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# TOWARDS COUPLED FINITE ELEMENT MODELING OF GRAIN GROWTH WITH PLASTICITY

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ABSTRACT

The purpose of this work is the finite element formulation of diffuse interface (continuum) model for the grain growth. Strategies for spatial (staggered/monolithic) and time (implicit/explicit) discretizations will be discussed and numerical results will be presented.

## INTRODUCTION

During industrial hot forming processes such as e.g. extrusion, hot rolling, or hot forging, materials undergo both mechanical deformation and recrystallization. Usually both phenomena influence each other in a complicated way, and it is exactly this influence of recrystallization on a material's ductility and strength that effects the appeal of a hot forming method.

The purpose of this work is (i) the formulation and application of a continuum field approach to the phenomenological modeling of the behavior of technological alloys undergoing recrystallization (grain growth-coarsening) and attendant plastic deformation and (ii) development of reliable numerical schemes for solution of arising coupled mechanical-grain growth models using finite element techniques [1]. At the current stage only the results for the grain growth are presented.

The interface between two phases on the atomic scale is a “mushy” one. Usual approach to model interfaces on the meso scale is to use a sharp interface model. This kind of the problem statement might be numerically quite complicated because one must impose boundary conditions on the moving interface. Contrary to this, here a relaxed (or diffused over a finite width) interface is employed (Fig. 1).

With the help of so called phase field[2,3], a field defined on the whole domain of the simulation and serving as a relaxed characteristic function and volume fraction for each phase, one can distinguish between different phases. It should be mentioned that the term “phase” here might be treated not only as a physical phase, but also in any other context. Particularly for the application in grain growth phase fields are used to describe grain orientations and consequently grain boundaries.

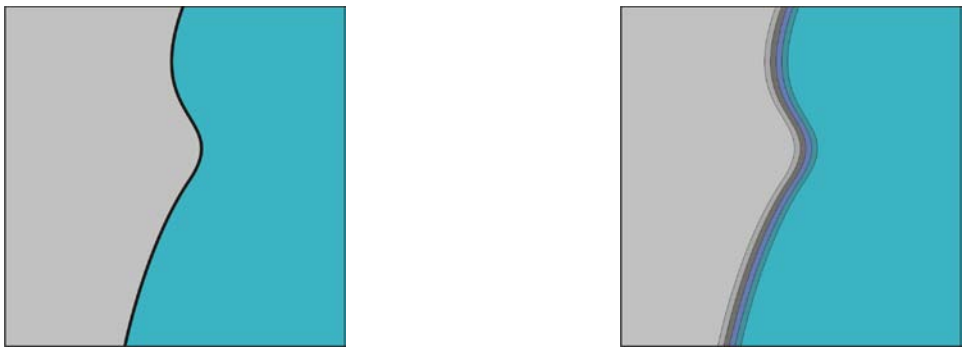

*Fig. 1 Sharp (left) vs diffuse (right) interface*

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## 1. MODEL FORMULATION

In this work a grain growth model developed in [4] is employed. This model utilize diffuse interface approach where each grain orientation is described by a separate relaxed characteristic function – a phase field, which is a function of space and time. Then Cahn-Allen type partial differential equations are derived for the evolution of phase fields:

$$\dot{\phi}_i = -L_i \left( -\alpha\phi_i + \beta\phi_i^3 + 2\gamma\phi_i \sum_{j\neq i}^{p} \phi_j^2 - \kappa_i \nabla\cdot\nabla\phi_i \right), \quad i = 1, 2, ..., p, \tag{1}$$

where $\phi_i$ is a phase field indicating the $i^{th}$ grain orientation, $p$ is a total number of grain orientations under considerations, $L_i$ are relaxation coefficients, $\kappa_i$ are gradient energy coefficients and $\alpha, \beta, \gamma$ are positive constants. Following[4] $\alpha = \beta = \gamma = L_i = 1$, $\kappa_i = 2$ and simplified model equations are:

$$\dot{\phi}_i = 2\nabla\cdot\nabla\phi_i + \phi_i \left( 1 + \phi_i^2 - 2\sum_{j}^{p} \phi_j^2 \right), \quad i = 1, 2, ..., p. \tag{2}$$

Problem formulation must be competed with the initial and boundary conditions. Initial conditions are set to random values in range $(-0.001; 0.001)$ for all $\phi_i$ to emulate initially "liquid" phase. Then crystallization takes place and grain microstructure is formed. Boundary conditions are set to homogeneous Neumann, i.e.$\nabla\phi_i \cdot \mathbf{n} = 0 \,\forall\, i$.

## 2. NUMERICAL TREATMENT

Numerically the above stated problem (2) is solved using tri-linear finite elements in space and semi-implicit first order scheme in time. All calculations are performed in open source finite element library `deal.II` [5] and post-processed in `ParaView`. Details are presented in the following subsections.

### 2.1 Spatial discretization

In space the problem is discretized using Bubnov-Galerkin approach and its weak form is:

$$\int_\Omega \phi^* \dot{\phi}_i \, dx = -\int_\Omega 2\nabla\phi^*\cdot\nabla\phi_i - \phi^*\phi_i \left( 1 + \phi_i^2 - 2\sum_{j}^{p} \phi_j^2 \right) dx, \quad i = 1, 2, ..., p, \tag{3}$$

where $\Omega$ is domain under consideration and $\phi^*$ is a test function.

There are two possibilities to discretize this problem in space: monolithic and staggered. Monolithic approach leads to definition in each finite element node $p$ degrees of freedom (DOFs), what in the final end leads to enormous system matrix size and makes problem numerically non-treatable. Staggered scheme leads to definition of only $p$ scalar finite element fields and sequential update of them. This scheme is employed here and actually written in the equation (3).

### 2.2 Time discretization

Explicit time discretization for a problem (3) leads to very small time steps. On the other hand fully implicit scheme leads to very long computation times due to re-assembly of the system matrix on each step and Newton-Raphson procedure. In this work semi-implicit scheme is used. In this case only linear part (mass matrix and discrete Laplacian) are sought in the new time step and the local nonlinear part is taken from the previous time step. This formulation allows firstly to build up system matrix only once and use it for all time steps and secondly to avoid Newton-Raphson iterations:

$$\int_\Omega \frac{1}{\Delta t}\phi^*\phi_i^{t+1} + 2\nabla\phi^*\cdot\nabla\phi_i^{t+1} \, dx = \int_\Omega \phi^*\phi_i \left( \frac{1}{\Delta t} + 1 + \phi_i^2 - 2\sum_{j}^{p} \phi_j^2 \right) dx, \quad i = 1, 2, ..., p, \tag{4}$$

where $\phi_i^{t+1}$ is unknown solution on the new time step, $\phi_i$is solution from the previous time step and $\Delta t$ is time step.

### 2.3 Numerical results

For numerical simulations following parameters were taken: $\Omega = [0, 200]^3$, $N_{elements} = 100^3$, $\Delta t = 0.5$, $t_{final} = 200\Delta t$, $p = 30$ (all dimensionless). On Fig. 2 two snapshots of the numerical solution are shown.

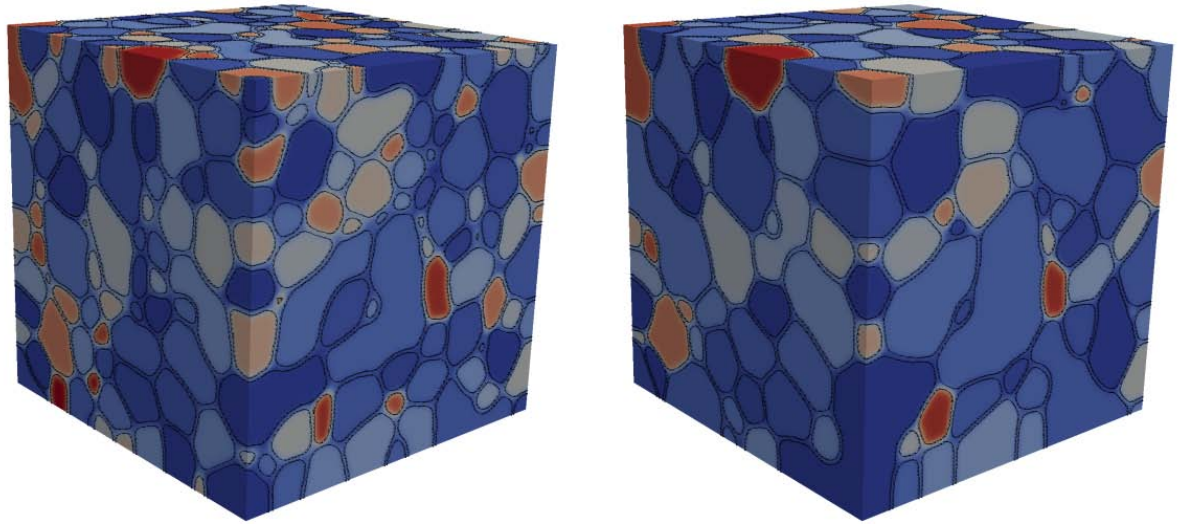

*Fig. 2 Snapshots of the grain structure for $t = 50$ (left) and $t = t_{final} = 100$ (right)*

## CONCLUSIONS AND OUTLOOK

Model formulation and numerical results for a grain growth were presented. Results show appropriate qualitative behavior for a normal grain growth/evolution. Next step is a coupling of the multi phase field (MPF) grain growth model of [6] with large strain plastic behavior based on the continuum mixture theory[7] and development of numerical methods for solutions of such problems. Several attempts in this direction were already reported mainly limiting to the case of small-strain plasticity. But to develop models for a case of large strain inelasticity we would like to describe the mechanical structure in the framework of a thermodynamic, internal-variable-based formulation in which the deformation and temperature are in general coupled[8]. Coupling between the mechanical fields, phase-fields and the temperature field arises via the mechanical dissipation during the deformation process as well as by the spatial distribution of the areas of different phases being modeled by the order parameter.

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