DIGIMU®: 2D and 3D Full Field Recrystallization Simulations with Coupled Micro-Macro Approaches

Doctor.-Ing. P.O. De Micheli
Transvalor S.A. / Development Department

Doctor.-Ing. L. Maire
MINES ParisTech, PSL-Research University / CEMEF-Centre for Material Forming

Doctor.-Ing. C. Moussa
MINES ParisTech, PSL-Research University / CEMEF-Centre for Material Forming

Prof. N. Bozzolo
MINES ParisTech, PSL-Research University / CEMEF-Centre for Material Forming

Prof. M. Bernacki
MINES ParisTech, PSL-Research University / CEMEF-Centre for Material Forming

Abstract

Microstructural predictions, specifically in multi-pass processes, are very challenging due to the strong evolution of the microstructure topology from the beginning to the end of the process. Grain growth (GG) and recrystallization (ReX) kinematics are strongly depending on grains size and shape. Minor variations of the process parameters (wait-times, reheating, temperature) may have huge effects, due to combined dynamic recrystallization (DRX), postdynamic recrystallization (PDRX) with more or less nuclei, and recovery meachanisms. Analytical or phenomenological models dedicated to grain size prediction can rapidly reach their limit. The microstructure of the metal must be fully described and its evolution must be simulated with *ad hoc* physical laws.

Recent improvements in full field finite element microstructural simulations enable to model in reasonable CPU times the discussed phenomena and their coupling: realistic polycrystal generation, grain growth driven by capillarity and stored energy jumps at the boundaries, hardening, recovery, and nucleation. The ongoing collaboration between CEMEF MINES ParisTech, 8 renowned French industries and TRANSVALOR leaded to the commercialization of the robust and easy to handle solution DIGIMU®. In the following, a micro-macro approach coupling the use of FE packages FORGE® and DIGIMU® will be illustrated on two industrial-like processes, in 2D and 3D.

1 Introduction

The microstructural state of metallic parts plays a major role on in-use properties and on the mechanical behavior during metal forming. It becomes necessary to master grain size and dislocations density evolutions during forming processes to fulfill always more severe specifications and to address efficiently new markets. However, the main involved physical phenomena still are not completely mastered yet even if they have been studied for more than 60 years. Boundary migration, recovery and nucleation remain open research subjects and the overall evolution resulting from the combination of all those effects even more [1].

Three famillies of models are available to address this issue. JMAK-like models (Johnson-Mehl-Avrami-Kolmogorov) [2] follow directly the evolution of mean field values as the mean grain size, the mean recrystallized fraction, sometimes also the mean dislocation densities, and more. They are very appealing because their cost for a computation on a whole part is almost neglictible. Because of the low number of variables, they may be computed at each point of a process macroscopic FEM simulation, and coupled to the material behavior in macroscopic simulations. However, it is of first importance to realize that their ranges of validity are extremely limited because the kinetics of the microstructural evolution is strongly dependant on the microstructural arrangement, which is not fully represented by means values. A set of parameters can sometimes fit the first cycle of recrystallization of a process if the initial microstructure is comparable to the one of the samples used for the identification. However, for a different initial material state, a process with several cycles of recrystallization, or a multipass process with non negligieble waiting times, predictions can't be any more reliable.

To go further, some Mean Field (MF) models follow a population of grains [3]. Even if the arrangement between the grains is not explicitely represented, the evolution of each grain is modelled by using more physical laws, and then mean values are deduced. In this case, a set of parameters is more independent of the grain size and arrangement. Following longer processes with several cycles of recrystallization becomes possible. The computation cost remain low enough to perform rapidly computations on a large number of specific points of the part, but the very high number of variables makes a computation at each integration point of a macroscopic process simulation impossible. It is then not possible to couple this model with the mechanical behavior. Moreover, the arrangement and connections between grains are not explicitely modeled, but only taken into account

using mathematical approaches. Those approaches remain then limited for complex size and shape distributions, or if the goal is to model very local phenomenon such as for example abnormal grain growth.

Full Field (FF) approaches appeared about 30 years ago [4]. The whole polycrystal evolution is explicitely modeled at a mesoscopic scale on a meshed Representative Volume Element (RVE) containing a representative number of grains. It gives them a much wider range of validity, making a set of parameters completely independent of the polycrystal arangement. Recent improvements in FF finite element microstructural simulation enable to compute accurately and in reasonable CPU time the discussed phenomena and their coupling: realistic polycrystal generation, grain growth driven by capillarity and stored energy jumps at the boundaries, hardening, recovery, and nucleation [5]. The CPU coast remains however much higher in this case than for the JMAK or MF approaches.

As all approaches have positive and negative aspects, it is essential today to combine them to get the best of what materials science can offer in terms of microstructure evolutions predictions. TRANSVALOR proposes to couple the software FORGE® with both the MF "NeighbourHood Model" NHM and the FF software DIGIMU®, developed in a wide ongoing collaboration with CEMEF MINES ParisTech and 8 renowned French industries in the French National Agency's Industrial Chair DIGIMU [6]. NHM and DIGIMU follow the same physical rules, modelling hardening and recovery using mean field laws, modelling grain growth driven by capillarity and enerjy jumps at grain boundary interfaces, modelling polycrystal and grain deformation and nucleation. Multi-scale and multi-approache analysis are then made much easier.

This article discusses the global microstructure simulation approach and its steps: macroscopic simulation of a process, material identification using MF or FF model, and industrial-like process simulations with DIGIMU®, illustrated by a 2D cogging computation on and a 3D close die forging computation.

2 Preliminary work

Reliable microstructure predictions require a non neglictible preliminary work for the user, to precisely know the thermomechanical pathes of its process, and to identify their material datas.

2.1 Macroscopic simulation of the process

A precise knowledge of the thermomechanical history of the process is required to make relevant microstructural predictions. Macroscopic simulations must be performed with a specific attention given to mechanical and thermal boundary conditions, as well as friction modelling. As the velocity gradient is a particularly unstable value in simulations, mesh must be fine enough to obtain smooth evolutions. In case of high temperature gradients at the boundaries, adapting the mesh is essential to describe accurately the temperature evolution. Once the temperature and strain rate range of the simulation is known, material caracterization can begin.

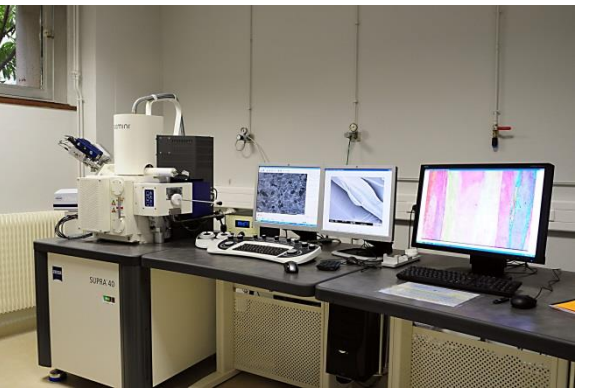
(a)  **(b)** 

Figure 1: **a)** MTS testing machine equiped with the oven financed by Opale ANR Industrial Chair. Maximal temperature is 1200°C, 800°C/hour heating rate, manual quenching in water. Sample temperature is measured by external thermocouples. **b)** Carl Zeiss Supra 40 field emission gun scanning electron microscope (FEGSEM) equipped with a Bruker Quantax system comprising EBSD e−FlashHR detector and the Esprit 2.1 software package.

2.2 Material parameters identification

Material identification is unavoidable to obtain accurate microstructural predictions, whatever the type or the complexity of the used model. The question is how much experiments need to be performed to obtain a broad enough description of the material. The identification of a set of parameters for a not physical model will require as many experiments as an identification for a physical one, but the range of validity of the physical model will be much better than the range of validity of the non physical one

(grain size distribution and grain shapes are naturally taken into account). Transvalor provides through the DIGIMU software a precise identification procedure, which has been setted up tested at CEMEF for material caracterisation of a 304L austenitic stainless steel [6]. The material used for this identification can be seen on figure 1.

2.2.1 Mobility parameters identification

The mobility parameters for GG simulations are relatively simple to identify. It requires heat treatments of different durations (4 or 5) at different temperatures (3 or 4). Grain size measurements can be done using optical micrography, and no specific care must be taken during the experiments. With 15 to 20 samples, a good knowledge of the material can be obtained. Second phase particles dragging forces does not need to be identified because they are naturally modelled in DIGIMU® by capillarity.

2.2.2 Hardening and recovery parameters identification

Hardening and recovery parameters are identified in the required range of temperature and strain rates using the beginning of stress-strain curves (where no recrystallization occurred). Interrupted tests are used for static recovery. No microscopic observation is required, as phenomenological models are deliberately used to describe those phenomena occurring at the dislocation scale.

2.2.3 Recrystallization parameters identification

The identification of recrystallization parameters remains the main and more delicate part of the experimental work. Recrystallized fractions (and eventually mean recrystallized grain size) must be identified on samples deformed at different stages (3 or more), temperatues (3 or more), and strain rates (3 or more) for dynamic recrystallization. A study of postdynamic recrystallization must also be done (3 or more times, temperature, strain rates). Caracterisations should be performed with EBSD microscopy. Experimental procedures are furthermore quite complex. The strain rain and the temperature must remain constant during the whole test. The samples must be quenched very quickly at the end of the experiments to obtain the required microstructure. Proper RX identifications at strain rates higher than 1 remain today very challenging, especially in an industrial context, and require high-end EBSD post-processing [7].

2.2.4 Available set of parameters for 304L

The 304L material has been caracterized for temperatures from 1000°C to 1100°C and strain rates from 0.01 /s to 0.5 /s. The inverse analysis steps required to determine some of the parameters have been done both with DIGIMU® and NHM model, leading to similar results. Please refer to [6] for more details on the model equations and parameter values.

3 2D cogging simulation and parameters variation analysis

3.1 Process Description

An industrial-like cogging sequence on a square bar of 304L steel is studied in a 2D approximation (the plane is perpendicular to the bar axis). Seven passes are simulated, every 10 seconds, followed by 40 seconds of final waiting time (see figure 2 and 3). At each pass, 10 strokes will be seen by the sensor, in the middle of the bar, with different directions (the bar is rotated between each stroke). At the beginning, the strokes are smaller (the sensor is not centered between the tools), then they grow up to a maximum (sensor is ventered between the tools), and then reduce again. In this demonstrator, the temperature is supposed to remain constant (1050°C). The initial mean grain size (equivalent radius in number) in the polycrystal is equal to 60 microns. Note that no FORGE® simulation has been done here to deduce the strain rate curves used in DIGIMU®, and that we only present here the feasibility of such approaches.

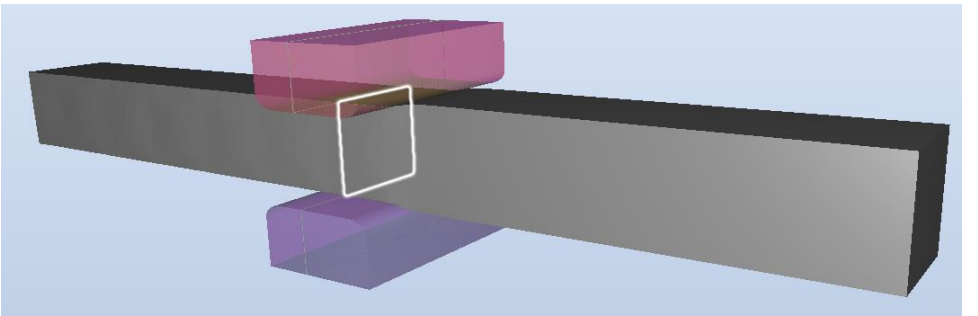


Figure 2: Illustration of the cogging process. DIGIMU uses a 2D assumption in the plane represented in white, studying the evolution of the microstructure on a point that could be located at the center of this plane. The bar is rotated on it axes at 90° between each stroke. Note however that no FORGE® simulation has been run on this process.

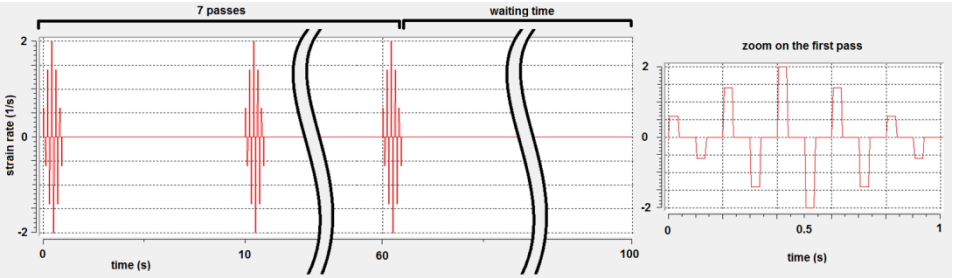


Figure 3: Strain rate history during the process, with a zoom on the first pass between the tools. A positive strain rate is a vertical compression, a negative one a horizontal compression

3.1.1 Results

The evolution of the microstructure can be followed very precisely thanks to the software, spotting wether the grain boundaries (see figure 4 and 5), or rather following mean values (see figure 6). Computation time is from 1 to 2 days on a desktop computer.

3.1.2 Parameters variation analysis

Some minor modifications in a process may have important effects on the final results, which can be very difficult to predict. With an initial mean grain size of 40μm, the recrystallization kinetics is slightly accelerated in comparaison with the 70μm initial grain size, as it could be expected (see figure 4, 5 and 6). With this accelerated kinetics, a new ReX cycle starts at the end of the 7^{th} pass, with only a few nuclei appearing. In comparison, with 70 μm initial radius, the 7^{th} pass was rather the end of the first ReX cycle, with a lot of nuclei appearing. Nuclei appearing at the last pass can grow during the 40 seconds of final waiting time because of their low energy, and consume the whole microstructure. Less nuclei at the last pass results then directly in higher final grain sizes. The mean radius evolution in the simulation with 70 μm initial mean radius (see figure 6) shows that at 100s, the microstructural state is close the equilibrium and the grain size do not evolve very fast. However, in the simulation with 40 μm initial mean radius, it can be seen in figure 5 and 6 that the mean grain nuclei have not finished to grow and would go on increasing rapidly if the process were a few seconds longer. Significantly higher grain sizes at the end of the process are then obtained with lower initial grain sizes. These results illustrate the necessity to follow precisely the microstructure evolution to optimize a complex process. Such observations would not be possible using a JMAK approach.

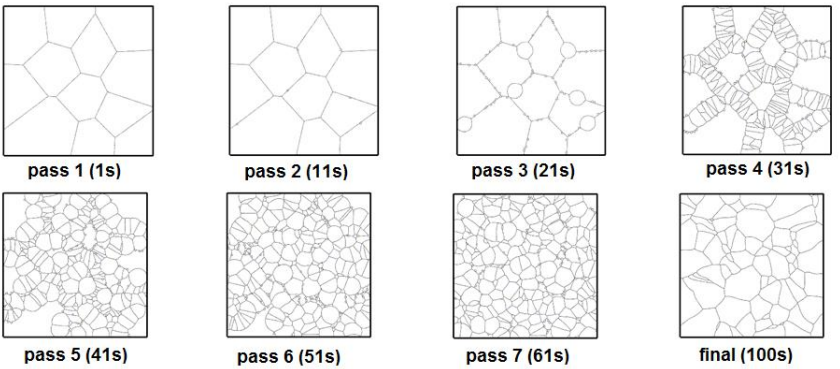


Figure 4: Overview of the grain boundaries in the polycrystal after each of the 7 passes, and after the final waiting time of 40 seconds, for an initial mean equivalent grain size of 70 µm.

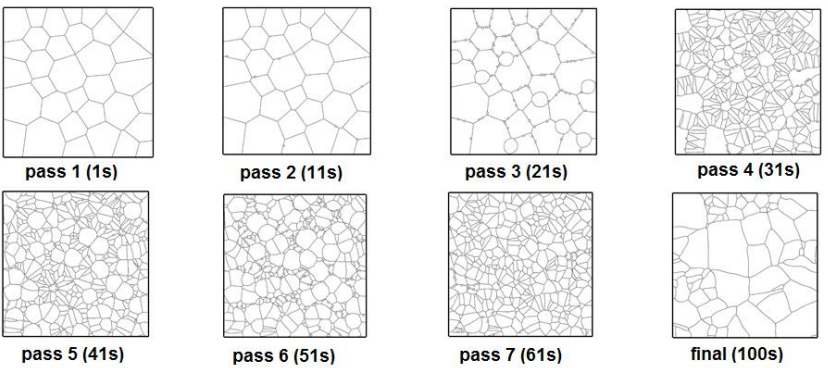


Figure 5: Overview of the grain boundaries in the polycrystal after each of the 7 passes, and after the final waiting time of 40 seconds, for an initial mean equivalent grain size of 40 µm.

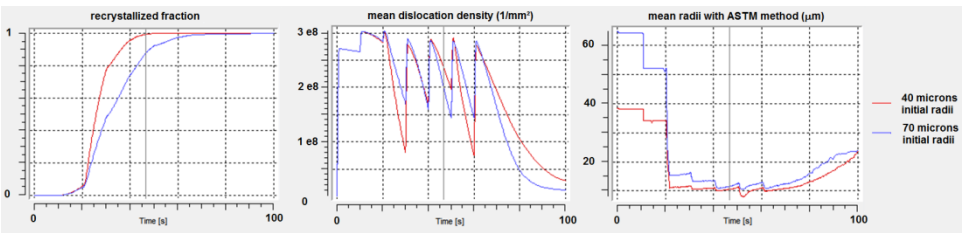


Figure 6: Recrystallized fractions, mean dislocation densities and mean raddi evolutions during the cogging process for different mean initial grains radii.

4 3D close die forging simulation

4.1 Description of the process

A 3D demonstrator with two passes, upsetting and close die forging, has been simulated with FORGE®. A sensor has been placed in the core of the part (see figure 7). The temperature can be considered as constant and equal to 1250°C. The velocity gradient tensor has been smoothed before to input it in DIGIMU. The initial mean grain size (equivalent radius in number) is 25 µm. Note that this study, with material and press velocities, does not correspond to an existing industrial process, but should be rather considered as a demonstrator.

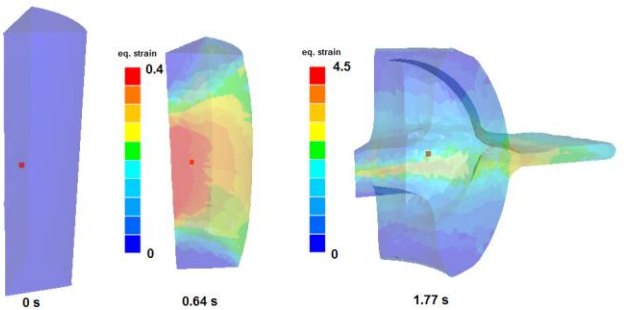


Figure 7: Overview of equivalent strain values and sensor position in the part at the initial state, at the end of the upsetting, and at the end of the close die forging operation.

4.2 Results

The grain boundaries evolution can be very clearly observed in this 3D simulation (see figure 8). Complex grain deformation due to the 3D deformation of the RVE is taken into account, and this modification of the volume-surface ratio of the grains plays an important role in the ReX kinetics. Parameters analysis done in the previous 2D example or mean value curves comparisons can also be lead in this 3D example. Computation time is 2 to 3 days on a multicore desktop computer, but the 3D RVE contains much less grains than the 2D one, and the forming process time is shorter than in 2D.

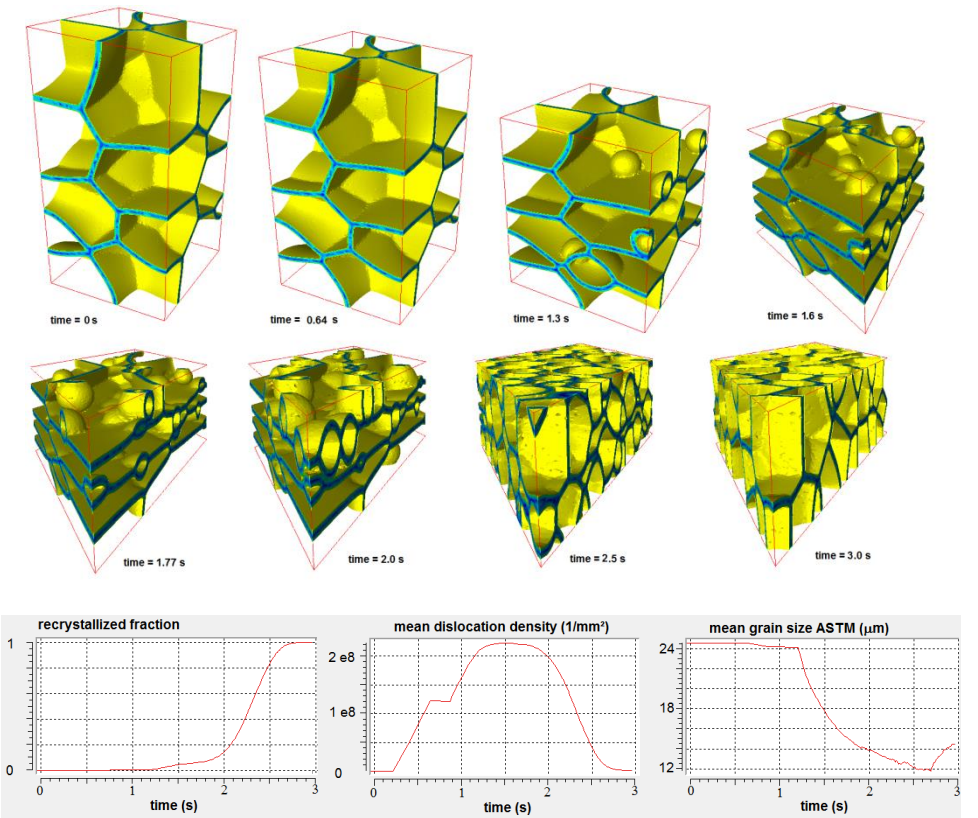


Figure 8: Overview grain size evolution in the two passes of the 3D forging example and corresponding mean value evolutions in the RVE.

5 Conclusion

Even if no perfect solution exists today to optimize rapidly a whole part microstructural state, it is already possible to combine the use of JMAK, MF and FF models to take the best out of the actual knowledge for those wanting to take a competitive advantage in grain size predictions. In addition to the software FORGE® dedicated to macroscopic simulations, TRANSVALOR proposes a FF simulation software DIGIMU® and soon a MF model NHM based on the same physical equations and taking the same set of parameters. Fine and intuitive simulations can be done at the mesoscopic level to predict microstructure evolutions during industrial processes or set up JMAK or mean field

models using “digital testing”. Simulations presented in this article have proven the feasilibitlity of the approach, but do not correspond exactly to existing industrial processes, and no comparison with experimental results on an industrial process has been done yet in recrystallization. However, it has been shown that the industry has the opportunity to take ownership concretly of the most cutting-edge advancements in RX predictions to reduce the cost of their microstructural study by combining experimental work with the use of efficient simulation tools. The dynamism of the research consortium (French National Research Agency, CEMEF MINES-ParisTech, ArcelorMittal, Aubert & Duval, Ascometal, CEA, Constellium, Framatome, Safran and Timet) guaranties future concrete improvement of DIGIMU and NHM, such as numerical optimizations and covering of new physical phenomena: second phase particules evolutions during a simulation, grain boundary anisotropy, and crystal plasticity.

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