Full field modeling of recrystallization and grain growth thanks to a level set approach: towards modeling by industry

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Introduction

Metal forming modeling can be predictive only if the strain rate, strain and temperature dependency of the flow behaviour are correctly described. The mechanical properties and behaviour of metallic materials mainly depends on the content and structure of dislocation network, this points out the need to incorporate microstructure concepts into the numerical 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, with 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 [10-12] making possible the use of these approaches in an industrial context.

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 in a statistical way by respecting the topological characteristics of the grains and the metallurgical properties. Efficient algorithms have been developed to respect a given grain size distribution and attributes [13,8]. The microstructural evolution is given by the displacement of interfaces (grain boundaries for example). The model considered here works around a LS description of the interfaces in a FE framework. This front capturing approach has the advantage of avoiding

the difficult problem of tracking interfaces and allows to naturally handle complex topological events occurring during grain boundary motion.

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 gathered 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 limiting 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 [11,12]. The interface of each GLS function is then displaced by solving a set of convective-diffusive equations [7] and a reinitialization procedure in order to keep the metric properties of the distance function. 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 reinitialization approach used in [7-9] consisting in solving an Hamilton-Jacobi equation for each GLS function.

As illustrated in Figure 1, the model works in 2D and in 3D. Realistic predictions necessitate a sharp description of the interfaces. This issue is achieved in 2D thanks to an anisotropic mesh adaptation around the interfaces allowing to reach this objective while conserving a high numerical efficiency. 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. If this meshing strategy is also usable in 3D (see Figure 1a), current developments concern the improvement of the associated remeshing numerical cost. Boundary conditions applied to the RVE are representative of what experiences a material point at the macroscopic scale (thermomechanical cycle of the point considered).

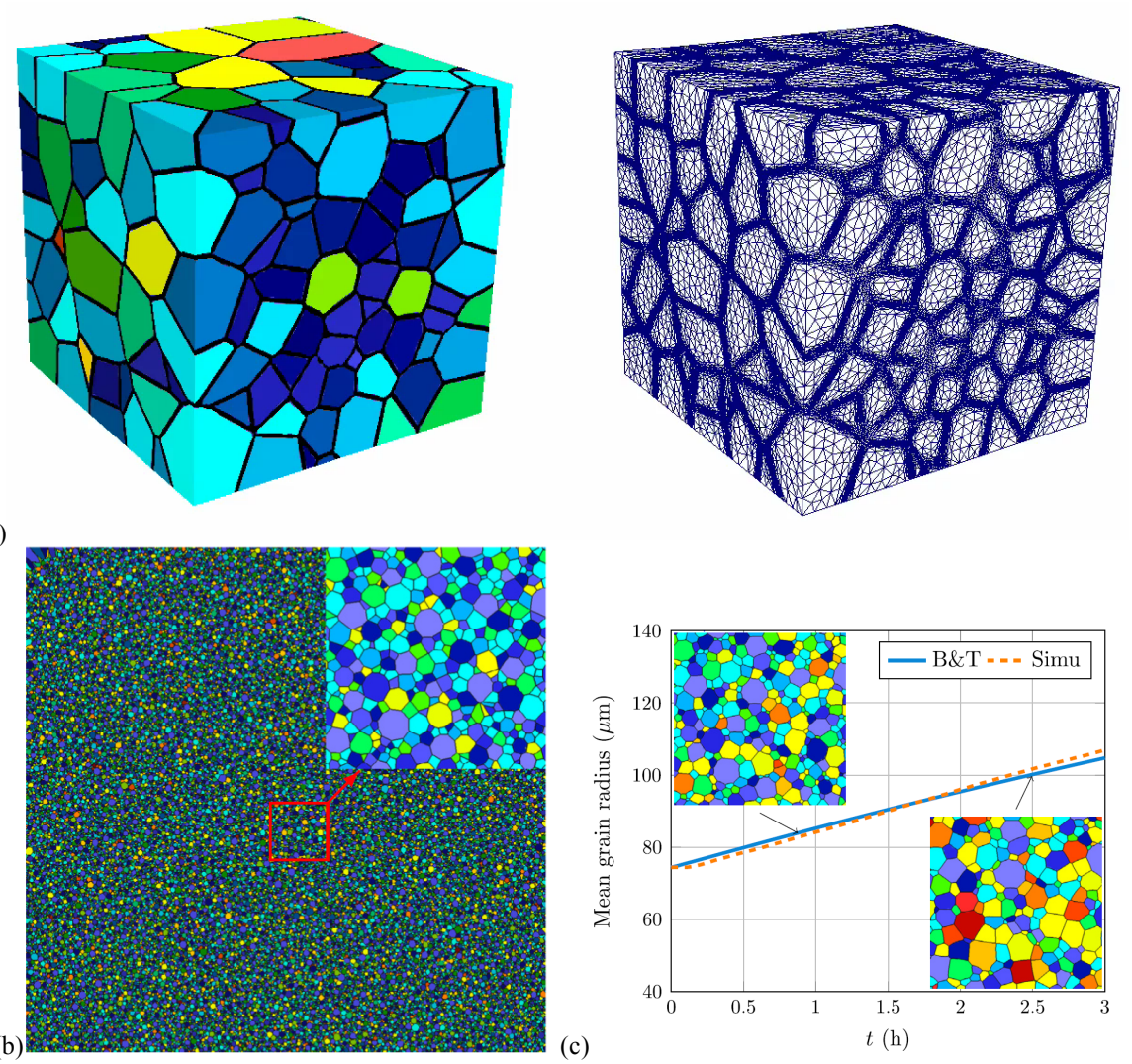


Figure 1. (a) 3D description of a polycrystal and corresponding finite element mesh (anisotropic meshing near grain boundaries), (b)

Initial 304L 2D polycrystal (50000 grains) and (c) microstructural evolution of this microstructure during an isothermal heat treatment (1050°C): comparison with the Burke and Turnbull model [11, 13].

3D large-scale representative simulations

Figure 2 represents, in context of static recrystallization, the microstructural evolution of a 304L austenitic stainless steel subjected to an isothermal heat treatment at 1050°C after deformation. The microstructural evolution is driven by the reduction of the total grain boundaries length/area and of the stored energy.

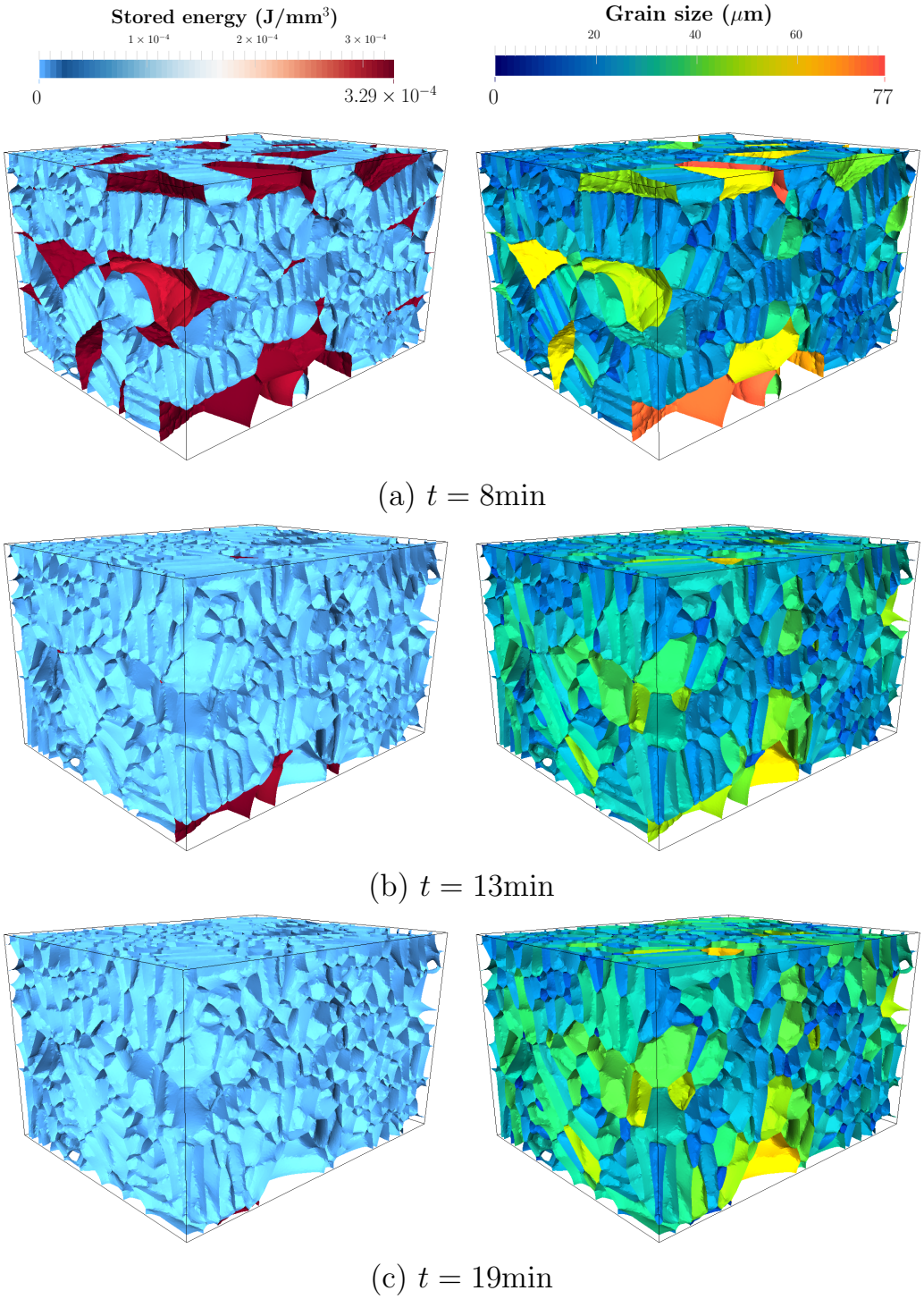
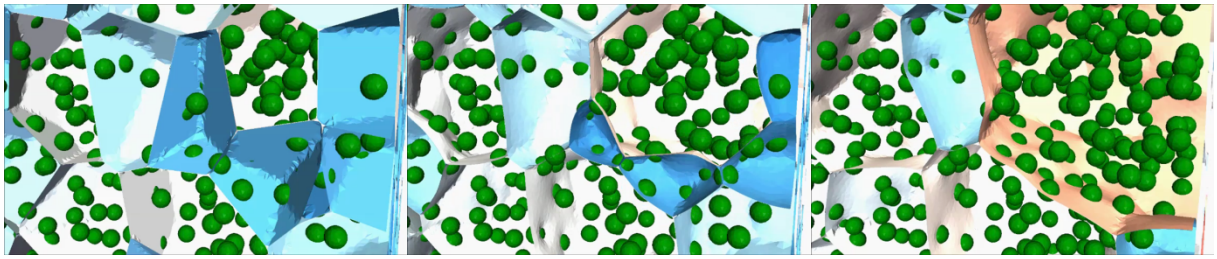


Figure 2. 3D microstructural evolution of a 304L steel during static recrystallization [12]. The color codes correspond to the stored energy (on the left column) and to the grain size (on the right column).

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 pinning 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 modeling tools able to account for the pinning phenomenon is necessary. Based on the work described in [9], the recent numerical developments [10-12] allowed performing 3D simulations as shown in Figure 3 [15]. SPPs are considered inert and are represented as holes in the FE mesh (green surfaces in Figure 3). In such a way, incoherent or coherent particle/grain interfaces can be considered through appropriate boundary conditions and the dragging effect is naturally modeled by the modification of the local curvature when the grain boundary passes through the particles.



t=0 t=T/8 t=T

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

Finally, the last figure (Fig. 4) illustrates the use of these new numerical tools in order to model the evolution of the microstructure during the last steps of a HIP-bonding of 316L austenitic stainless steel [16]. Hot Isostatic Pressing-diffusion bonding of grooved plates is a potentially attractive technique for manufacturing compact heat exchangers. During the process, microstructural changes must be controlled and groove deformation must be minimised. First, plastic deformation processes result in collapse of the surface asperities, the interfacial void closure is then achieved by diffusion controlled mechanisms such as creep and grain boundary diffusion, bonding is finally achieved by grain growth. The process parameters must be accurately calibrated in order to ensure the disappearance of the initial diffusion welding plane while controling the final grain size distribution. Modeling at the microscale is then a precious tool to reach these goals. Figure 4 illustrates the 3D modeling of the last step of a HIP-bonding process (grain growth phenomenon) for 316L thanks to the LS approach, the color code corresponds to the grain size and more than 20,000 grains are considered in the simulation.

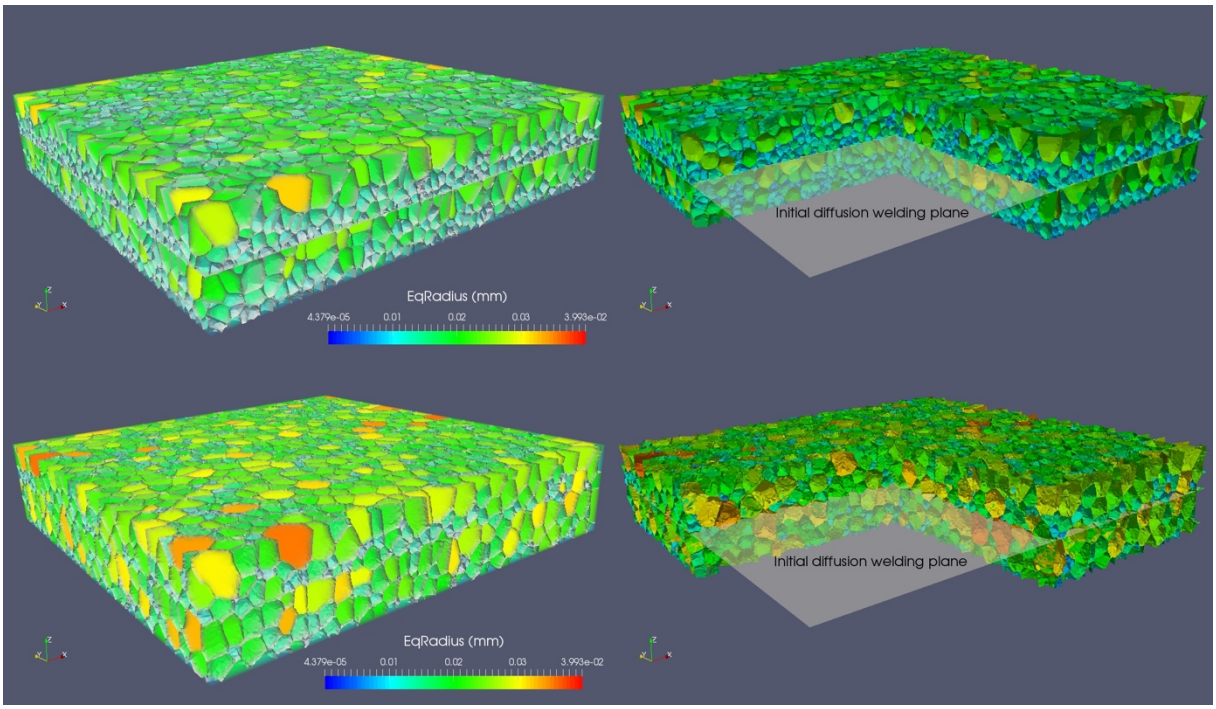


Figure 4. 3D modeling of the last step of a HIP-bonding process (grain growth phenomenon) for 316L thanks to the LS approach, the color code corresponds to the grain size (mm). In the left side, the white surface corresponds to the grain boundary network. On the right side, a cutting view of the grain boundary network is described with the bonding plane (defined by the middle Z-plane). More than 20,000 initial grains are considered in the simulation. (Top) Representative microstructure at the beginning of the grain growth mechanism (where T-junctions are then present in the bonding plane). (Bottom) Evolution of the microstructure after 600s at 1100°C.

Conclusion

A full field approach using the LS method in a FE context has been developed to simulate the microstructural evolution during forming processes. Modeling at the mesoscopic scale can give insight into the understanding of 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 high computation times generally associated with these models make possible now their use for industrial applications.

The objective of the industrial partners of these developments is to provide the best possible quality for the final product of their customers within the shortest delivery time. With that aim, the development of numerical models able to predict microstructure evolution, at the mesoscopic scale is nowadays of prime importance. These digital models will allow being very reactive to new markets with high enough confidence in the proposed manufacturing sequences and parameters. The final aim is the capitalization of this knowledge and of these tools in a multiscale software package framework usable in an industrial context. This is exactly what it is proposed through the DIGIMU® software package dedicated to the industrialization of these developments [15]. Furthermore, scientific perspectives in terms of understanding and modeling of metallurgical phenomena and development of the LS methodology are then as ambitious as the industrial perspectives in terms of applications. Figure 5 illustrates the consortium involved in the development of the DIGIMU® software package.

Figure 5. Consortium involved in the development of the DIGIMU® software package.

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