5.3 Numerical materials

A. Context

What are the evolutions of microstructure induced by forming and heat treatment operations? How can one model them? What are the appropriate lengthscales? What are the different strategies to build a bridge between the different scales?

Through the development of numerical methods dedicated to multiscale modeling and high performance computing in material sciences, the CEMEF tries to provide new answers and methods to these different questions. Furthermore, all these numerical techniques enable to build, to structure and to improve the scientific finite element library (CIMLib) developed by the CEMEF. CEMEF is a research center of MINES ParisTech located in Sophia Antipolis and dedicated to materials processing. About 150 persons including more than 60 PhD students are working at CEMEF on essential topics for the understanding of forming processes for all types of materials, and in close collaboration with industrial partners. CEMEF has notably a worldwide recognized expertise in numerical modeling of materials and related processes.

It is well known that the micro (or nano) structure of materials is a key factor for determining the constitutive law during forming and for predicting the final properties of the work-piece. To treat in an average way, the evolution of the material microstructure during thermal and thermomechanical treatments, the classical method, well known as "mean field approach", consists in fact in a macro description, selecting representative material parameters (grain size, inclusions, phase percentage, precipitates, porosities, etc.) and to identify physical laws which govern the evolution of these parameters, and their influence on the mechanical behavior. The macro approach is quite convenient for coupling thermal, mechanical and physical computation, but it suffers severe limitations and needs a large amount of experiments to identify the physical laws describing microstructure evolution.

On the other hand, computation at the microscale is now possible and is developed for a potentially more realistic description of materials under the concept of "full field approach". Nowadays, mesoscale modeling is then a crucial realm in materials science.

Success in the integration of multiscale modeling activities requires an effective means to organize the data that defines structure, its variability over many scales, to model accurately the physical mechanisms of interest and to develop the *ad hoc* numerical strategies. These requirements are addressed using a modeling system referred as the Digital/Numerical Materials. Thanks to the explosion of computer capacities, mesoscopic modeling techniques for materials are now available. Future of materials will also be numerics.

B. Current activity

First research axis concerning the modeling of microstructure at the mesoscopic scale concerns the ability to be representative, with real description or statistical one, of the microstructures of interest through the concept of Representative Volume Element (RVE). We develop accurate numerical tools to generate complex 2D and 3D statistical virtual microstructures or to immerse experimental data in finite element (FE) mesh. These techniques, based on mathematical morphology, capturing methods (level-set or phase field description of the interfaces) and anisotropic meshing adaptation was validated for some RVEs. The methodology developed in terms of virtual generation, implicit description of the interfaces and meshing adaptation, is now used, as illustrated in Figure 1, for a large variety of applications as polycrystal [1-3], granular semi-solid [4], foam, powder [2][5], heterogeneous microstructures with particles and voids in a metallic matrix [6-7], polymer composites... Moreover constant work concerning this topic concerns the minimization of the numerical cost. As illustrated, this numerical tools are generic and could be used in the *C4P0* project to describe a large variety of objects at different scales **(cf Themes 5.4-5.5-11.6).**

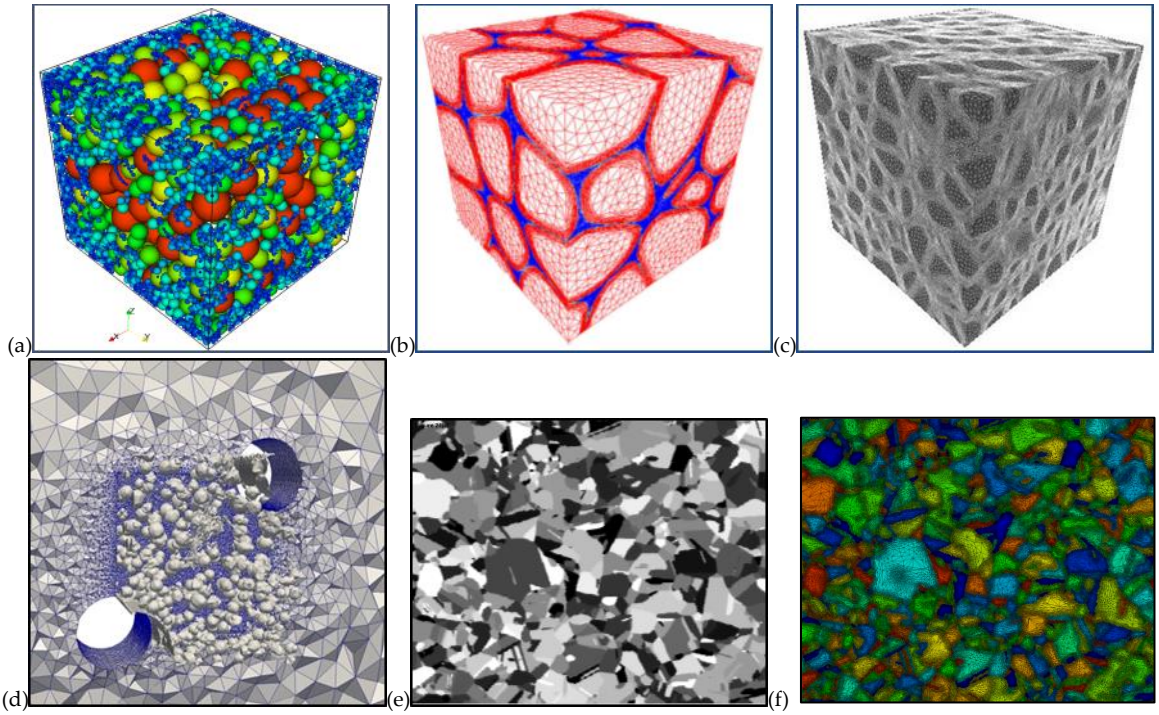

Figure 1. Some RVEs respecting initial statistical data: (a) a 304L powder, (b) semi-solid granular with liquid in blue, FE mesh is anisotropically adapted to the interfaces, (c) 304L polycrystal with anisotropic finite element mesh in white, (d) immersion of a real microstructure of a metallic composite, (f) 2D FE immersion of a SEM image of a polycristal described in (e).

Mechanical and functional properties of materials are strongly related to their microstructures, which are themselves inherited from thermal and mechanical processing. For example, fatigue resistance is a critical attribute that is affected by the heterogeneity of the grain size distribution for metals. Hence, the understanding, the predicting and so the modeling of microstructure evolutions during thermomechanical treatments are of prime importance in a theoritical point of view but also for industrial applications. This aspect is definitely a cornerstone of the innovation concerning the future materials and the main problematic of the numerical materials realm.

This second research axis undermines the development in context of HPC of full field numerical strategies in order to describe a wide range of dynamic microstructural mechanisms and, secondly, the development of a powerful multiscale strategy in order to develop more and more accurate main field models. These aspects constitute the main activities of the Numerical Materials team. Thus an important number of numerical methods dedicated to interfaces tracking or capturing problems at the microscopic scale (level set, phase field, stochastic approaches, discrete methods) are developped.

Moreover, collaboration with other teams is essential in order to perform well designed experiments with the aim of deriving physically consistent models and of validating the previous numerical developments (cf Theme 5.2). Figure 2 and Figure 3 illustrated some recent concrete applications concerning the modeling of microstructure evolutions thanks to front-capturing/front tracking methods and *ad hoc* meshing/remeshing ability:

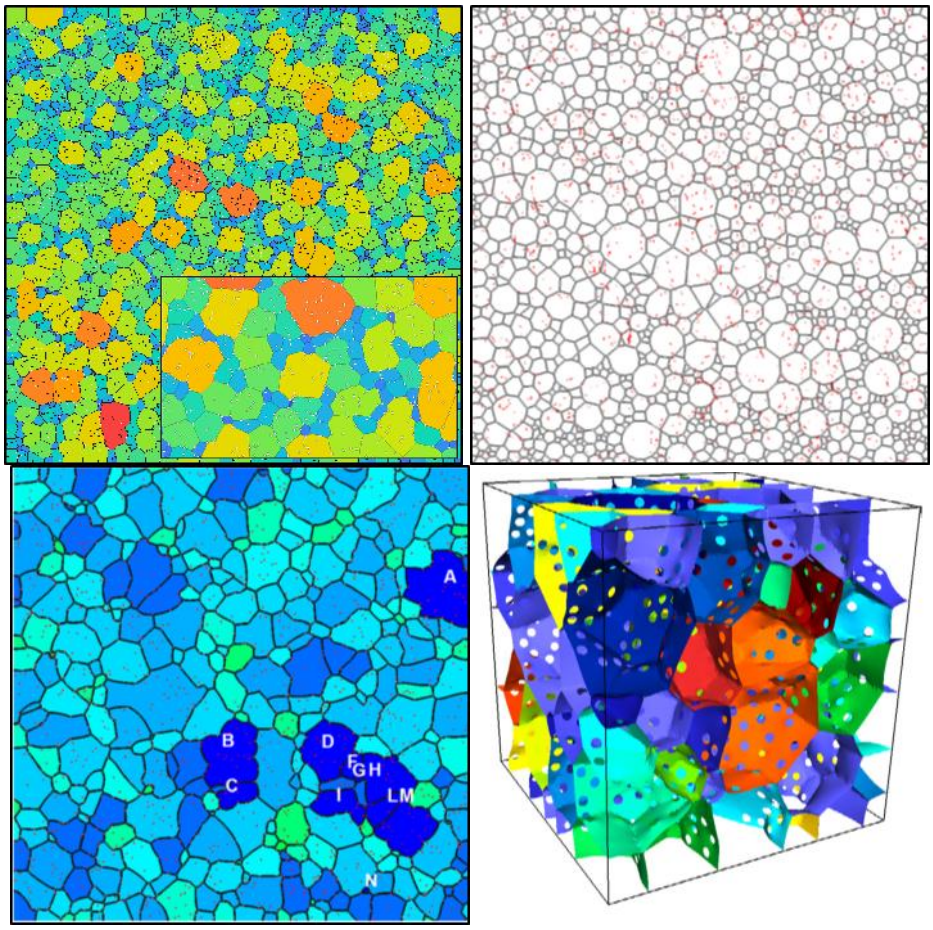

Figure 2. Level Set modeling of grain boundary motion during annealing of a Inconel 718 sample: (a) 2D grain growth, pinned microstructure [8] - (b) 2D grain growth with real shape of second phase particles (SPP) [9] -- (c) 2D grain growth with stored energy, abnormal grain growth configuration [10] - (d) 3D pure gain growth for few grains and spherical SPP, pinned microstructure [3].

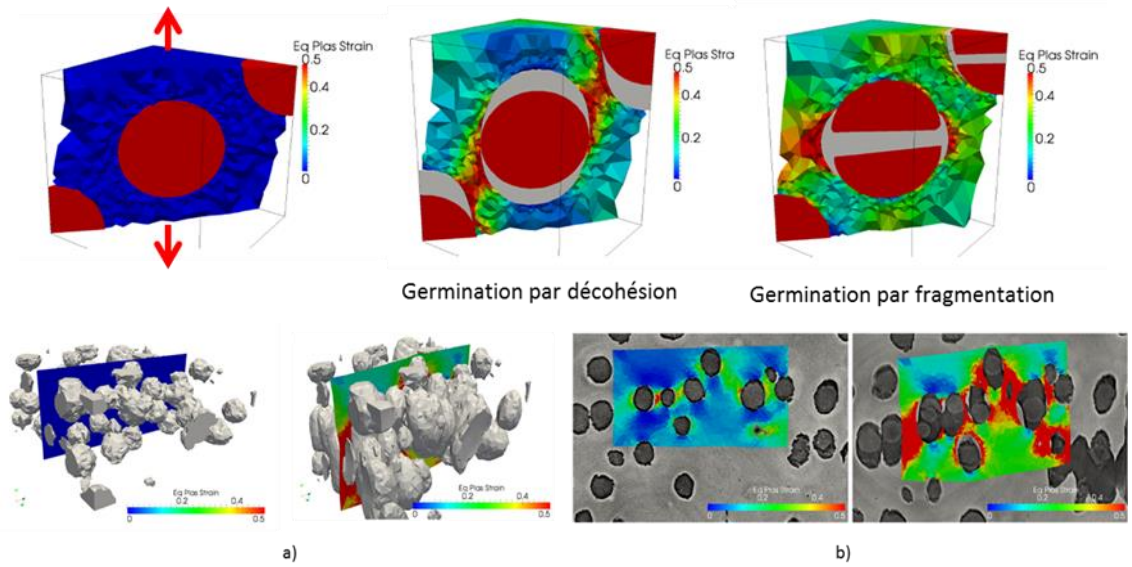

Figure 3. Application in ductile damage prediction at the microscale (cf Theme 11.1): (top) 3D full field modeling of nucleation mechanism by interface debonding or particle failure in a 3D microstructure and (bottom) 3D computation on nodular cast iron microstructure with boundary conditions coming from digital volume correlation and superimposition of numerical simulation strain field and laminography pictures at two loading steps.

The full field numerical models for simulating recrystallization phenomena and predicting the microstructure obtained after a given thermomechanical path are in addition implemented into a **software package**: DIGIMU® **[11]**. This package software is being developed at CEMEF in cooperation with a large industrial consortium :

This brief description of some results could be completed by another realized developments concerning modeling of microstructural evolutions at the RVE scale. In fact, all these developments converge toward the same objectives, i.e. to provide a set of numerical tools in order to improve macroscopic models thanks to simulations realized at the microscopic scale but also to provide a better understanding of heterogeneous microstructural evolutions which can not be predicted by mean field approaches.

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[8] B. Scholtes, D. Ilin, A. Settefrati, N. Bozzolo, A. Agnoli, and M. Bernacki. *Full field modeling of the Zener pinning phenomenon in a level set framework - discussion of classical limiting mean grain size equation*. Accepted in proceedings of the 13th International Symposium on Superalloys, 2016.
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[11] *https://www.transvalor.com/fr/cmspages/digimu.86.html*

C. Future steps

Future developments aim at improving numerical efficiency, implementing new models and methods to allow for representing more and more complexe (*i.e.* realistic) microstructures and physical mechanisms. Some of those developments will be made thanks to the support of the DIGIMU industrial consortium. Moreover, we hope to get a positive answer to the ERC grant proposal submitted in 2016, which would allow faster developments.

D. International collaborations

Our main academic collaborations abroad are briefly listed below with names and topics :

- **Carnegie Mellon University (USA)**: collaboration with Prof. A.D. Rollett and Prof. G.S. Rohrer**.** Characterization of grain boundary character distributions. 3D data for full field modeling.
- **EPFL (Switzerland):** collaboration with Prof. R.E. Logé**.** Mean field modelling and full field modeling of recrystallization phenomena.
- **CONICET (Argentina)** collaboration with Prof. J. Signorelli. Development of advanced methods for CPFEM calculations
- **LMT Cachan (France)**: collaboration with Prof. F. Hild (expert in DIC and DVC analyses) within the COMINSIDE ANR project dedicated to the understanding and modeling of ductile fracture at the microscale.
- **CdM Mines ParisTech (France)**: collaboration with Dr. T. Morgeneyer (expert in X-Ray laminography at ESRF) within the COMINSIDE ANR project dedicated to the understanding and modeling of ductile fracture at the microscale.
- **ENSAM Angers (France)**: collaboration with Prof. F. Morel on the modeling of shot-peening and its impact of steel fatigue properties.
- **Ecole des Mines de Saint-Etienne (France):** collaboration with Prof. F. Montheillet, Prof. G. Kermouche and Prof. D. Piot. Full field modeling of recrystallization.

E. List of people involved in the project

Permanent :

- Marc BERNACKI (Pr, Numerical Metallurgy)
- Nathalie BOZZOLO (Pr, Physical Metallurgy)
- Pierre-Olivier BOUCHARD (Pr, Numerical Metallurgy)
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- Charbel MOUSSA (Assistant Pr, Mechanical Metallurgy)
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Engineers:

- Selim KRARIA (Computer Engineering)

Post-doc :

- Dmitrii ILIN (Full field modelling of crystal plasticity)

PhD :

- Benjamin SCHOLTES (Development of the DIGIMU software)
- Danai POLYCHRONOPOULOU (Full field modeling of globularisation in titanium alloys)
- Romain BOULAIS-SINOU (Full field modelling of dynamic recrystallization)
- Ludovic MAIRE (Coupling of mean filed and full field models)
- Modesar SHAKOOR (Numerical methods for failure of heterogeneous materials)
- Victor TREJO NAVAS (Ductile Fracture at Microscale)
- Abdelouahed CHBIHI (Model for modeling voids closure during hot metal forming)

- Fang LU (Full field modeling of polymer composites)

F. Most significant publications of the team

M. Bernacki, Y. Chastel, T. Coupez and R. Logé, Level set framework for the numerical modelling of primary recrystallization in polycrystalline materials. *Scripta Mat.* **58:12**, 1129-1132 (2009).

B. Scholtes, M. Shakoor, A. Settefrati, P.-O. Bouchard, N. Bozzolo, and M. Bernacki. New finite element developments for the full field modeling of microstructural evolutions using the level-set method. Computational Materials Science, 109:388–398, 2015.

Y. Jin, N. Bozzolo, A.D. Rollett, and M. Bernacki. 2D finite element modeling of anisotropic grain growth in polycrystalline materials: level set versus multi-phase-field method. Computational Materials Science, 104:108–123, 2015.

K. Hitti, P. Laure, T. Coupez, L. Silva and M. Bernacki, Precise generation of complex statistical represen- tative volume elements (RVEs) in a finite element context. *Comp. Mat. Sci.*, **61**, 224–238 (2012).

E. Roux, M. Shakoor, M. Bernacki and P.-O. Bouchard, A new finite element approach for modelling ductile damage void nucleation and growth – analysis of loading path effect on damage mechanisms. *Modelling and Simulation in Materials Science and Engineering*. **22**, 1-23 (2014).

M. Shakoor, M. Bernacki and P.-O. Bouchard. A new body-fitted immersed volume method for the modeling of ductile fracture at the microscale: analysis of void clusters and stress state effects on coalescence. *Engineering Fracture Mechanics*, **147**, 398–417 (2015).

M. Bernacki, R. Logé, and T. Coupez. Level set framework for the finite-element modelling of recrystal- lization and grain growth in polycrystalline materials. *Scripta Mat.*, **64 :6**, :525–528, (2011).

Short CV of the main participants

M. Bernacki, Professor in Numerical Metallurgy at CEMEF MINES-ParisTech. Expert in development of numerical methods and HPC in materials science. His Main activities concern the simulation of microstructure evolution during materials forming. Applicant for an ERC grant in 2016. Head of the "Numerical Materials" committee of the SF2M. Head of the research group "MultiScale Modelling".

N. Bozzolo, Professor in Physical Metallurgy at CEMEF MINES-ParisTech. Expert in quantitative analysis of microstructures and textures, identification of metallurgical mechanisms and recrystallization phenomena. Holder of the OPALE ANR-Safran industrial chair. Member of the national board of the French Society for Metallurgy and Materials (SF2M). Head of research group "Metallurgy, Structure, Rheology"

C. Moussa, Assistant Professor in Mechanical Metallurgy at CEMEF MINES-ParisTech. Expert in mechanical testing and mean field modelling of recrystallization phenomena in relation to the constitutive behavior. Member of research group "Metallurgy, Structure, Rheology".

P.-O. Bouchard, is Professor at Mines ParisTech and in charge of the Computational Mechanics and Physics department at the Center for Material Processing, Sophia-Antipolis. Laureate of the ESAFORM Scientific Prize in 2005. P.-O. Bouchard is expert in damage and fracture modeling at multiple scales. He is the coordinator of the French ANR project COMINSIDE (2014-2018). He is in charge of the MECAMAT association working group dedicated to “Physics and Mechanics of Damage and Fracture”. About 50 refereed publications.

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relation to the constitutive behavior. Member of the research group "Mechanical Physics of Industrial Polymers".

T. Toulorge, Assistant Professor at CEMEF MINES-ParisTech. Expert in numerical methods and advanced meshing techniques for finite element simulations. Member of the research group "MultiScale Modelling ".

D. Pino Muñoz, Assistant Professor at CEMEF MINES-ParisTech. Expert in mechanical metallurgy, powder metallurgy and finite element simulations. Member of the research group "MultiScale Modelling ".