

# Fluid Model of Crystal Plasticity - Mathematical Properties and Computer Simulations

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An extended abstract of the PhD dissertation

## 1 Introduction

The main purpose of this dissertation is to investigate model of a plastic flow of a highly viscous fluid that describes the ultrafine structure formation induced by severe plastic deformation. The idea behind is to apply and further develop methods known from fluid mechanics to modelling crystal solids. We aim to describe very large deformations, that are typical for fluid models, thus the Eulerian formulation is employed. Numerical simulation equipped with necessary mathematical analysis, can predict microstructure evolution, including the material hardening, shear band formation and strain localization.

The thesis focuses on three broad areas: mathematical modelling of responses of elasto-viscoplastic materials (Chapter 1), mathematical analysis of newly developed models (Chapter 2), and the development of numerical schemes to capture the behaviour of such materials (Chapter 3 and Chapter 4). In the centre of attention are, fully Eulerian models of crystal plastic materials under large deformations.

### 1.1 Motivations

The title of the thesis is Fluid Model of Crystal Plasticity - Mathematical Properties and Computer Simulations. The topic arises from the material science where the investigation of polycrystalline materials, is of a great importance. In particular, the properties of materials are strongly related to their microstructure. Crystalline matter is mechanically anisotropic. This means that the instantaneous and time-dependent deformation of crystalline aggregates depends on the direction of the mechanical loads and geometrical constraints imposed. An essential consequence of the crystalline anisotropy of material is that its mechanical properties are orientation dependent.

We are interested in modelling and investigating large deformations of advanced materials, that outperform conventional materials with superior mechanical properties such as toughness, hardness, accompanied by relatively good ductility, and durability. Moreover, advanced materials may have also novel properties including the ability to memorize shape or respond to environmental changes, this is however beyond the scope of the dissertation.

The mechanical properties of crystalline materials are determined by several factors, the average grain size of the material plays a significant, and often a dominant, role. A new advanced materials can be developed by further grain refinement. In general, the smaller the grain size, the bigger the strength of a material. This behaviour is described through the Hall–Petch relation  $\sigma_y = \sigma_0 + k_y d^{-\frac{1}{2}}$ , where  $\sigma_y$  stands for yield stress,  $\sigma_0$  is friction stress,  $k_y$  is a constant of yielding, and  $d$  is grain size

[1, 2]. Expected mechanical properties are exhibited by ultra fine grain (UFG) materials, namely polycrystals having very small grains with average grain sizes less than  $1\mu\text{m}$ .

Experimental studies show that applying severe plastic deformation (SPD) is suitable to obtain small grain size. SPD techniques are characterized by imposing high strains without introducing any change in the overall dimensions of the material. Several metal forming processes achieving severe plastic deformations are now available. We chose the equal channel angular extrusion [3, 4] and high pressure torsion [5, 6] because it has proven highly suitable for experimental and theoretical studies. The nature of the imposed deformation is simple shear.

## 2 Modelling of large deformation crystal plasticity

To start with, we employ the continuum description of matter at length scales that are large compared to the molecular scale. Continuum physics aims to describe materials with variables such as velocity, density, stress, etc., under an assumption that a given number of molecules is large enough to warrant the use of a smooth continuum description. We briefly recall basic concepts of solid and fluid mechanics, introduce necessary quantities, and derive balance laws.

After a review of kinematics, balance equations, and the second law of thermodynamics we discuss one-dimensional mechanical analogues of elasto-visco-plastic elements. We present different classes of constitutive responses, namely stress-strain behaviour under a uni-axial loading. It provides a motivation for consideration of a rate type material models.

Later we address a constitutive theory, focusing on a stress-strain relation. Starting point to the modelling of large deformation plasticity is to employ the multiplicative decomposition of the deformation gradient. We present two approaches to modelling large deformations. Multiplicative decomposition by Kroner [7, 8] and natural configuration by Rajagopal [9, 10], both lead to the additive decomposition of the deformation gradient, but are based on different thermodynamical basis. As pointed out by Rajagopal and Srinivasa [9] within classical plasticity literature it is usual to specify some evolution equation for the plastic strain and then to define the rate of dissipation as the inner product of the stress with the rate of plastic strain, see e.g. [11]. On the other hand, one can choose different set of assumptions, namely make constitutive assumptions on the nature of the work done, the Helmholtz potential and the rate of dissipation. By postulating that the rate of dissipation per unit volume is the maximum possible.

Following the paper by Rajagopal and Srinivasa [12], 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,

$$f(\dot{\mathbf{T}}, \mathbf{T}, \mathbf{L}) = 0,$$

where the constitutive relation contains the Cauchy stress  $\mathbf{T}$ , the rate of stress  $\dot{\mathbf{T}}$ , and the velocity gradient  $\mathbf{L}$ , we refer to [13, 12]. The comparison between the derivation of the rate type stress-strain relation using the Helmholtz and the Gibbs potential is given. The emphasis is on the application of the Gibbs potential to obtain a model of a rate-type, describing flow of crystal plastic material.

Next step is to equip the derived model with plastic effects. We provide the description of crystal plastic behaviour and introduce all necessary variables and constitutive assumptions. For formulation of rate dependent flow rule and hardening law, we refer to early references, such as Asaro et al.[14, 15] and Hill et al. [16].

Furthermore, we propose possible extensions of the flow rule by a rate independent implicit constitutive relation [17, 18], namely rewrite perfect plastic flow rule as an implicit scalar equation.

Several variants of an implicit formulae and description of preliminary numerical studies are given.

Finally we employ a maximization of the rate of entropy production principle [9, 10] to identify the rate of plastic strain. The goal is to replace the single crystal hypothesis, by postulating proper rate of dissipation function.

The obtained model is fully Eulerian. The important feature is the Eulerian description of the evolution of the crystal lattice. To sum up we present the system of equations we aim to solve. Let  $T > 0$ ,  $\Omega \subset \mathbb{R}^d$  open,  $\varrho_0 : \Omega \rightarrow \mathbb{R}$ ,  $\mathbf{v}_0 : \Omega \rightarrow \mathbb{R}^d$ ,  $\mathbf{S}_0 : \Omega \rightarrow \mathbb{R}^{d \times d}$ ,  $\mathbf{a}_{i0} : \Omega \rightarrow \mathbb{R}^d$ ,  $i = 1, 2, \dots, d$ ,  $\mathbf{v}_D : \Gamma_D \rightarrow \mathbb{R}^d$ ,  $\mathbf{t} : \Gamma_N \rightarrow \mathbb{R}^d$ . The system is satisfied inside the domain  $\Omega \subset \mathbb{R}^d$ , the boundary  $\partial\Omega$  consists of two non-intersecting parts  $\Gamma_D$  and  $\Gamma_N$  corresponding to the Dirichlet and the Neumann boundary conditions, respectively. We look for the density  $\varrho$ , the velocity  $\mathbf{v}$ , the Kirchhoff stress  $\mathbf{S}$ , and the lattice vectors  $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_d$  ( $\mathbf{s}^{(\alpha)}$  and  $\mathbf{m}^{(\alpha)}$  are given through lattice vectors) satisfying

$$\dot{\varrho} + \varrho \operatorname{div} \mathbf{v} = 0 \quad \text{in } \Omega \times (0, T), \quad (1a)$$

$$\varrho \dot{\mathbf{v}} = \operatorname{div} (\varrho \mathbf{S}) \quad \text{in } \Omega \times (0, T), \quad (1b)$$

$$\mathcal{A} \overset{\nabla}{\mathbf{S}} = \mathbf{D} - \sum_{\alpha=1}^N \nu^{(\alpha)} \operatorname{sym} \left( \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} \right) \quad \text{in } \Omega \times (0, T), \quad (1c)$$

$$\sum_{i=1}^d \dot{\mathbf{a}}_i \otimes \mathbf{a}^i = \nabla \mathbf{v} - \sum_{\alpha=1}^N \nu^{(\alpha)} \left( \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} \right) \quad \text{in } \Omega \times (0, T). \quad (1d)$$

The system (1) is equipped with following boundary conditios

$$\varrho(x, 0) = \varrho_0(x) \quad \forall x \in \Omega,$$

$$\mathbf{v}(x, 0) = \mathbf{v}_0(x) \quad \forall x \in \Omega,$$

$$\mathbf{S}(x, 0) = \mathbf{S}_0(x) \quad \forall x \in \Omega,$$

$$\mathbf{a}_i(x, 0) = \mathbf{a}_{i0}(x) \quad \forall x \in \Omega,$$

$$\mathbf{v} = \mathbf{v}_D \quad \text{on } \Gamma_D \times (0, T),$$

$$\mathbf{S} \mathbf{n} = \mathbf{t} \quad \text{on } \Gamma_N \times (0, T).$$

Chapter 2 is devoted to the mathematical analysis of the simplified problem in a two dimensional spatially periodic domain. We assume incompressibility, namely the mass balance (1a) is equivalent to the divergence free condition. We put  $\varrho = 1$ ,  $p = -\frac{1}{2} \operatorname{tr} \mathbf{S}$  and for the sake of brevity denote the deviatoric part of stress as  $\mathbf{S}$ . Moreover, plastic effects are neglected, thus equation (1d) and corresponding unknowns are not taken into account.

Let  $T > 0$ ,  $\Omega \subset \mathbb{R}^2$  periodic,  $\mathbf{v}_0 : \Omega \rightarrow \mathbb{R}^2$ ,  $\mathbf{S}_0 : \Omega \rightarrow \mathbb{R}^{2 \times 2}$ . Find the velocity  $\mathbf{v}$ , the pressure  $p$ , and the Kirchhoff stress  $\mathbf{S}$ , such that

$$\begin{aligned}
\operatorname{div} \mathbf{v} &= 0, & \text{in } \Omega \times (0, T), \\
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \nabla \mathbf{v} + \nabla p &= \operatorname{div} \mathbf{S}, & \text{in } \Omega \times (0, T), \\
\frac{\partial \mathbf{S}}{\partial t} + \mathbf{v} \nabla \mathbf{S} + \mathbf{W} \mathbf{S} - \mathbf{S} \mathbf{W} &= \mathbf{D} & \text{in } \Omega \times (0, T), \\
\mathbf{v}(x, 0) &= \mathbf{v}_0(x) & \forall x \in \Omega, \\
\mathbf{S}(x, 0) &= \mathbf{S}_0(x) & \forall x \in \Omega.
\end{aligned}$$

In Chapter 4 we provide a numerical solutions to the system (1), however it can reformulated according to the specific experimental setting.

### 3 Mathematical analysis of a rate-type fluid model arising from crystal plasticity

The mathematical theory of initial and boundary value problems involving visco-elastic fluids gained attention during the last three decades. For the incompressible model Oldroyd-B model, there is a vast amount of results in the literature. We aim to provide the analytical result for a rate-type fluid model originated in crystal plasticity. In comparison with Oldroyd-B model our system lacks viscous contribution to the momentum balance, thus the momentum equation is similar to the Euler equation. This makes the analysis of the complete problem (1) difficult. We propose a regularisation of the rate type equation for the extra (elastic) stress  $\mathbf{S}$ . This regularization helps us to improve a priori estimates that are then shown to be sufficient to establish the large data existence of a weak solution. There exists studies of stress diffusive Oldroyd-type models, see e.g. [19], but to the author's knowledge the system investigated in this chapter have not been studied so far.

The system (1) derived in Chapter 1 describes behaviour of crystal plastic material. For the sake of mathematical analysis of the system we make the following simplifications: consider the incompressible case and neglect plastic effects. The following problem captures essential mathematical difficulties, find  $(\mathbf{v}, \mathbf{S}, p)$  spatially periodic in  $[0, L]^2 \times (0, T)$  such that

$$\operatorname{div} \mathbf{v} = 0, \tag{2a}$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \nabla \mathbf{v} + \nabla p = \operatorname{div} \mathbf{S}, \tag{2b}$$

$$\frac{\partial \mathbf{S}}{\partial t} + \mathbf{v} \nabla \mathbf{S} + \mathbf{W} \mathbf{S} - \mathbf{S} \mathbf{W} = \mathbf{D} \tag{2c}$$

Despite our effort we were unable to show the existence of the solution to the system (2). Therefore, we propose two different regularizations, namely adding a regularization term  $-\Delta \mathbf{S}$  or  $-\Delta \frac{\partial \mathbf{S}}{\partial t}$ .

We will not give the physical justification for proposed regularizing term. In the literature one can find visco-elastic models with a diffusive term appearing in the evolution equation for the visco-elastic stress tensor that are an outcome of modelling, see e.g. diffusive Peterlin model [19] or [20, 21].

We consider the model 2 regularized by  $-\Delta \frac{\partial}{\partial t} S$ . It describes a flow of crystal plastic material in a two dimensional periodic domain. Note that one can multiply the regularization term by an arbitrary small constant  $-\varepsilon \Delta \frac{\partial}{\partial t} S$ , however we are unable to pass to the limit with  $\varepsilon \rightarrow 0$  so for the sake of brevity we put  $\varepsilon = 1$ .

The system of governing equations reads. Find  $\mathbf{v}(x, t) : \Omega \times [0, T) \mapsto \mathbb{R}^2$ ,  $p(x, t) : \Omega \times [0, T) \mapsto \mathbb{R}$ , and  $\mathbf{S}(x, t) : \Omega \times [0, T) \mapsto \mathbb{R}_{\text{sym}}^{2 \times 2}$  such that

$$\operatorname{div} \mathbf{v} = 0, \quad (3a)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \nabla \mathbf{v} + \nabla p = \operatorname{div} \mathbf{S}, \quad (3b)$$

$$\frac{\partial \mathbf{S}}{\partial t} + \mathbf{v} \nabla \mathbf{S} + \mathbf{W} \mathbf{S} - \mathbf{S} \mathbf{W} - \varepsilon \Delta \frac{\partial}{\partial t} \mathbf{S} = \mathbf{D}, \quad (3c)$$

$$\mathbf{v}(x, 0) = \mathbf{v}_0, \quad (3d)$$

$$\mathbf{S}(x, 0) = \mathbf{S}_0. \quad (3e)$$

Let us now define a weak solution and state the main result.

**Definition 1.** Let  $\Omega \subset \mathbb{R}^2$  open. Let  $\mathbf{v}_0 \in L^2_{0,\operatorname{div}}(\Omega)$  and  $\mathbf{S}_0 \in L^2(\Omega)$ . Then the couple

$$(\mathbf{v}, \mathbf{S}) \in L^\infty(0, T; W^{1,2}_{0,\operatorname{div}}(\Omega)) \times L^\infty(0, T; W^{1,2}(\Omega)) \cap L^2(0, T; W^{2,2}(\Omega))$$

with  $\frac{\partial \mathbf{v}}{\partial t} \in L^1(0, T; (W^{1,2}_{0,\operatorname{div}}(\Omega))^*)$  is called a global weak solution to the system (3) corresponding to data  $\mathbf{v}_0$  and  $\mathbf{S}_0$ , if

$$\int_{\Omega} \frac{\partial \mathbf{v}}{\partial t} \boldsymbol{\varphi} \, dx + \int_{\Omega} (\mathbf{v} \cdot \nabla \mathbf{v}) \boldsymbol{\varphi} \, dx = - \int_{\Omega} \mathbf{S} : \mathbf{D}(\boldsymbol{\varphi}) \, dx \quad \forall \boldsymbol{\varphi} \in \{C_0^\infty(\Omega \times (-\infty, T))^2, \operatorname{div} \boldsymbol{\varphi} = 0\}, \quad (4a)$$

$$\begin{aligned} \int_{\Omega} \frac{\partial \mathbf{S}}{\partial t} \boldsymbol{\Sigma} \, dx + \int_{\Omega} \mathbf{v} \nabla \mathbf{S} : \boldsymbol{\Sigma} \, dx + \int_{\Omega} \mathbf{S} \mathbf{W} : \boldsymbol{\Sigma} - \mathbf{W} \mathbf{S} : \boldsymbol{\Sigma} \, dx \\ + \varepsilon \int_{\Omega} \nabla \frac{\partial \mathbf{S}}{\partial t} : \nabla \boldsymbol{\Sigma} \, dx = \int_{\Omega} \mathbf{D} : \boldsymbol{\Sigma} \, dx \quad \forall \boldsymbol{\Sigma} \in \{C_0^\infty(\Omega \times (-\infty, T))^{2 \times 2}\}, \end{aligned} \quad (4b)$$

**Theorem 1.** *Existence of Weak Solution.* There exists a global weak solution to the problem (3) such that (4) is satisfied.

Moreover we show the local-in-time existence and global existence for small initial data of a weak solution to the  $\Delta \mathbf{S}$ -regularised system. The proofs rely on the logarithmic Sobolev inequality and second order a priori estimates. The key inequality reads as follows.

Let  $f \in W^{s,p}$  for  $n < sp$ , then

$$\|f\|_{L^\infty} \leq C \left( 1 + \|\nabla\|^{\frac{n}{p}} f\|_{L^p} (1 + \ln(e + \|f\|_{W^{s,p}}))^{1 - \frac{1}{p}} \right).$$

For  $n = p = s = 2$  we obtain Brezis–Gallouet inequality, see [22]

$$\|f\|_{L^\infty} \leq C \left( 1 + \|\nabla f\|_{L^2} (\ln^+(\|f\|_{W^{2,2}}))^{1/2} \right),$$

where  $\ln^+ = \begin{cases} 1 & \text{for } x < e \\ \ln x & \text{for } x \geq e \end{cases}$ .

## 4 Numerical methods and simulations

Numerical analysis of the derived models is based on the Finite Element Method. In Chapter 3 we give a thorough description of the numerical methods used in the dissertation. To start with we provide a brief overview of Crystal Plasticity Finite Element Method together and methods dedicated to visco-elastic problems is given. We recall necessary tools in order to discretize the fluid in model of crystal plasticity both in space and time, such that: triangulation of a domain, proper finite dimensional spaces and time discretization schemes. The discrete system resulting from the weak formulation of the considered system is solved by means of the Newton's method. Also the discussion on the choice of finite elements focuses on velocity-pressure-stress triples, that satisfy the stability condition is provided. Moreover, we cover an Arbitrary Lagrangian Eulerian (ALE) method. The crystal plasticity equation are reformulated in ALE coordinates, which enables us to solve free boundary problems in time-varying domains. We formulated a finite element discretization schemes, which has been used to solve the fully coupled problem. Our solver is monolithic.

Finally, in Chapter 4 the results of performed numerical simulations are discussed in detail. We present three numerical examples: channel-die compression, micropillar compression, and 2-turn equal channel angular extrusion. The first two settings refer to experimental studies and are dedicated to comparison of the results, see [23, 24].

In the case of compression the Arbitrary Lagrangian Eulerian (ALE) approach has been used in the sense that we use the Eulerian formulation on a moving mesh which captures the free boundary. The results of channel-die compression simulations are in agreement with experimental observations. Our model predicts that the lattice reorientation of the single crystals of various initial crystallographic orientations tends to bring the crystals toward the geometry coincided with a stable state of symmetric slip. The simulations in the case of symmetric double slip lead to the formation of the shear bands. The method is able to reproduce a solutions obtained by Lagrangian based methods, and exceed them to higher strains.

The 2-turn ECAP is a novel computational example, motivated by papers of Rosochowski and Olejnik, [25, 26]. 2-turn channel enables us to introduce high strains within one ECAP pass. For this setting the introduction of the elastic stretches was important. They allow us to reduce high values of stress in the vicinity of inner turns.

Since our method is based on Eulerian formulation we proved that it is capable of solving deformations with very large strains for suitably defined problems, in particular in the case of compression we are able to cover nominal strain up to 0.4. The reason is that the priority is not the displacement and the strain but the velocity of the material flow and the distortion of the crystal lattice space. All numerical computations are performed for system describing crystal plasticity in Eulerian coordinates and we solve fully coupled problems. The computational results where published in [27, 28].

Numerical methods described in the thesis are implemented as a FEniCS based Python module, see [29, 30]. We use following linear algebra backends: PETSc - Portable, Extensible Toolkit for Scientific Computation and MUMPS: a MULTifrontal Massively Parallel sparse direct Solver.

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