DIGIMU®: Full Field Recrystallization Simulations for Optimization of Multi-Pass Processes

P.O. De Micheli[1,a)], L. Maire[2], D. Cardinaux[3], C. Moussa[2], N. Bozzolo[2] and M. Bernacki[2,b)]

[1]TRANSVALOR S.A. Parc de Haute Technologie SOPHIA-ANTIPOLIS, 694. Av. Dr. Maurice Donat, 06255 Mougins Cedex, France.
[2]MINES ParisTech, PSL-Research University, CEMEF-Centre for Material Forming, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia-Antipolis CEDEX, France.
[3]ArcelorMittal INDUSTEEL, CRMC, 56 rue Clemenceau, 71201 Le Creusot Cedex, France.

[a)]Corresponding author: pascal.demicheli@transvalor.com
[b)]marc.bernacki@mines-paristech.fr

Abstract. Microstructural predictions on multi-pass processes are very challenging because the grains topology evolves in a very wide range, due to the coupled action of hardening, recovery, grain growth (GG), discontinuous dynamic and post dynamic recrystallization (DRX and PDRX). Classical models reach their limits. More physical approaches taking into account the complexity of the topology becomes necessary. In this article, DIGIMU®, the first commercial full field (FF) simulation software dedicated to grain growth and recrystallization modeling will be presented. Its ability to model industrial processes will be illustrated on an industrial-like 2D plate rolling process.

INTRODUCTION

Microstructural state of metallic parts plays a major role on in-use properties and on the mechanical behavior during forming. It becomes nowadays necessary to master grain size and dislocations density evolution during industrial processes to fulfill always more severe specifications and to address efficiently new markets.

However, microstructural predictions on multi-pass processes are very challenging due to the strong evolution of the microstructure topology from the beginning to the end of the process. The competition between boundary migration, recovery and nucleation leads to complex coupled effects. Only minor variations of the process parameters (inter-pass waiting and reheating times, temperature and strain rates values at each pass) may have huge effects on the way dynamic and post dynamic recrystallization take place. Actual forming simulation software packages propose different models based on phenomenological or mean fields (MF) approaches. However, their range of validity associated with a given set of material parameters is often limited to a given process and initial material state. Facing multi-pass process, they rapidly reach their limits.

During the last 30 years, academical full field (FF) modeling approaches appeared [1]. Whole polycrystal evolution is explicitly modeled on a Representative Volumic Element (RVE) containing several grains. Taking into account directly the grain topology gives to those models a much wider range of applications for a given set of parameters. Recent improvements in FF 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 wide ongoing collaboration between CEMEF MINES ParisTech, 8 renowned French industries and the software editor TRANSVALOR in a French National Agency's Industrial Chair leaded to the industrialization of the robust and easy to handle commercial solution DIGIMU®dedicated to GG and ReX modeling in industrial processes conditions. The actual version is restricted to 2D, but 3D will be

available in the upcoming version 2019. This article will first describe rapidly the software and illustrate it capabilities on a realistic industrial-like plate hot rolling sequence with eleven passes.

MODEL DESCRIPTION

This section will briefly present the commercial software package DIGIMU®and the underlying models. A more detailled description of the models and simulation settings can be found in [2] [3].

Polycrystal Generation

Grain boundaries are tracked using a 2D or 3D FE formulation associated to a level set method [4],[5],[6]. To optimize CPU times, each grain is not associated to its own level set funtion ψ, but non adjacents grains are grouped together in the same function using a coloring/recoloring algorithm [7], which reduces importantly the number of necessary level set functions. An initial polycrystal can be generated using Laguerre-Voronoï algorithm coupled to sphere packing algorithms, for a given initial grain size distribution [8]. Grains can be equiaxed or elongated (see Fig. 1). It is possible to import experimental data to reproduce a specific microstructure.

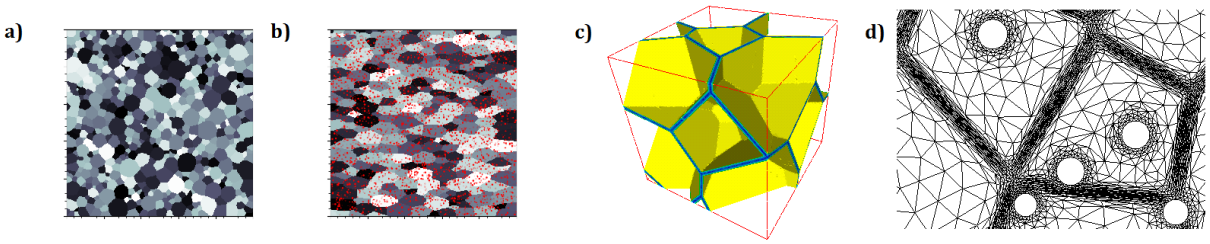

FIGURE 1. Initial polycrystal generation from statistical data: a) equiaxed grains from grain size histogram, b) elongated grains (ratio 2) from lognormal distribution with a bimodal Second Phase Particles (SPP) radius distribution in red, c) 3D isotropic grains from lognormal distribution, d) Automatic Adaptive Anisotropic meshing overview around grains boundaries and SPP in 2D.

An automatic mesh adaptation algorithm is used to optimize the mesh at each situation, isotropically or anisotropically. Convergency and accuracy is ensured, without that the user has to specify numerical parameters (see Fig. 1 d)) [4, 5, 8].

The software also enables to define an initial dislocation density per grain in the polycrystal. This dislocation density distribution can either be described by statistical data, by an histogram, or imported from experimental EBSD data analysis [9].

Grain boundary migration

Grain boundary migration is leaded by two physical mechanisms. The first one is the pressure due to capillarity, i.e. the tendency to reduce the grain boundary energy by reducing the boundary overall surfaces (or length in 2D). The second one is the pressure due to the stored energy jump at the boundary between two grains, that will promote the growth of the grain with the lowest energy. Under the condition that the LS functions remain distance functions ($\left\|\vec{\nabla}\psi\right\| = 1$), the grain velocity can then be split into two terms $\vec{v}_c$ and $\vec{v}_e$ with :

$$\vec{v} = \vec{v}_c + \vec{v}_e \quad with \quad \vec{v}_e = M_b \delta(\dot{\varepsilon}) [\![E]\!] \vec{\nabla}\psi \quad and \quad \vec{v}_c = -M_b \gamma_b \Delta\psi \vec{\nabla}\psi, \tag{1}$$

with M_b being the grain boundary mobility, $\delta(\dot{\varepsilon})$ a parameter depending on the strain rate, $[\![E]\!]$ the stored energy jump at the boundary and γ_b the grain boundary energy. Solving the grain boundary migration problem consists then in solving a convection-diffusion problem on all the level set functions.

Second phase particles (SPP) can be taken into account in the computation, without having to consider pinning pressure. They are represented by holes in the mesh, imposing their curvature to the grain boundaries, and then modifying their velocity simply because of the capillarity effect. Several studies have shown the accuracy of this model by comparing the simulation results to experimental ones [10].

Polycrystal Deformation, Hardening and Recovery

The software can deal with very large polycrystal deformations, and to follow the dislocation density evolution during the computation by using simple mean fields models, in order to avoid the numerical cost of a crystal plasticity FE formulation. Dislocation density is supposed to be constant per grain.

During grain boundary migration, the zone swept by the boundary is supposed to have a dislocation density ρ_0 corresponding to an undeformed material. The new dislocation density of the grain is computed by averaging the previous one and ρ_0, weighted by the corresponding area or volumes (resp. 2D or 3D).

Yoshie-Laarsaoui-Jonas model has been chosen to link dislocation density evolution to deformation, through its hardening coefficient K_1 and its dynamic recovery coefficient K_2. Both coefficients can depend on strain rate and temperature [11]. Static recovery is taken into account on a similar way, with a static recovery parameter K_s depending on temperature ([12],[13]) .

$$if\ (\dot{\epsilon} > 0) :\ \frac{\partial \rho_j}{\partial \varepsilon^p_{eff}} = K_1 - K_2 \rho_j \quad else :\ \dot{\rho_j} = -K_s \rho_j. \tag{2}$$

Static, Dynamic and Post-Dynamic Recrystallization

Simulation of necklace recrystallization is enabled thanks to a nucleation model. As the dislocation density per grain is constant in the model, the position of the nuclei can't be localized specifically. It is then asumed that nucleation only occurs at the boundaries because it is where dislocation accumulate generally [14]. A critical dislocation density ρ_{cr} is defined, and all the nodes adjacent to the boundary of a grain whose dislocation density overpasses ρ_{cr} are flagged as eligible for nucleation. ρ_{cr} is computed iteratively, function of the grain boundary mobility M_b and of the grain boundary energy γ_b [13] :

$$\rho_{cr} = \left[-2\gamma_b \dot{\epsilon} K_2 M_b \delta(\dot{\varepsilon}) \tau^2 ln\left(1 - K_2 K_1 \rho_{cr}\right) \right]^{1/2}. \tag{3}$$

The nuclei are supposed to be spherical and appear with a dislocation density ρ_0. The initial radius is defined by the Bailey-Hirsch criterion [15]. It is the minimal radius that ensure nucleus to grow with an energy jump from ρ_0 to ρ_{cr}, in spite of the capillarity pressure, with a security factor ω which generally equals 1.5. The parameter *dim* is here the spacial dimension of the computation.

$$r^* = \omega \frac{(dim - 1)\,\gamma_b}{\rho_{cr} \tau}. \tag{4}$$

Nucleation rate $\dot{V}$ is fixed by the probability of nucleation of the electible grain boundaries $K_g(T, \dot{\varepsilon})$, and the length (2D) or surface (3D) of this boundary Φ :

$$\dot{V} = K_g \Phi \Delta t. \tag{5}$$

Once a nucleus appeared, its evolution is simply governed by capillarity and energy jumps at the interface pressures presented in this section.

ROLLING SIMULATION

Description of the Process

An industrial-like hot plate rolling process has been set up with the collaboration of ArcelorMittal Industeel. The process lasts 120 seconds, with 11 passes between the rolls, and different waiting times between those passes. A sensor has been placed in the middle of the product in a FORGE®simulation.

Temperature is supposed to be constant in this simulation, equal to 1050°C. Strain rate history was analyzed, and simplified to create the strain rate function of time tabulated file for DIGIMU®(see figure 2). The material is a 304L austenitic stainless steel, lightly derived from the material file available in the solution package. The initial polycristal in the simulation was generated with the Laguerre-Voronoï algorithm following a lognormal distribution with a mean grain size of 40 microns (equivalent grain radius in number).

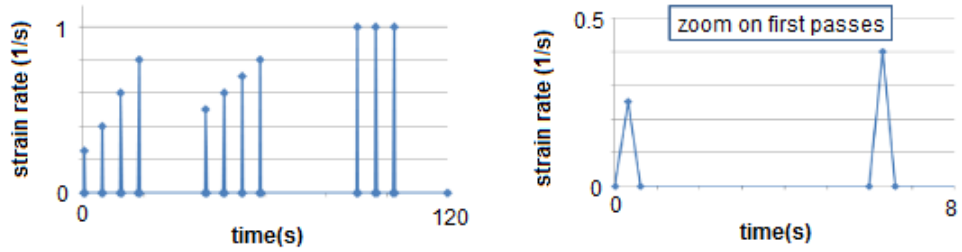

FIGURE 2. Strain rate function of time in the RVE derived from a FORGE®simulation for a plate hot rolling process simulation with 11 passes.

Simulation Results

The computation has been launched with the commercial version of DIGIMU®3.0, in 2D. Mean grain size and mean dislocation density evolution, as well as a graphical evolution of the polycrystal at each pass are visible in Fig. 3 and 4.

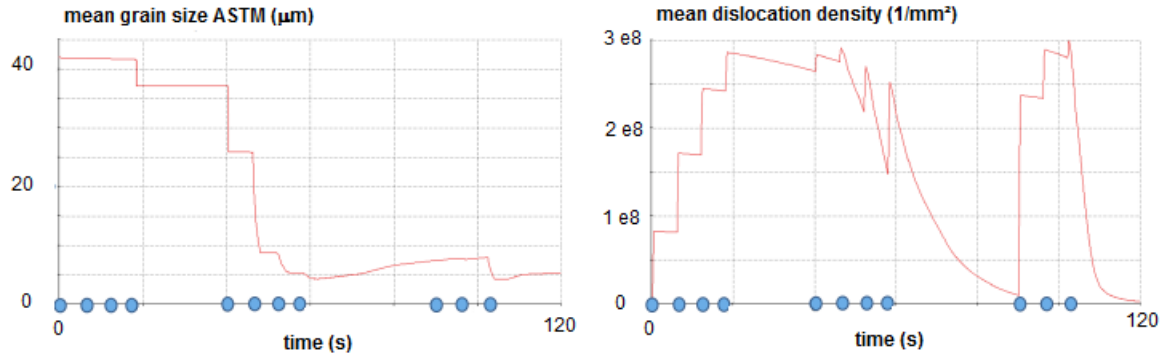

FIGURE 3. Mean grain radius evolution (ASTM), and mean dislocation density evolution (average in surface) during the process. Each blue point on the time axis represent a pass between in the rolling mill.

CONCLUSION AND PROSPECTS

The commercial finite element software package DIGIMU®, dedicated to full field microstructure modeling, has proven in this paper to be able to treat industrial multipass processes, such as this plate rolling demonstrator, set up with the help of ArcelorMittal and FORGE®simulations. Eleven rolling passes have been simulated, with the corresponding DRX and PDRX sequences. The topology and the dislocation density of each grain can be easily followed during the whole simulation (see Fig. 4). A lot of well known phenomena are here clearly visible. The bigger grains are the last ones to be totally recrystallized, because of the necklace nucleation. Sometimes, a second cycle of recrystallization begins before that the previous one have been finished (see dislocations densities at 60 seconds). If only few nuclei appear before a static period, those will grow importantly and reach important size rapidly (see difference between 20s and 40s in the simulation). However, if more grains nucleate just before this static period, they are in competition and reach lower radii.

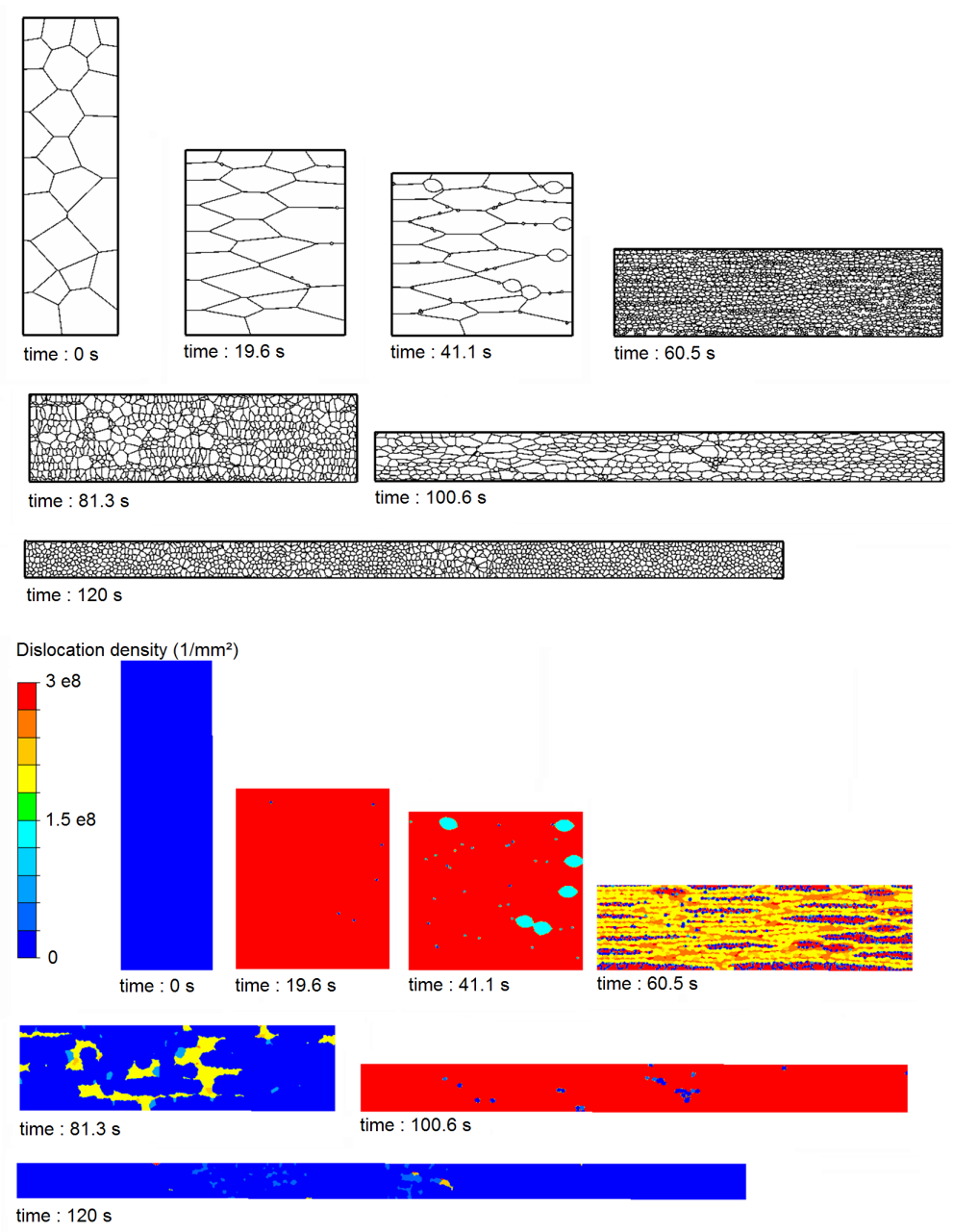

FIGURE 4. Grain boundaries and dislocation density evolution in the polycrystal during the rolling process.

Full field modeling enables also to give smooth and very interesting mean size and mean dislocation densities evolution, through the wide range of phenomena that occurred during the process (see Fig. 3). Mean grain size evolution allows to localize precisely when recrystallization occurs, and the subsequent grain growth. The competition between recrystallization and recovery is also clearly visible on the mean dislocation density evolution. If the waiting time between the passes is too long, recovery can simply prevent the part to reach the critical dislocation density in spite of the applied deformation. The important effect of PDRX during waiting times can also be easily analyzed on the curve. All those results give a very comprehensive description of the microstructure evolution during the whole process.

At this time, no comparison between experiments and simulation has been done on this industrial process, but this work is actually in progress, with a proper identification of material parameters. However, this rolling simulation perfectly illustrates the capability of the software to deal with multipass industrial processes. It would have been also possible to work on cogging, ring rolling, becking and other different open die forging processes, as long as the 2D plane strain hypotheses makes sense. 3D simulations would be necessary for the other ones (Fig. 5), but actual computational times made them more dedicated to shorter forging sequences or heat treatments in an industrial context for the moment.

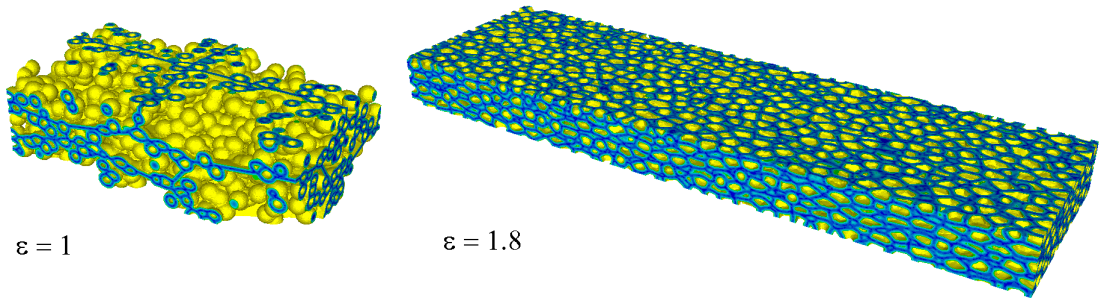

FIGURE 5. Grain boundaries during a 3D DRX simulation, at a partially and fully recrystallization stage, with up to 5000 grains.

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