropy (Clausius–Duhem inequality), takes the form

$$\varrho\dot{\eta} + \operatorname{div}\left(\frac{\boldsymbol{q}}{\theta}\right) - \frac{\varrho r}{\theta} \geq 0. \tag{10}$$

We identify the rate of dissipation (the rate of entropy production per unit mass) as

$$\xi = \boldsymbol{S} : \left(\boldsymbol{D} + \frac{\partial^2 G}{\partial \boldsymbol{S}^2}\dot{\boldsymbol{S}}\right) = \boldsymbol{S} : \left(\boldsymbol{D} - \boldsymbol{\mathcal{A}}\dot{\boldsymbol{S}}\right), \tag{11}$$

where $\boldsymbol{\mathcal{A}} = -\frac{\partial^2 G}{\partial \boldsymbol{S}^2}$ stands for the fourth order symmetric elastic compliance tensor.

In order to obtain an objective stress-strain constitutive relation (1) we follow Rajagopal and Srinivasa (2011). The right hand side of (11) consists of $\boldsymbol{D}$ and $\boldsymbol{\mathcal{A}}$, both objective tensors, and $\dot{\boldsymbol{S}}$, which itself is not objective (however $\boldsymbol{S} : \boldsymbol{\mathcal{A}}\boldsymbol{S}$ is objective). To overcome this difficulty we notice that, due to the fact that function $\boldsymbol{\mathcal{A}}\boldsymbol{S}$ is linear we can observe that $(\boldsymbol{\mathcal{A}}\boldsymbol{S})\boldsymbol{S} = \boldsymbol{S}(\boldsymbol{\mathcal{A}}\boldsymbol{S})$. Now let us consider an arbitrary tensor $\boldsymbol{W}$ and the expression $\boldsymbol{S} : \boldsymbol{\mathcal{A}}(\boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W})$. From the symmetry of $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{S}$ ($\boldsymbol{S} = \boldsymbol{S}^T$) together with the above observation we obtain

$$\boldsymbol{S} : \boldsymbol{\mathcal{A}}(\boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W}) = \boldsymbol{\mathcal{A}}\boldsymbol{S} : (\boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W}) = \boldsymbol{W} : ((\boldsymbol{\mathcal{A}}\boldsymbol{S})\boldsymbol{S} - \boldsymbol{S}(\boldsymbol{\mathcal{A}}\boldsymbol{S})) = 0. \tag{12}$$

By adding (12) to (11) we get

$$\xi = \boldsymbol{S} : \left(\boldsymbol{D} - \boldsymbol{\mathcal{A}}(\dot{\boldsymbol{S}} + \boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W})\right). \tag{13}$$

Let us denote the dissipative part of $\boldsymbol{D}$ by $\boldsymbol{D_p}$ and the inversion of $\boldsymbol{\mathcal{A}}$ by $\boldsymbol{\mathcal{C}}$,

$$\boldsymbol{D_p} = \boldsymbol{D} - \boldsymbol{\mathcal{A}}(\dot{\boldsymbol{S}} + \boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W}), \quad \dot{\boldsymbol{S}} + \boldsymbol{W}\boldsymbol{S} - \boldsymbol{S}\boldsymbol{W} = \boldsymbol{\mathcal{C}}(\boldsymbol{D} - \boldsymbol{D_p}). \tag{14}$$

To reformulate (14) in terms of the Cauchy stress we substitute $\boldsymbol{S} = \boldsymbol{T}/\varrho$ and deduce

$$\dot{\boldsymbol{T}} + \boldsymbol{T}\operatorname{div}\boldsymbol{v} + \boldsymbol{W}\boldsymbol{T} - \boldsymbol{T}\boldsymbol{W} = \varrho\boldsymbol{\mathcal{C}}(\boldsymbol{D} - \boldsymbol{D_p}). \tag{15}$$

Finally we obtain the material rate of Cauchy stress. By choosing an arbitrary tensor $\boldsymbol{W}$ as the skew-symmetric part of the velocity gradient $\boldsymbol{W} = \frac{1}{2}\left(\nabla\boldsymbol{v} - (\nabla\boldsymbol{v})^T\right)$, we conclude that the evolution of the Cauchy stress is described by the Jaumann rate (15).

In what follows we confine ourselves to an isotropic elastic response, by specifying the fourth order elastic tensor $\boldsymbol{\mathcal{C}}$ as $\boldsymbol{\mathcal{C}}(\boldsymbol{D}-\boldsymbol{D_p}) = \lambda(\operatorname{tr}(\boldsymbol{D}-\boldsymbol{D_p}))\boldsymbol{I} + 2\mu(\boldsymbol{D}-\boldsymbol{D_p})$, where λ and μ are the Lame coefficients, $\boldsymbol{\mathcal{C}} = \lambda\boldsymbol{I}\otimes\boldsymbol{I} + 2\mu\boldsymbol{I}$, $\boldsymbol{\mathcal{C}}_{IJKL} = \lambda\delta_{IJ}\delta_{KL} + \mu(\delta_{IK}\delta_{JL} + \delta_{JK}\delta_{IL})$.

1.3 Single Crystal Hypothesis

Plastic effects are modelled as the deformations of a material due to the flow of material dislocations through the lattice. The single-crystal hypothesis is based on the assumption that the motion of dislocations in crystalline materials take place in preferred slip directions on preferred slip planes. The slip directions are described by the constant, orthonormal, unit vectors $\boldsymbol{s}_0^{(i)}$ and $\boldsymbol{m}_0^{(i)}$, where $\boldsymbol{s}_0^{(i)}$ is in the direction of the slip and $\boldsymbol{m}_0^{(i)}$ is normal to the slip plane. These two vectors indicate slip systems ($i = 1, 2, \ldots, N$) and are given by the crystallographic structure. The plastic part of the velocity gradient $\boldsymbol{L}_p$ is assumed to be given by (Rice, 1971)

$$\boldsymbol{L}_p = \sum_{i=1}^{N} \nu^{(i)} \boldsymbol{s}_0^{(i)} \otimes \boldsymbol{m}_0^{(i)}, \quad \boldsymbol{D_p} = \sum_{i=1}^{N} \nu^{(i)} \mathrm{sym}\left(\boldsymbol{s}_0^{(i)} \otimes \boldsymbol{m}_0^{(i)}\right), \tag{16}$$

with the slip rates $\nu^{(i)}(x,t)$ given by a flow rule (18). Moreover, we introduce the current slip directions and those normal to the current slip directions, which depend on the deformation gradient through the relation $\boldsymbol{s}^{(i)} = \boldsymbol{F_e} \boldsymbol{s}_0^{(i)}$, $\boldsymbol{m}^{(i)} = \boldsymbol{F_e}^{-T} \boldsymbol{m}_0^{(i)}$. Finally we obtain the flow rule

$$\boldsymbol{L} = \boldsymbol{L_e} + \sum_{i=1}^{N} \nu^{(i)} \boldsymbol{F_e} \boldsymbol{s}_0^{(i)} \otimes \boldsymbol{m}_0^{(i)} (\boldsymbol{F_e})^{-1} = \boldsymbol{L_e} + \sum_{i=1}^{N} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)}. \tag{17}$$

To complete the system of equations, the slip rates $\nu^{(i)}$ have to be specified. Following Peirce et al. (1983), we employ the common assumption that the rate-sensitivity function is a power-law function

$$\nu^{(i)} = \nu_0 \mathrm{sgn}\left(\tau^{(i)}\right) \left(\frac{|\tau^{(i)}|}{\tau_c^{(i)}}\right)^{1/m}, \tag{18}$$

where the resolved shear stresses $\tau^{(i)}$ represent the Cauchy stress resolved on each slip system $\tau^{(i)} = \boldsymbol{s}^{(i)} \cdot \boldsymbol{T} \boldsymbol{m}^{(i)}$, $1/m$ is a rate sensitivity parameter, ν_0 a reference slip rate, and τ_c is a critical resolved shear stress. The critical stresses $\tau_c^{(i)}$ representing dissipative internal forces that oppose the slip are assumed to be governed by the evolution equation

$$\dot{\tau_c}^{(i)} = \sum_j H_{ij} |\nu^{(j)}|, \tag{19}$$

where the hardening coefficients H_{ij} are functions of accumulated slip rate and $\tau_c|_{t=0} = \tau_0$.

Let us notice that under the above assumptions the second law of thermodynamics is satisfied

$$\xi = \boldsymbol{T} : \boldsymbol{D_p} = \sum_{i=1}^{N} \nu^{(i)} \boldsymbol{T} : \left(\boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)}\right) = \sum_{i=1}^{N} \nu^{(i)} \tau^{(i)} = \sum_{i=1}^{N} \nu_0 |\tau^{(i)}| \left(\frac{|\tau^{(i)}|}{\tau_c^{(i)}}\right)^{\frac{1}{m}} \geq 0. \tag{20}$$

1.4 Evolution of the Slip Systems

Our goal is to formulate a system of equations in the current configuration independently of the deformation gradient. To this aim we employ ideas from Cazacu and Ionescu (2010b,a). By taking the time derivative of the relation $\boldsymbol{s}^{(i)} = \boldsymbol{F_e} \boldsymbol{s}_0^{(i)}$ and substituting $\dot{\boldsymbol{F}}_{\boldsymbol{e}}$ from (5), we obtain the equation that describes the evolution of the slip directions

$$\dot{\boldsymbol{s}^{(i)}} = \left(\nabla \boldsymbol{v} - \sum_i \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)}\right) \boldsymbol{s}^{(i)}. \tag{21}$$

In Section 2 we will restrict ourselves to the plane strain case. We consider projections of three dimensional slip systems onto the plane. Due to the geometrical restrictions of the in-plane model of FCC crystal, we will consider only three slip systems (for detailed discussion see Cazacu and Ionescu (2010b)). Two dimensional vectors corresponding to the $i-$th slip system can be described by their angle of lattice rotation φ_i and the scalars s_i, m_i responsible for elastic stretching. Since all three slip systems are rotating together, we can characterise the rotation by specifying the angles φ_i for $i \in \{1, 2, 3\}$ as $\varphi_1 = \varphi + \phi$, $\varphi_2 = \varphi$, and $\varphi_3 = \varphi - \phi$, where $\phi = 54.7°$,

$$\boldsymbol{s}^{(i)} = s_i(\cos\varphi_i, \sin\varphi_i), \quad \boldsymbol{m}^{(i)} = m_i(-\sin\varphi_i, \cos\varphi_i). \tag{22}$$

We reformulate the vectorial equations (21) in terms of the scalar unknowns (φ, s_1, m_1, s_2, m_2, s_3, m_3),

$$\dot{\varphi} = (-\sin\varphi, \cos\varphi) \cdot \left(\nabla \boldsymbol{v} - \sum_{i=1}^{3} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} \right) s_2 (\cos\varphi, \sin\varphi), \tag{23}$$

$$\dot{s}_i = (\cos\varphi_i, \sin\varphi_i) \cdot \left(\nabla \boldsymbol{v} - \sum_{i=1}^{3} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} \right) s_i (\cos\varphi_i, \sin\varphi_i);\ i \in \{1, 2, 3\}, \tag{24}$$

$$\dot{m}_i = (-\sin\varphi_i, \cos\varphi_i) \cdot \left(\nabla \boldsymbol{v} - \sum_{i=1}^{3} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)} \right) m_i (-\sin\varphi_i, \cos\varphi_i);\ i \in \{1, 2, 3\}. \tag{25}$$

2 2-turn Equal Channel Angular Extrusion

ECAE is based on forcing a specimen through an L-shape channel of a constant cross-section. Simple shear takes place in the thin layer at the channel turn. The process is repeated a couple of times (typically up to 10) in order to obtain a very large (severe) plastic deformation and a fine grain structure. The first report on the use of a 2-turn channel is due to Liu et al. (1998). Later the idea was extended to multi-pass ECAE by Nakashima et al. (2000).

The Eulerian system of equations derived in Section 1 allows us to consider more than one turn in a single domain. We chose a 2-turn channel to show the main features of the presented approach. For experimental and numerical studies of a 2-turn ECAE we refer to Rosochowski and Olejnik (2002, 2008).

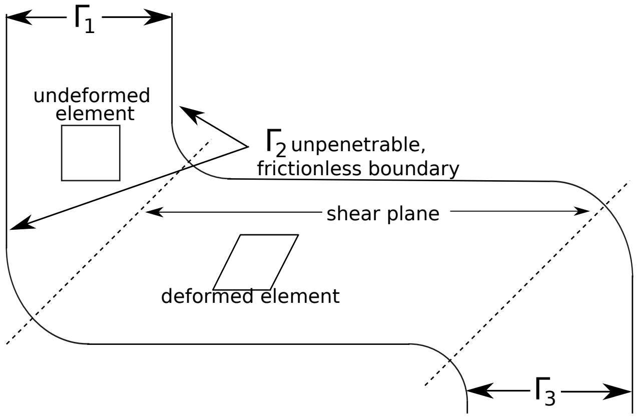

Figure 1: Scheme of 2-turn ECAE experiment

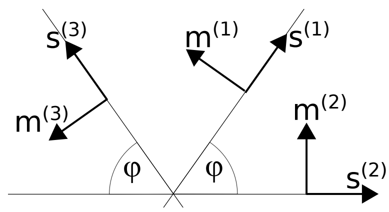

Figure 2: Scheme of slip systems

2.1 Initial-boundary Value Problem

Our domain Ω is the 2-turn channel (see Figure 1). In the Eulerian description of plane-strain crystal plasticity the unknowns are: the velocity $\boldsymbol{v}(x,t)$, the Cauchy stress $\boldsymbol{T}(x,t)$, the density $\varrho(x,t)$, and the orientation of the lattice $\varphi(x,t)$. The boundary of the domain is divided into three parts: the inflow boundary Γ_1, the impenetrable boundary Γ_2 and the outflow boundary Γ_3. The boundary conditions are set to be: the Dirichlet inflow condition on the velocity and the lattice orientation, $\boldsymbol{v}|_{\Gamma_1} = \boldsymbol{v}_{in} = (0,-1), \varphi|_{\Gamma_1} = \varphi_{in} = 0$, the perfect-slip on Γ_2, and the stress free condition on Γ_3. The material parameters and characteristic values are taken to be: the density $\varrho_0 = 3000\frac{kg}{m^3}$, the velocity $V = 10^{-5}\frac{m}{s} = 10\frac{\mu m}{s}$, the length $L = 10^{-2}m$, the reference slip rate $\nu_0 = 10^{-3}\frac{1}{s}$, the reference stress $\tau_0 = 70MPa$, the Young's modulus $E = 1000\tau_0$, the Poisson's ratio $\nu_{pois} = 0.35$, and the rate sensitivity parameter $m = 0.05\,(1/m = 20)$. The material parameters correspond to aluminium and the characteristic values reflect ECAE experiments. As initial values we put $\boldsymbol{v}(x,0) = 0$, $\boldsymbol{T}(x,0) = 0$, $\tau_c(x,0) = \tau_0$, $\varrho(x,0) = 1$, $\varphi(x,0) = 0$ and $m_i(x,0) = s_i(x,0) = 1,\ \forall i \in \{1,2,3\}$.

After rescaling of the system we get the following set of equations

$$\begin{aligned}
&\varrho_{,t} + \mathrm{div}\,(\varrho \boldsymbol{v}) = 0\\
&R_1 \varrho \dot{\boldsymbol{v}} - \mathrm{div}\,\boldsymbol{T} = 0\\
&\dot{\boldsymbol{T}} + \boldsymbol{T}\mathrm{div}\,\boldsymbol{v} + \boldsymbol{W}\boldsymbol{T} - \boldsymbol{T}\boldsymbol{W} = \varrho \boldsymbol{\mathcal{C}}(\boldsymbol{D} - \boldsymbol{D_p})\\
&\dot{\varphi} = (-\sin\varphi, \cos\varphi)\cdot\left(\nabla \boldsymbol{v} - R_2 \sum_{i=1}^{3} \nu^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{m}^{(i)}\right) s_2(\cos\varphi, \sin\varphi)
\end{aligned} \tag{26}$$

where $\boldsymbol{D_p}$, $\nu^{(i)}$, m_i, s_i and $\dot{\tau_c}^{(i)}$ are given by (16), (18), (24), (25) and (19), respectively.

Two characteristic numbers appear in the system, $R_1 = \frac{\varrho_0 V^2}{L\tau_0} \approx 10^{-12}$ and $R_2 = \frac{L\nu_0}{V} = 1$. The very small value of R_1 justifies the restriction to the quasi-static case, which is common in plasticity. However we keep the time derivative in the balance equation (7).

Moreover, we specify the hardening matrix $H_{ij} = H = H_0 \mathrm{sech}^2\left(\frac{H_0 \nu_{acc}}{\tau_s - \tau_0}\right)$, where the initial hardening rate $H_0 = 8.9\tau_0$, the saturation strength $\tau_s = 1.8\tau_0$ and the accumulated slip $\nu_{acc}(t) = \sum_i \int_0^t |\nu^{(i)}|\mathrm{dt}$, see Peirce et al. (1983).

2.2 Finite Element Formulation

Inspired by the numerical methods of fluid dynamics, a finite element Eulerian representation is formulated and applied to a solution of the flow adjustment initial-boundary value problem for the 2-turn equal channel angular extrusion, see Section 2.1.

The domain Ω is approximated by a simplical triangulation $\mathcal{T}_h$. Time is discretized by a one step finite difference. The discretization in space consists of P2 elements for the velocity, P1 for the density and the lattice rotations (all continuous) and P1-discontinuous for the Cauchy stress and the slip rates. We define the finite-dimensional spaces

$$\begin{aligned}
\mathbb{V}_h &= \{v_h \in W^{1,2}(\Omega;\mathbb{R}^2);\ \boldsymbol{v}|_{\Gamma_1} = (0,-1),\ \boldsymbol{v}|_K \in \mathcal{P}_2(K)^2\ \forall K \in \mathcal{T}_h\},\\
\mathbb{R}_h &= \{\varrho_h \in W^{1,2}(\Omega;\mathbb{R});\ \varrho_h|_{\Gamma_1} = 1,\ \varrho_h|_K \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\},\\
\mathbb{T}_h &= \{\boldsymbol{T}_h \in W^{1,2}(\Omega;\mathbb{R}^{2\times 2}_{sym}); \boldsymbol{T}_h|_K \in \mathcal{P}_1(K)^{2\times 2}\ \forall K \in \mathcal{T}_h\},\\
\mathbb{N}_h &= \{\nu_h \in L^2(\mathbb{R}); \nu_h|_1 \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\},\\
\mathbb{A}_h &= \{\varphi_h \in W^{1,2}(\Omega;\mathbb{R});\ \varphi_h|_{\Gamma_1} = 0,\ \varphi_h|_K \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\}.
\end{aligned}$$

The slip rates are added to the system (26) as variables. We discretize the system (26) in a mixed finite element space and solve the following problem. Find $(\boldsymbol{v}_h, \varrho_h, \boldsymbol{T}_h, \nu_{1h}, \nu_{2h}, \nu_{3h}, \varphi_h) \in \mathbb{V}_h \times \mathbb{R}_h \times \mathbb{T}_h \times \mathbb{N}_h \times \mathbb{N}_h \times \mathbb{N}_h \times \mathbb{A}_h$, such that

$$\begin{aligned}
&(\varrho_{h,t}, z_\varrho) + (\boldsymbol{v}_h \nabla \varrho_h, z_\varrho) + (\varrho_h \mathrm{div}\,(\boldsymbol{v}_h), z_\varrho) = 0 \quad \forall z_\varrho \in \mathbb{R}_{h0},\\
&R_1(\varrho_h \dot{\boldsymbol{v}}_h, \boldsymbol{z_v}) + (\boldsymbol{T}_h, \nabla(\boldsymbol{z_v})) + (\boldsymbol{T}_h \boldsymbol{n}\cdot\boldsymbol{n}, \boldsymbol{z_v}\cdot\boldsymbol{n})_{\Gamma_2} + \frac{\beta}{h}(\boldsymbol{v}_h\cdot\boldsymbol{n}, \boldsymbol{z_v}\cdot\boldsymbol{n})_{\Gamma_2} = 0 \quad \forall \boldsymbol{z_v} \in \mathbb{V}_{h0},\\
&\left(\dot{\boldsymbol{T}}_h + \boldsymbol{T}_h \mathrm{div}\,\boldsymbol{v}_h + \boldsymbol{W}_h\boldsymbol{T}_h - \boldsymbol{T}_h\boldsymbol{W}_h, \boldsymbol{Z_T}\right) - \left(\varrho\boldsymbol{\mathcal{C}}(\boldsymbol{D}_h - \boldsymbol{D_p}_h), \boldsymbol{Z_T}\right) + (\boldsymbol{Z_T}\boldsymbol{n}\cdot\boldsymbol{n}, \boldsymbol{v}_h\cdot\boldsymbol{n})_{\Gamma_2} = 0 \quad \forall \boldsymbol{Z_T} \in \mathbb{T}_h,\\
&\left(\nu_h^{(i)} - \mathrm{sgn}\,(\boldsymbol{T}_h : \boldsymbol{s}_h^{(i)} \otimes \boldsymbol{m}_h^{(i)})\left(\frac{|\boldsymbol{T}_h : \boldsymbol{s}_h^{(i)} \otimes \boldsymbol{m}_h^{(i)}|}{\tau_c^{(i)}}\right)^{20}, z_{\nu i}\right) = 0 \quad \forall z_{\nu i} \in \mathbb{N}_h \text{ and } i \in \{1,2,3\},\\
&\left(\dot{\varphi}_h - (-\sin\varphi_h, \cos\varphi_h)^T\left(\nabla \boldsymbol{v}_h - R_2\sum_{i=1}^{3}\nu_h^{(i)}\boldsymbol{s}_h^{(i)}\otimes\boldsymbol{m}_h^{(i)}\right) s_{2h}(\cos\varphi_h, \sin\varphi_h), z_\varphi\right) = 0 \quad z_\varphi \in \mathbb{A}_h,
\end{aligned} \tag{27}$$

where $(\cdot,\cdot)$ is the standard L_2 inner product. The boundary conditions on the impenetrable, frictionless boundary Γ_2 are imposed by the Nitsche's method: $(\boldsymbol{Z_T}\boldsymbol{n}\cdot\boldsymbol{n}, \boldsymbol{v}\cdot\boldsymbol{n})_{\Gamma_2} + (\boldsymbol{T}\boldsymbol{n}\cdot\boldsymbol{n}, \boldsymbol{z_v}\cdot\boldsymbol{n})_{\Gamma_2} + \frac{\beta}{h}(\boldsymbol{v}\cdot\boldsymbol{n}, \boldsymbol{z_v}\cdot\boldsymbol{n})_{\Gamma_2}$ with $\beta = 10$, see Freund and Stenberg (1995).

To solve the system (27) we employ a non-linear Newton-Ralphson solver with an analytic Jacobian. Implementation is done in the software package FEniCS (Logg et al., 2012). A linear system is solved by a direct solver.

Moreover, the critical resolved shear stresses and the stretch of slip directions are updated after each time step according to (19), (24), and (25).

2.3 Results

We present the results of computations at the moment when a steady state is reached (see Figure 3). We treat the plastic material as a fluid so it fills the entire domain, as opposed to models where empty zones (close to outer turn) are reported (Rosochowski and Olejnik, 2008). The velocity profile is typical of flow problems.

We can observe that plastic slip occurs only in the vicinity of shear planes where the channel turns. The accumulated slip has its highest values close to the inner turns. Its density is almost constant, although it changes in the neighbourhood of the curved part of the boundary and it is higher before the first turn than in the rest of the domain. The lattice rotation also changes nearby the shear planes in the direction of turn.

In Figure 4 we observe the behaviour of individual slip systems. The arrangement of slip directions is presented in Figure 1. We notice that the activation of a particular slip system depends on its position relative to the shear plane. The second slip system is almost inactive but we need to take it into account due to compressibility.

Simulations were conducted for two different meshes: 5278 vertices (10252 cells) and 21289 vertices (41974 cells). We conclude that the problem is mesh independent. The resented results were computed with the finer mesh.

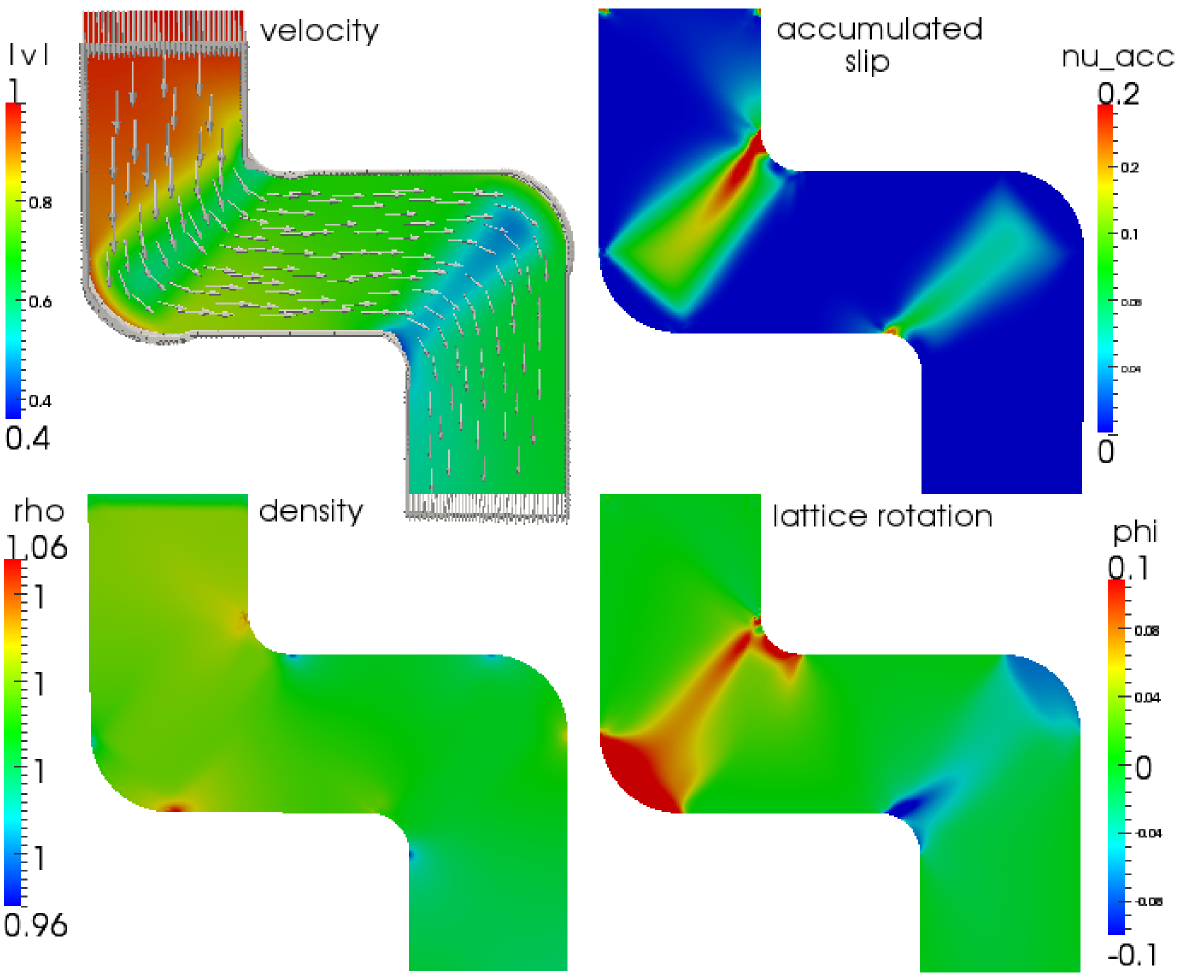

Figure 3: Computed variables: velocity magnitude (top-left), accumulated slip (top-right), density (bottom-left), lattice rotation (bottom-right).

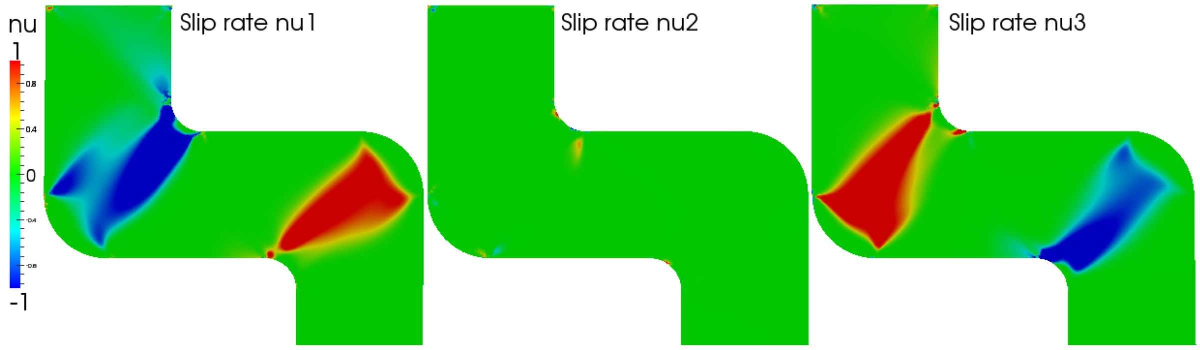

Figure 4: Behaviour of slip rates on individual slip systems in the 2-turn channel.

3 Conclusions

In this paper we derived a model of crystal plasticity that includes compressible linear elasticity, namely stretches and rotations of the slip systems have been taken into account. Moreover, the evolution of the Cauchy stress has been justified by thermodynamical discussion.

We formulated a finite element discretization scheme, which has been used to solve the fully coupled problem. Performed numerical simulations show the capabilities of the method applied. Important elements of the model are the elastic stretches, because they allow us to reduce high values of stress in the vicinity of inner turns.

The presented approach is purely Eulerian and its main advantage is the ability to capture high strains, due to ECAE with multiple turns. In the future we plan to abandon the plane strain assumption and compute 3D models including the full set of the slip systems, even though this will require the use of parallel computing.

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Address: Piotr Minakowski, University of Warsaw, Institute of Applied Mathematics and Mechanics, Banacha 2, 02-097 Warszawa, Poland
email: `minak@mimuw.edu.pl`