Numerical simulations of shear bands formation for single-slip crystal

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Abstract

The aim of this paper is to investigate fluid model of single-slip crystal plasticity. We give detailed description of the model and present results of finite element numerical simulations performed in Eulerian coordinates. The constitutive relation between slip rate and resolved shear stress is formulated in two ways, explicit and implicit. We introduce the numerical treatment of implicitly constituted materials and compare it with classical explicit approach.

Keywords: finite element method, Eulerian plasticity
AMS Classification: 74S05, 74C15

1 Introduction

Within the last 20 years it was recognized that severe plastic deformation of certain material allows to achieve exceptionally high strength accompanied by relatively good ductility. Several metal forming processes achieving severe plastic deformation are now available. Our motivation is experiment ECAE (Equal Channel Angular Extrusion) where the material is forced through the curved channel [7]. Very high strains can be achieved without interruption, one can look at various amount of strains in one specimen, due to relatively simple loading conditions strain can be defined approximately by compression.

In presented approach plastic behaviour of crystalline solid is treated as a highly viscous material flow through an adjustable crystal lattice. Looking at severe plastic deformations experiments [7,8] it seems that crystalline materials at yield behave as a special kind of incompressible, anisotropic, highly viscous fluid.
2 Higher-order gradient crystal plasticity

2.1 Kinematics of crystal plasticity

Let $\Omega$ denote the reference configuration of the body and $\Omega_t$ denote current configuration at time $t$. The point which was at position $X \in \Omega$ in the reference configuration is in the current configuration in time $t$ in the position $\chi(X,t) \in \Omega_t$.

$$x = \chi(X,t).$$ (1)

The deformation gradient $F$ is defined through

$$F = \frac{\partial \chi(X,t)}{\partial X}.$$ (2)

The multiplicative (Kröner) decomposition of the deformation gradient $F$ is employed as a basis for the kinematics of a single crystal [1,6],

$$F = F_e F_p,$$ (3)

where $F_e$ stands for elastic distortion (stretch and rotation of the lattice) and $F_p$ for plastic distortion (distortion of the lattice due to formation of dislocations). All the volumetric changes are assumed to result from elastic stretches in the lattice,

$$\det F_p = 1, \quad \det F = \det F_e.$$ (4)

By the virtue of Kröner decomposition (3) we obtain

$$\nabla v = \dot{F} F^{-1} = \dot{F}_e (F_e)^{-1} + F_e (\dot{F}_p (F_p)^{-1}) (F_e)^{-1} = \dot{F}_e F_e^{-1} + F_e L_p (F_e)^{-1},$$

where superposed dot denotes material-time derivative.

We introduce slip directions by constant vectors $s_0$ and $m_0$, $s_0$ in the direction of slip and $m_0$ unit normal to slip plane and are given by crystallographic structure (see Figure 2.1). Current slip directions and the normals (to slip directions) depend on deformation gradient through the relation

$$s = F_e s_0,$$ (5)

$$m = F_e^{-T} m_0.$$ (6)

Moreover, the plastic flow is governed by slip rate $v(x,t)$ on the individual slip systems. $L_p$ is assumed to be given by $L_p = \nu s \otimes m$.

Finally we obtain the flow rule

$$\nabla v = \dot{F}_e F_e^{-1} + \nu F_e s_0 \otimes (F_e)^{-T} m_0 = \dot{F}_e F_e^{-1} + \nu s \otimes m.$$ (7)

Resolved shear stresses $\tau$ represent the Cauchy stress $T$ resolved on slip system

$$\tau = s \cdot T m.$$ (8)

In the considered process Cauchy stress satisfies the balance equation

$$\text{div} \ T = 0.$$ (9)
2.2 Constitutive equations.

We adopt the following constitutive relation in terms of the material Jaumann rate of the Kirchhoff stress $\mathbf{T}$ ($\mathbf{T} = \det(F)\mathbf{\Sigma}$ for Cauchy stress $\mathbf{\Sigma}$). As it was proposed in [6] we introduce evolution equation for the Kirchhoff stress tensor $\mathbf{T}$

$$\dot{\mathbf{T}} - WT + TW = \mathbf{C} : D - \nu (\mathbf{C} : P + QT - TQ),$$

(10)

where $\mathbf{D} = \text{sym}(\nabla \mathbf{v})$, $\mathbf{W} = \text{skew}(\nabla \mathbf{v})$ and $\mathbf{Q} = \text{skew}(\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)})$, $\mathbf{P} = \text{sym}(\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)})$. Elastic part is described by Young modulus $E$, Poisson ratio $\nu_p$ and fourth order elastic tensor $\mathbf{C}$ reads as follows

$$\mathbf{C} : \mathbf{D} = \lambda (\text{tr} \mathbf{D}) \mathbf{I} + 2\mu \mathbf{D},$$

where $\lambda = \frac{E\nu_p}{(1+\nu_p)(1-2\nu_p)}$ and $\mu = \frac{E}{2(1+\nu_p)}$ are Lame coefficients.

To complete the system, slip rate $\nu$ have to be specified. Here we use power law slip rate relation [6]

$$\nu = \nu_0 \text{sgn} (\tau - \tau_b) \left( \frac{|\tau - \tau_b|}{\tau_c} \right)^{1/m},$$

(11)

where $1/m$ is rate sensitivity parameter, $\nu_0$ reference slip rate, $\tau_b$ stands for backstress and $\tau_c$ is constant critical resolved shear stress.

Backstress is described by equation

$$\tau_b = b\tau_0 \mathbf{l} \nabla \varrho \cdot \mathbf{s},$$

(12)

where $b, \tau_0, l$ are respectively: Burgers vector, reference stress, length scale. Moreover in (12) we introduced Geometrically Necessary Dislocations densities $\varrho$ given by

$$\dot{\varrho} = -\frac{1}{b} \nabla \nu \cdot \mathbf{s}.$$  

(13)
Implicit constitutive relation

In the constitutive relation (11) exponent $\frac{1}{m}$ is responsible for material rate sensitivity and the rate independent limit is $m \to 0$. In that case material response is given by the yield condition:

$$\nu = 0 \implies |\tau - \tau_b| < \tau_c$$

$$|\nu| > 0 \implies \tau - \tau_b = \tau_c \frac{\nu}{|\nu|} = \tau_c \text{sgn}(\nu)$$

The above conditions are equivalent to the relation

$$f(|\tau - \tau_b|, \nu) + (|\tau - \tau_b| - \tau_c)_+ = 0,$$

where $(x)_+ = \max\{x, 0\}$. Function $f$ satisfies following conditions

$$f(X) = 0 \iff X = 0$$

and for $|\tau - \tau_b| > \tau_c$

$$f(X) = - (|\tau - \tau_b| - \tau_c).$$

In computations we will restrict ourself to $f(X) = \frac{1}{2} \arctan(X)$.

### 2.3 Dimensionless form

To obtain dimensionless form of considered system we scale equations (7-13) in the following way.

$$\text{div} \, T^* = 0$$

$$\nabla \nu^* = \hat{F}_e F_e^{-1} + \mathcal{R}_1 \nu^* \otimes s \otimes m$$

$$T^* - W^* T^* + T^* W^* = C : D^* - \mathcal{R}_1 \nu^* (C : P + Q T^* - T^* Q)$$

$$\tau^* = s^{(i)} \cdot T^* m^{(i)}$$

$$\nu^* = \text{sgn} (\tau^* - \tau_b^*) \left( \frac{|\tau^* - \tau_b^*|}{\tau_c^*} \right)^{1/m}$$

$$\tau_b^* = \mathcal{R}_2 \nabla \psi^* \cdot s$$

$$\dot{\psi}^* = \frac{\mathcal{R}_1}{\mathcal{R}_2} \nabla \psi^* \cdot s$$

where $\mathcal{R}_1 = \frac{l_0 \nu_0}{\tau_0}$ and $\mathcal{R}_2 = b l_0 \varrho_0$ are dimensionless parameters and star denotes dimensionless variables: length $x^* = \frac{l_0}{l_0} x$, velocity $v^* = \frac{v_0}{v_0} v$, time $t^* = \frac{l_0}{v_0} t$, Kirchoff stress $T^* = \frac{l_0}{l_0} T$, resolved shear stress $\tau^* = \frac{l_0}{l_0} \tau$, backstress $\tau_c^* = \frac{l_0}{l_0} \tau_c$, critical stress $\dot{\tau}_c^* = \frac{l_0}{l_0} \tau_c$, slip rates $\nu^* = \frac{1}{v_0} \nu$, GND-dislocations densities $\varphi^* = \frac{1}{\varrho_0} \varphi$. In what follows, we will omit star to keep the notation transparent.

We choose dimensionless characteristic numbers $\mathcal{R}_1$ and $\mathcal{R}_2$ to be equal unity, corresponding scales are presented in the table below.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l_0$ [mm]</td>
<td>1</td>
</tr>
<tr>
<td>$\nu_0$</td>
<td>0.001</td>
</tr>
<tr>
<td>$v_0$ [m/s]</td>
<td>10</td>
</tr>
<tr>
<td>$b$ [nm]</td>
<td>0.1</td>
</tr>
<tr>
<td>$\varrho_0$ [m$^2$]</td>
<td>$10^{12}$</td>
</tr>
</tbody>
</table>
3 Finite element formulation and computational results

We are dedicated to the Equal Channel Angular Extrusion experiment. This section consists of the results of numerical simulations for compression of rectangular-shaped single-slip single crystal under plane strain conditions. The scheme of the setting is presented in the figure 2.1.

The finite $P^2 - P^1$ elements choice reads as follows:

$$P^1 : F_e, \nu, \tau, \eta, \varrho$$

$$P^2 : v, T$$

Domain is discretized by unstructured rectangular mesh, figure 2. Discretization in time is given by one step finite difference. For solving non-linear system of equations (15-21) we use non-linear Newton solver. All computations were made with use of the FEniCS package [5].

3.1 Compression of a single-slip single crystal

The model problem considered in this paper is the compression of a single-slip single crystal. Slip system is oriented at $\phi = 45^\circ$ $(s_0 = (\sin(\phi), -\cos(\phi)), \quad m_0 = (\cos(\phi), \sin(\phi)))$. The boundary conditions are given by

$$v_{x_2} = -0.5 \text{ along } x_2 = H$$

$$v = (0, 0) \text{ along } x_2 = 0$$

$$\nu = 0 \text{ along } x_2 = 0 \text{ and } x_2 = H$$

$$\varrho = 0 \text{ along } x_1 = 0 \text{ and } x_1 = L$$

For other variables zero Neumann boundary condition is applied. At the initial time we put $F_e = I$ and zero for remaining variables. Moreover we specify material constants $E = 130\text{MPa}$, $\nu_p = 0.3$, $\tau_0 = 50\text{MPa}$, $0.1 \leq m \leq 0.05$. The aspect ratio of the specimen is $H = 3L$.

We present accumulated slip on the deformed mesh at strain 0.1, figure 2. The result shows the formation of the regions where slip is accumulated. The regions are aligned with slip direction what is compatible with the model and physical motivations.

Furthermore, comparison between explicit and implicit approach was investigated, figure 3. We used in equation (14) function $\arctan$

$$f(|\tau - \tau_b|\nu - \nu \tau_c) = \frac{1}{2} \arctan (|\tau - \tau_b|\nu - \nu \tau_c).$$

We present magnitude of velocity (upper part of figure 3) and accumulated slip (lower part of figure 3) at strain 0.1 on the original mesh (Eulerian coordinates). The result shows similar behaviour for both cases. However the crucial point is that accumulation of slip is faster in implicit case (one can observe that looking at changes in time) and regions where the slip is localised differs.
Figure 2: Accumulated slip on a unstructured deformed mesh

Figure 3: Comparison between explicit (a) and implicit (b) approach
Acknowledgement

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