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Large scale FE simulations of recrystallization and grain growth thanks to a level set approach, illustrations in context of industrial forming processes

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Abstract. Recently, an original full field model using the level set method in a finite element framework has been introduced and validated at the Mines ParisTech - Center for Materials Forming. This approach has demonstrated its potential for the simulation of 2D or 3D large scale grain growth and recrystallization problems. Through the development of the DigiMu® software by Transvalor, this methodology is now considered for industrial applications.

1 Introduction

Metal forming modelling can be predictive only if the strain rate, strain and temperature dependency of the flow behaviour is correctly described. The mechanical properties and behaviour of metallic materials depending mostly on the dislocation content and structure, this points out the need to incorporate microstructure concepts into those models. The goal is to correctly describe the main physical mechanisms occurring in metals during thermomechanical processes i.e. work-hardening, recovery, grain boundary migration, nucleation and grain growth related to dynamic, static or metadynamic recrystallization. Macroscopic and homogenized models are widely used in the industry, mainly due to their low computational cost [1, 2]. If this mean field framework is quite convenient, it can be synonymous for a given material of a large amount of experiments with advanced laboratory devices. Moreover, the homogenization of the microstructure does not permit to capture some very local phenomena.

Over the last decades, lower-scale models (called full field models) have been developed in order to simulate explicitly the microstructural evolution [3-5]. The idea behind these mesoscale simulations is that the morphology and the topology of the grain boundary network play a non-negligible role in the evolution of the microstructure. Recently a new full field approach, based on a Level Set (LS) description of the interfaces in a finite element (FE) context has been introduced to model 2D and 3D primary recrystallization, including the nucleation stage, and has been extended to take into account the grain growth stage [6-8]. Moreover in this LS context, Smith-Zener pinning (SZP) phenomenon can be taken into account in a natural way [9]. These full field approaches are generally associated with an elevated computational cost making them hardly usable for 3D computations. Moreover they require many numerical parameters whose calibration is not straightforward. Recent major developments and improvements addressed these issues [10, 11] making possible the use of these approaches in an industrial context.

2 Numerical model description

Simulations are performed on a Representative Volume Element (RVE) at the mesoscopic scale where the microstructural features are explicitly represented. The polycrystal is constructed respecting the topological characteristics of the grains and the metallurgical properties. The RVE is generated from a statistical method. Efficient algorithms have been developed to respect a given grain size distribution [12] (Figure 1).

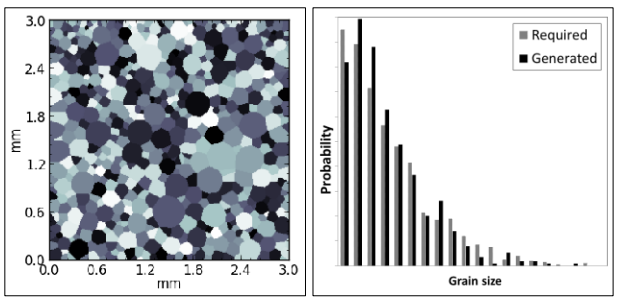


Figure 1. 2D RVE generation (500 grains) respecting a given grain size distribution.

The microstructural evolution is given by the displacement of interfaces (grain boundaries for example). The model considered here works around a LS

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description of the interfaces in a FE framework. This method has the advantage of avoiding the difficult problem of tracking interfaces. Indeed a LS function ψ is defined over a domain Ω as the signed distance function to the interface of a sub-domain G of Ω. The values of ψ are calculated at each mesh node and the sign is defined as positive inside G and negative outside:

$$\forall t \begin{cases} \psi(x,t) = \pm d\big(x, \Gamma(t)\big), x \in \Omega \\ \Gamma(t) = \{x \in \Omega, \psi(x,t) = 0\} \end{cases} \quad (1)$$

where *d(.,.)* corresponds to the Euclidean distance. The interface is given by the level 0 of the function ψ.
Theoretically, each grain must be represented by its own LS function. In practice, non-neighbouring grains in the initial microstructure (separated by a certain number of grains) can be grouped to form global LS (GLS) functions. This approach allows using a small number of functions N_p compared to the total number of grains constituting the microstructure N_g and thus limits the numerical cost. The initial separation between grains belonging to the same GLS function must be chosen small enough to limit the computation time and sufficiently high to avoid a numerical coalescence. To address this issue, an efficient grain recoloring algorithm has been recently developed [11]. The interface of each GLS function is then displaced by solving a set of convective-diffusive equations [7]:

$$\forall p \in \{1, \dots, N_p\}: \quad \begin{cases} \frac{\partial \psi_p(x,t)}{\partial t} - m\gamma \Delta \psi_p(x,t) + v_e . \nabla \psi_p(x,t) = 0, \\ \psi_p(x, t=0) = \psi_p^0(x) \end{cases} \quad (2)$$

where m and γ are respectively the grain boundary mobility and energy. The diffusive term refers to capillarity effects while the convective one is related to stored energy gradients throughout the microstructure.
The distance function must be reinitialized at each time step in order to keep the metric property $\|\nabla \psi_p\| = 1$ during all the simulation. Indeed, even if reinitialization is favourable for the regularity of the LS function, this treatment is especially crucial in order to verify that the capillarity effects are properly describe by the diffusive part of Eq. (2). An efficient and parallel reinitialization algorithm based on a direct approach and using optimized searching procedures has been recently developed [10] leading to significant computational cost reductions in comparison to the classical approach used in [7-9] consisting in solving an Hamilton-Jacobi equation for each GLS function.

The model works in 2D and in 3D. Realistic predictions necessitate a sharp description of the interfaces. This issue is achieved thanks to an anisotropic mesh adaptation around the interfaces (Figure 2). As the interface moves, periodic remeshing is performed such that the refinement zone always coincides with the interface position. This technique allows improving precision and reducing computation times. Boundary conditions applied to the RVE are representative of what suffered a material point at the macroscopic scale (thermomechanical cycle of the point considered).

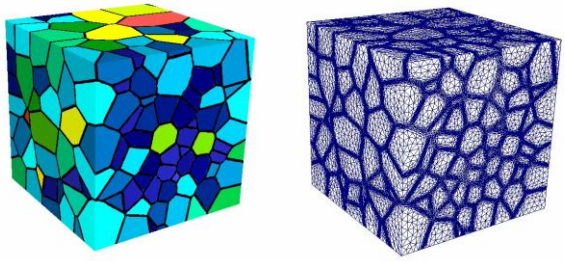


Figure 2. Polycrystal description in 3D with the used finite element mesh (anisotropic meshing near grain boundaries).

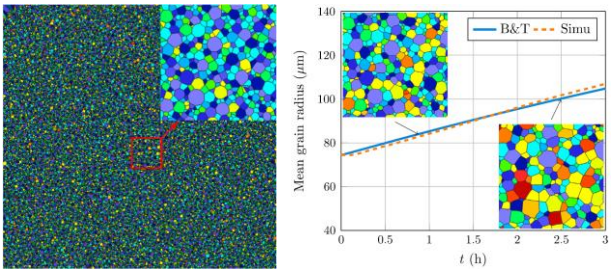


Figure 3. Left: Initial 304L 2D polycrystal (50000 grains). Right: Microstructural evolution during an isothermal heat treatment (1050°C): comparison with the Burke and Turnbull model [11, 13].

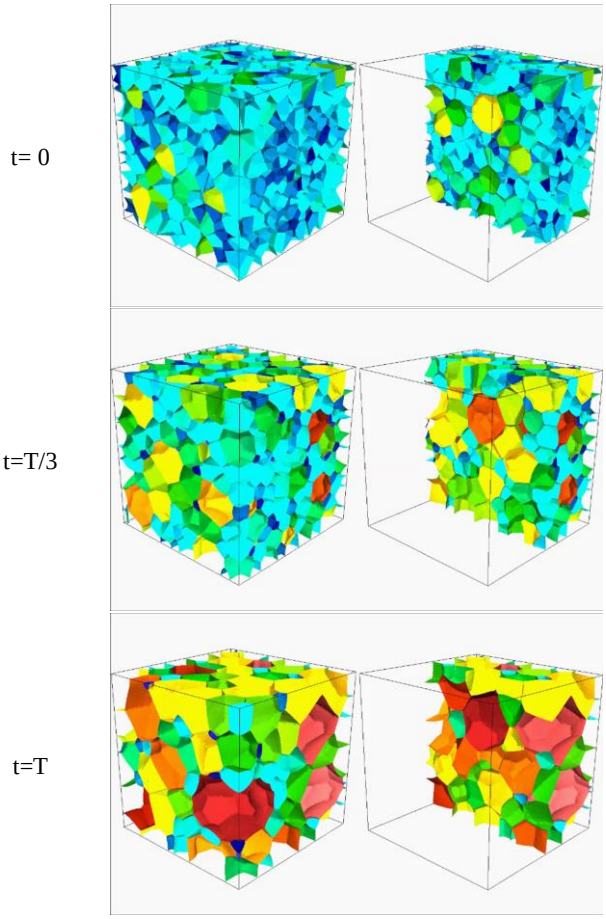
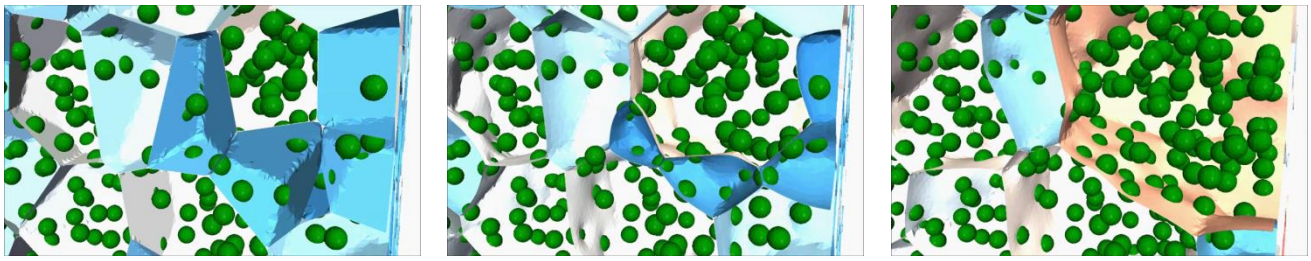


Figure 4. 3D microstructural evolution of a 304L steel (grain growth simulation, the initial polycrystal contains 1700 grains).



t=0 t=T/8 t=T

Figure 5. A 3D grain growth simulation for Inconel™ 718. The green spheres represent the precipitates.

3 Large-scale simulations

Different 2D and 3D large-scale simulations enabled by the new major developments described previously, and which would not have been performed in acceptable computation times before, are illustrated below.

Figures 3 and 4 represent the microstructural evolution of a 304L austenitic stainless steel subjected to an isothermal heat treatment at 1050°C. Simulations are performed respectively on a 2D and a 3D polycrystal. In both cases, the microstructural evolution is only driven by the reduction of the total grain boundaries length/area. With isotropic grain boundary mobility and energy, the well-known Burke and Turnbull equation [13] is used to validate the results obtained through these full field simulations. The comparison is plotted on Figure 3 showing a good agreement between both models.

In order to limit the final grain size which can be detrimental for the mechanical properties, a classical method consists in precipitating second phase particles (SPP) that can hinder the grain boundaries motion. If this approach is usually efficient, under specific conditions, abnormal grain growth (AGG) may occur. AGG can be described as the selective growth of only a few grains while other grains do not grow in the microstructure. It may occur as a result of a heterogeneous stored energy field leading to a driving force for some grain boundaries that overcomes the SZP force, or as a result of grain boundary energy anisotropy, or as a result of a heterogeneous SPP distribution. Mean field models cannot predict such a local phenomenon (because of the microstructure homogenization); therefore the development of efficient and accurate 3D modelling tools able to account for the SZP phenomenon is necessary. Based on the work described in [9], the recent numerical developments [10, 11] allowed performing 3D simulations as shown in Figure 5. SPPs are considered inert and are represented as holes in the FE mesh (green surfaces in Figure 5). In such a way, incoherent or coherent particle/grain interfaces can be considered through appropriate boundary conditions and the dragging effect is naturally modelled by the modification of the local curvature when the grain boundary passes through the particles.

The full field approach described here has also been applied to the modelling of recrystallization. In that case, the driving force for grain boundaries motion is given by both grain boundaries curvature and stored energy gradients between neighbouring grains (recrystallized or non-recrystallized). Preferential sites for nucleation of newly recrystallized grains can also be controlled by a suitable choice of nucleation criteria (topological and/or stored energy based).

4 Conclusion

A full field approach using the level set method in a finite element context has been used to simulate the microstructural evolution during forming processes. Modelling at the mesoscopic scale can be a help for understanding complex microstructural phenomena but it can also be used to optimize/calibrate higher scale models (like mean field models). These simulations allow describing in a natural way the materials in terms of microstructural features. The recent improvements done to reduce the high computation times generally associated with these models make possible now their use for industrial applications.

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