PhD position at Mines ParisTech CNRS
Phase field and Cosserat simulation of recrystallization in polycrystals
2020-2023

Location : Centre des Matériaux Mines ParisTech, CNRS UMR 7633, PSL University
Funding : Contrat doctoral CNRS
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Wanted skills: Continuum mechanics, Computational mechanics, Mechanics of Materials
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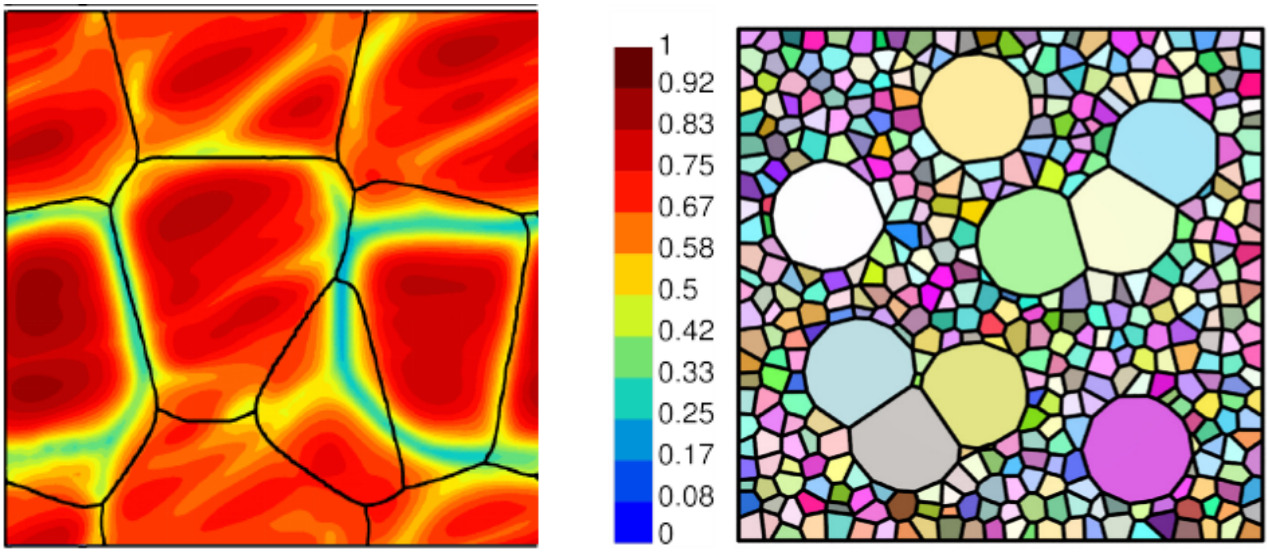

Champ de phase dont les valeurs minimales sont atteintes dans les joints de grains (à gauche) à l'aide du modèles de Cosserat-champ de phase (les traits noirs indiquent les joints de grains initiatux) après déformation par cisaillement du polycristal périodique. Microstructure synthétique de polycristal bimodal (à droite, utilisée par (Flipon et al. 2019) pour étudier le comportement mécanique).

Abstract : The objective of the project is to develop the most recent multi-scale methodologies from physical metallurgy and continuum mechanics in order to contribute to the design of bimodal microstructures, i.e. with two populations of distinct grain sizes, of metal alloys with high work hardening and sufficient ductility. The mechanisms involved are grain growth and recrystallization induced by the energy stored in polycrystals due to plastic deformation. The proposed approach combines Cosserat media mechanics applied to crystal plasticity with the phase field method suitable for mobile interface modeling. The three-field theory (displacement, crystal orientation, crystal order) will be informed by atomic simulations of grain boundary properties. Validated in the case of harmonic microstructures available at the GPM of INSA Rouen, the approach will be extended to hexagonal alloys to take advantage of their strong anisotropy. Numerical simulations will be carried out in 2D and 3D using the nonlinear finite element method.

Keywords: Polycristal, Crystal plasticity, Recrystallization, Grain growth, Cosserat mechanics, Phase field method, Bimodal microstructure, Grain boundaries, Finite Element Simulation

State of the art: Microstructural engineering has developed considerably over the last twenty years by relying on grain size refinement processes and by playing on their morphology: nanocrystalline grains (Meyers et al., 2006) and lamellar or wire structures (Thilly et al. 2002, Gu et al. 2019). Produced by powder

metallurgy, severe deformation or hyper-deformation, these materials reach unprecedented elasticity limits but generally suffer from low ductility. More recently, so-called harmonic microstructures have been designed to combine hardening and ductility by associating two grain populations, in terms of size and spatial distribution: a "matrix" of fine grains hardening the material, and coarse grains improving ductility by supporting most of the plastic deformation. Since the first works proposing this type of material (e.g. Jin et al. 2004, and Srinivasrao et al. 2008), most studies have focused on metals and alloys with a cubic structure (Guo et al. 2017). These materials are generally produced by powder metallurgy involving a grinding step prior to sintering (e.g., by SPS) or by severe plastic deformation (SPD). In both cases, the grain growth and recrystallization steps are essential for the genesis of the bimodal microstructure. Finally, it appears that the behaviour is sensitive to the preferred crystalline orientations of the grains as well as to the spatial distribution of large grains within the fine grain matrix (Mompiou et al. 2018, Flipon et al., 2019). Understanding the deformation modes of these bimodal polycrystals requires finite element calculations of their plastic deformation using the laws of crystal plasticity, calculations recently performed by (Wang et al. 2019, Flipon et al. 2019).
At the atomic scale, the study of the structure of grain boundaries, their static (energy) and dynamic (mobility) properties has progressed considerably since the first numerical work of Sutton et al. (1983). Interatomic potentials have become more reliable thanks to their parameterization using DFT results and machine learning techniques (Zhang et al. 2015). Massively parallel molecular dynamics codes allow to perform calculations on many grain boundary configurations by scanning the geometrical parameter space (Frolov et al. 2013). In parallel, molecular dynamics has been used to determine the mobility of grain boundaries for a smaller number of configurations (Hoyt 2014). These atomic scale studies concern cubic metals and alloys, with the exception of a study on symmetrical bending joints for hexagonal materials (Wang et al. 2012).
The design of new optimal microstructures requires the modelling of grain growth and heterogeneous recrystallisation. The full-field simulation of these phenomena has progressed significantly, first through cellular automata or vertex methods, then through level line approaches (Bernacki et al. 2009, Ilin et al. 2018) or phase fields for monitoring grain joints and multiple junctions. The latter approaches have the advantage of being able to be coupled to the mechanical behaviour involving competition between the energies and curvature of grain boundaries and the energy stored by dislocations resulting from deformation (Abrivard et al. 2012, Kamashali et al., 2015). Phase field methods are based on a thermodynamic formulation and thus allow the integration of the different physical contributions recorded in the free energy potential and the dissipation potential. Among the phase field models applied to growth and recrystallization, a distinction must be made between the so-called multi-phase field approaches, due to I. Steinbach, assigning one phase field per grain, and the 2-field, crystal orientation and crystal order parameter (minimum in grain boundaries) approaches based on the Kobayashi-Warren-Carter (KWC) model. The latter are the only ones capable of describing the orientation gradients induced within grains by deformation and likely to develop into grain subgrains or even nuclei of new grains. They have recently been coupled with crystalline plasticity (Ask et al. 2018, 2019, Admal et al. 2018, 2019).
Such methods have not yet been applied to the design of harmonic microstructures.

Scientific challenges: Two main challenges have been identified. The first is the representation and determination of jograin boundary energies and associated anisotropy. So far, isotropic functions have been used by (Ask et al. 2019) which only account for Read-Shockley type relationships. A 5-variable representation (relative orientation between the two grains, normal to the grain boundary) has been addressed by (Admal et al. 2019). It remains to identify such a parameterization in the case of metals with marked anisotropy, such as hexagonal. The methods of exploration of this 5-dimensional space nowadays use kriging or genetic algorithms. Similar difficulties are encountered concerning the mobility of grain joints and the quantification of stored energy.
The second hurdle is that the current field of use of physical models of recrystallization of the KWC class is limited: small rotations, small curvatures, low number of grains, two-dimensional simulations, insufficient consideration of crystallographic textures, role of temperature. The results obtained to date are qualitative and rather modest due to the strong non-linearities of this class of models and the insufficient knowledge of the energies involved.

The **objective of the project** is to propose a Cosserat phase field formulation capable of simulating grain growth as a function of strong deformation heterogeneities within grains and from grain to grain, and of the anisotropy of grain boundary energies. The Cosserat model reconciles the KWC approach with mechanics

(Ask et al. 2018) while the phase field describes a diffuse and mobile grain boundary as a function of lattice curvature and local dislocation densities. The stress tensor is non-symmetrical in this theory and the non-symmetrical part is treated as the driving force of crystal reorientation within the diffuse grain boundary. The interdisciplinary character of the project lies in this combination of the most advanced thermodynamic, metallurgical and mechanical approaches, mixing order parameters, crystallography and mechanical variables of elasto-visco-plastic behaviour. The project brings together physical concerns as well as those of the engineer concerned with the forming and strength of industrial alloys. The sustainable pooling of skills in physical (phase fields) and mechanical (plasticity, fracture) simulations is necessary today to propose a new, more fundamental treatment of the engineer's problems, such as the shaping or lightening of structures, for example. The proposed class of models is attractive because of the clear physical content of the different variables involved, but has not been applied to date to realistic microstructures of the engineer's materials (3D polycrystalline aggregates, high strain rates). The exploratory nature of the project then consists in evaluating the robustness of the approach with respect to the increasing level of requirement in terms of the physics represented and the realism of the microstructure. It is at this price that the tool can be inserted in a microstructure optimization approach.

Methodologies to be implemented: Four stages are distinguished in the project, some of which will be carried out in parallel:

1. Determination of grain boundary energies for hexagonal systems

Atomic scale calculations will be performed combining DFT and empirical atomic potentials for grain boundary energies in Ti, Zn or Mg (depending on the difficulty). They will be performed at the IJL institute, in parallel with the mesoscopic calculations to start building a bank of grain boundary energies that can then be used in the mesoscopic model. The interatomic potentials from the literature most suitable for the study of hexagonal metals will be selected by comparing their predictions of the most relevant quantities for the study of grain boundaries with DFT calculations on a few judiciously chosen configurations (Tamura et al. 2017). An automatic learning technique will be used to scan the space of the five geometrical parameters characterizing the grain boundaries. After the construction of the energy landscape of grain boundaries, the description of the grain boundaries by their atomic structure (Gomberg et al. 2017) will be linked to the order parameter of the phase field.

2. Numerical platform for Finite Element and FFT simulation

A finite element formulation of the Cosserat model is available in Zset code (http://www.zset-software.com) for small deformations, small rotations and curvatures, in 2D. The extension to the 3D case and to large finite element deformations and misorientations is ambitious but indispensable. The difficulty lies in the treatment of finite rotations, a delicate problem well known for example in the mechanics of shells. In order to ensure the extensibility of the approach to the case of realistic microstructures with a sufficient number of 3D grains, an implementation of the Cosserat model in a FFT code will also be carried out.

3. Numerical characterization of the critical strain-hardening concept

A key to obtaining bimodal microstructures is the ability to control levels of stored energy allowing certain classes of grain to grow at the expense of other grains. This requires mastery of the basic concept of critical strain hardening at a given temperature, i.e. a strain level leading to rapid growth in areas that are sufficiently deformed according to the mobility parameters of the grain joints and dislocation densities. Tensile simulations of trapezoidal specimens will be carried out to determine, as is done experimentally, the level of critical strain-hardening predicted by the model.

4. Link between localization of plastic deformation and recrystallization nucleation

In microstructure optimization, recrystallization is the second lever after growth. The germination of new grains is often considered as a random and sometimes mysterious process. We believe that the proposed approach is able to predict the spontaneous germination of new grains in areas of strong localization of network deformation and curvature, for example at the intersection of shear bands. Elementary situations will be studied in large deformation in grain undergoing strain localization. They will be followed by a digital heat treatment to observe the germination of new grains, places of intense recovery by scanning through subgrain boundaries formed locally by the localization of the curvature. Stability studies of certain elementary configurations will also be carried out in a semi-analytical manner to monitor the germination mechanisms in the proposed complex approach.

Expected results: The expected product is first of all a mesoscopic model of growth and recrystallization valid for the engineer's material grain sizes (from a few microns to mm), with information on grain boundary energies and stored energy induced by the deformation. It will be parameterized by the temperature to predict

a local critical strain hardening in order to optimize the recrystallization heat treatments. This is an important step forward compared to the current physical modelling, which is still rudimentary.
The expected results also include simulations of bimodal structures in the cubic case based on experimental and numerical results available at INSA Rouen in F. Barbe's team within the GPM. The fields of orientations available before and after heat treatments will allow us to carry out first calculations of privileged growth of certain aggregates. Comparisons with experiments already carried out will concern growth kinetics and grain size ratios between the two modes. Simulations will be first two-dimensional and then three-dimensional.
The expected results will then concern similar simulations in the case of metals or alloys of hexagonal structure. The anisotropy of growth and deformation will constitute a greater degree of freedom allowing to play not only on the size of the grains obtained but also on their morphology: ellipsoidal or even lamellar grains.
A framework for optimizing microstructures will finally be formulated in terms of bimodal morphology maps as a function of dislocation densities, grain boundary energies and temperature. These maps will serve as a basis for an optimization approach for which a reduced base or a meta-model will be necessary due to the numerical cost of individual microstructure calculations.

The involvement of the teams:
Mines ParisTech: The PhD student, S. Forest and K. Ammar, in close cooperation with Anna Ask (ONERA), will contribute to the development of the theory and its implementation in the Zset finite element code. They will also work on the parameterization of the model thanks to the results obtained at the IJL and data from the literature. They will contribute to the setting up and realization of numerical simulations that will be carried out on the Mines ParisTech cluster as well as the ONERA cluster.
University of Lorraine (IJL): B. Appolaire and M. Cottura will work, on the one hand, on atomic scale calculations for the determination of surface energies and, as far as possible, interface mobilities, and, on the other hand, on the FFT numerical formulation of a simplified version of the model in order to increase the efficiency of calculations for larger grain populations.
ONERA (DMAS): Anna Ask, following her post-doc Marie Scklodowska-Curie at the Materials Centre, masters and develops the coupled Cosserat-phase model in close cooperation with Mines ParisTech and IJL. She is a specialist in particular in the parameterization of the current model with respect to grain boundary energies. The project is structuring to efficiently pursue this cooperation with ONERA.
INSA Rouen Normandie (GPM): F. Barbe supervised the thesis of B. Flipon who worked on the development of 304 and 317 stainless steels with bimodal grain size distribution, in cooperation with CRISMAT, as well as on the finite element modelling of their mechanical behaviour, also characterised by mechanical tensile tests. It provides the project with a rich database in terms of grain sizes and proportions of grains of the same size. These data include EBSD characterizations that can be directly used for project simulations. F. Barbe will bring to the project the knowledge of the behaviour of these materials as well as the guides for the choice of treatments adapted to the elaboration.

Doctoral student's mission: The role of the doctoral student is central to the project because of the significant work and the theoretical and numerical synthesis to be carried out. S. Forest and B. Appolaire will be the thesis co-directors, Anna Ask and Kais Ammarwill be the official co-supervisors. The role of the doctoral student will consist in :
1. Develop a 3D finite element in finite deformations for a Cosserat medium coupled to the phase field. It will be based on the theory proposed by (Ask et al. 2019) and will extend it to integrate the temperature dependence of the parameters involved. It will set up a cooperation between Mines-IJL-ONERA to stabilize a robust formulation of the model. In consultation with the IJL, the PhD student will propose validation tests for comparison with the FFT numerical model developed at the IJL. If necessary, he/she will be able to perform calculations with this simulation tool.
2. Perform the junction with the results obtained at the IJL on grain boundary energies.
The identification of grain boundary energies for FCC and hexagonal crystals will be the subject of close cooperation with the IJL. It will be carried out on the basis of multi-scale data from the literature and atomic calculations performed at the IJL.
3. To demonstrate the capability of the modelling to account for the concept of critical strain hardening.
The PhD student will examine, with the help of theoretical and numerical analyses, whether the model as it stands is able to account for this key concept of recrystallization. If necessary, adapted constitutive laws will be developed.

4. To simulate the development of bimodal microstructures in the case of stainless steels.
The PhD student will benefit from the database of bimodal steels developed during B. Flipon's thesis and whose textures and mechanical behaviour have been characterized. He will exchange with F. Barbe from INSA Rouen.
5. Explore the approach proposed in the case of hexagonal metals.
With the developed tools, the PhD student will then be able to explore an additional lever, i.e. the optimization of grain morphology in addition to grain size. By playing on the strong anisotropy of hexagonal metals, a bimodality of morphology (spherical grains vs. ellipsoidal or lamellar grains) is expected.

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