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Full field Continuous dynamic recrystallization simulations considering precipitates evolutions with DIGIMU®

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Abstract. Full field simulations have proven to be an efficient tool for grain size prediction in industrial processes, with wider ranges of validity and more comprehensive results than other approaches. DIGIMU® is a level-set based solution able to simulate grain growth, Smith-Zener pinning, discontinuous dynamic, post-dynamic, and static recrystallization, and very recently Continuous Dynamic Recrystallization (CDRX). The goal of this work is to explore the capabilities of DIGIMU® to CDRX with evolving second phase particles. First, a new formalism has been implemented to describe particles boundaries with a level-set function. It is then possible to apply growth or dissolution velocities to the boundaries, and to make new particles appear. Secondly, the orientation has been defined in each grain, and the grain boundary energy can then be computed from the intergranular disorientation with Read-Shockley model. A boundary migration solver which considers heterogeneous grain boundary energy is used, which enables the simulation of structure and substructure evolutions. The Gourdet-Montheillet CDRX model is adapted from a mean field to a full field framework, and the corresponding parameters for Zircaloy-4 are identified. Thanks to all those developments, DIGIMU® can simulate full field CDRX in high stacking fault energy materials, coupled with precipitates evolution. Several examples will be presented, some of them compared to experimental results.

Introduction

Mastering grain size, solid phase transformations, and dislocations density evolution during industrial processes becomes necessary to fulfill more and more severe microstructure and properties specifications of the processed materials. In multi-pass processes, the competition between boundary migration, recovery and the different types of recrystallizations leads to complex coupled effects, and minor variations of the process parameters may have huge consequences. A correct modelling of the main physical microstructural mechanisms becomes then necessary [1].

Thanks to the explosion of computer capacities, mesoscopic modeling techniques for metallic materials at the solid-state are now available. These lower scale approaches, the so-called full-field models, are based on a full description of the microstructure topology and have demonstrated an exciting potential for an extensive range of microstructure evolutions. First, it is possible to use more physics in the models because of the better description of the microstructure, leading to a wider range of validity [1]. Secondly, observing directly the polycrystal microstructure evolution, in addition to curves and histograms, allows to analyze the results much more comprehensively [1]. Several numerical frameworks are available: Monte Carlo Potts (MC) [1], Cellular Automata

(CA) [2], Multi-Phase Field (MPF) [3, 4], Vertex [5] or LS models [6,7]. Transvalor distributes for several years the software DIGIMU®, based on a FE-LS framework associated with remeshing algorithms, which is the most adapted framework to simulate large polycrystal deformations. DIGIMU® enables full field simulations of industrial processes and heat treatments with grain growth, discontinuous DRX, PDRX or SRX, with or without second phase particles (SPP) [8,9,10,11,12,13,14]. User-friendliness, CPU time and accuracy have been optimized, and a userroutine module is proposed to modify and adapt default hardening, recovery and nucleation models.

Recently, two new functionalities have been added to broaden the scope of DIGIMU® in terms of thermomechanical conditions and material types. First, an evolutive precipitates formalism is proposed, where a LS function is used to describe the boundaries of an evolutive precipitates population [15,16]. It allows to perform simulations close to solvus, at temperatures where the precipitation state can evolve significantly. Secondly, DIGIMU® can now model the evolution of grain boundaries with heterogeneous energies, and a recent full-field adaptation of the mean field Gourdet-Montheillet model [17, 18] has been implemented to propose a full field CDRX model. It opens the door to the simulation of high stacking fault energy materials, tending to recrystallize continuously [1]. The model was applied to Zircaloy-4 recrystallization and compared with experimental observations [18,19,20].

However, in CDRX, the evolution of the microstructure during the post-dynamic phase is very important, and for numerous materials, this post dynamic phase occurs in presence of precipitates, that may evolve during the heat treatment or the cooling. This is for example the case for several zirconium and aluminum alloys. This article will present more in detail the coupling between precipitates evolution and CDRX models, showing how they can interact to better simulate more advanced CDRX processes with precipitates dissolution, and what are the actual limits. Examples will be provided for Zircaloy-4.

Simulate coupled SPP and grain evolutions

Grain boundaries pinning by second phase particles (SPP) was first discussed by Smith [21] and then detailed by Zener one year after [22]. Under certain conditions, SPP can pin the grain boundaries, slowing down the grain growth process or even stopping it at a limit grain size. The idea in DIGIMU® is to model the dragging pressure induced by the SPP on grain boundaries naturally, by representing the local curvature modification of the grain boundaries induced by the SPP geometry, without the use of any additional parameter [23,13]. The SPP populations are simply geometrically generated in the polycrystal from a statistical distribution law, or directly imported from microscopy images.

In the evolutive formalism, several distinct SPP populations can be described, each one using its own LS function [15,16]. For each population, one evolution law is provided, describing the normal velocity of the SPP boundary in function of a wide range of variables (temperature, particle radius, mean particle radius, mean particle fraction, particle fraction at equilibrium for this temperature…) and the precipitation rate and radius if precipitation is considered (function of the actual temperature, mean particle fraction, equilibrium particle fraction for this temperature …). Of course, more advanced phenomena like the dissolution and immediate reprecipitation after the grain boundary passed through a precipitate (the precipitate seems cut by the grain boundary), are not taken into account. However, this simple framework enables to render quite efficiently precipitation, particles growth or dissolution, and Ostwald ripening (see Fig. 1).

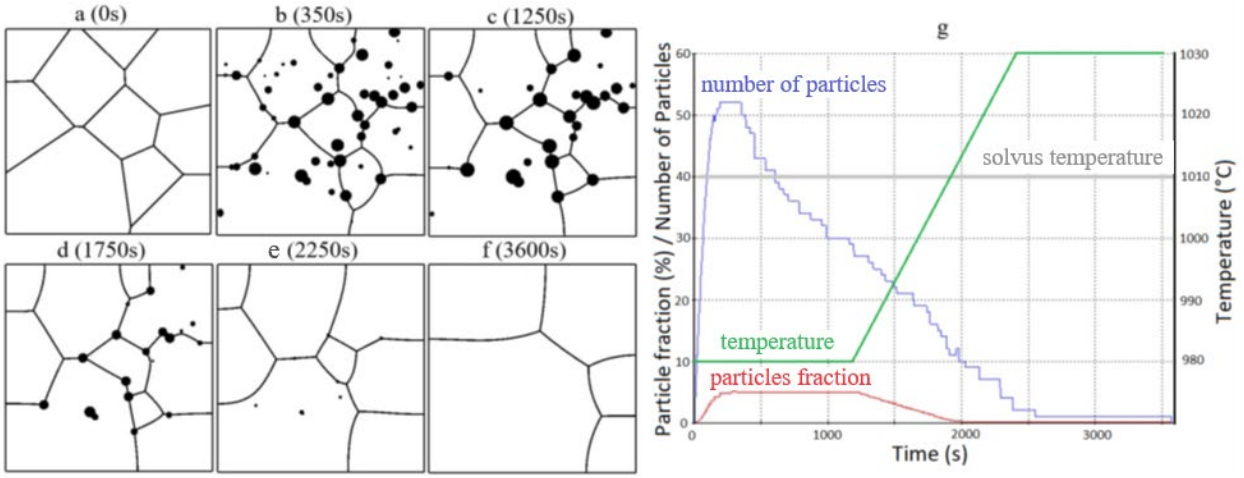

Fig. 1: Simulation of a heat treatment with a wide range of precipitates evolution mechanisms. From a to b) Precipitation and growth of the particles, from b to c) Ostwald ripening, particles with higher radius growth at the expend of the smaller ones, from c to f) increase of the temperature, and lowering of the equilibrium fraction up to the solvus point, followed by the effective particles dissolution, with a progressive release of the grain boundaries. g) Evolution of the simulated particle fraction, number of particles and temperature in the polycrystal during the heat treatment.

Simulate grain substructure evolution and CDRX

Even if the LAGB's energies are lower than the HAGB's energies, their effect on microstructure evolution can however sometimes be of first order. This is especially the case in high stacking fault energy materials, where the progressive formation of a sub grain structure and its progressive evolution to an unhardened grain structure is the main mechanism of recrystallization, the so called CDRX. In this case, the evolution of LAGB cannot be neglected anymore, and must be considered by using a grain boundary migration solver working with heterogeneous grain boundary energies. Recent developments in DIGIMU® enable to define and store the crystallographic orientation for each grain. The grain boundary energy is computed from the intergranular disorientation using the Read-Shockley model, and the grain boundary migration has been adapted and is now able to deal reliably with high energy gradients [24,25,26]. In order to deal with sub boundaries creation and progressive disorientation, the model has been coupled to an adaptation of the CDRX Gourdet-Montheillet model in a full field context [18,19,26,27]. The dynamically recovered energy provided by the Yoshi-Lasraoui-Jonas hardening law is split into two terms.

- Some dislocations stacks together, leading to the creation of new sub boundaries dS^+, converted in the full field model into the creation of new closed sub grains:
$$dS^+ = \frac{\alpha\, b\, dE_r}{h\theta_0}.$$
- Some dislocations are stacking into existing boundaries, leading to their disorientation, converted in the model into the rotation of the existing sub grains by an angle $d\theta$:
$$d\theta = \frac{(1-\alpha)\, b\, D\, dE_r}{2h}.$$

Here, α is a coefficient describing the balance between the two phenomena, function of the current grain diameter D and of a reference grain diameter D_0:
$$\alpha = 1 - exp\left(\frac{D}{D_0}\right)^m,$$

where b is the Burger vector norm, dE_r the computed dynamically recovered energy at this time step, h the number or of sets of dislocations, θ_0 the disorientation angle of newly formed sub grains and m a fixed coefficient.

Parameters for Zircaloy-4 have been identified by Framatome Components Research Center [18,19]. More details about parameters identification and values can be found in [20]. The simulation of the hot deformation of a sample at 650°C, at a strain rate of 1/s up to a strain value of 1, followed by a heat treatment of 100s has been performed. Substructure formation and evolution (Fig. 2) and dislocation density evolution (Fig. 3) show an interesting agreement with the experimental results. Even if the first inserted circular closed sub grains are not really comparable to the physical open sub boundaries which are created, after a few seconds, the simulated substructure evolves in something much closer to the reality and allows reasonably representative simulations.

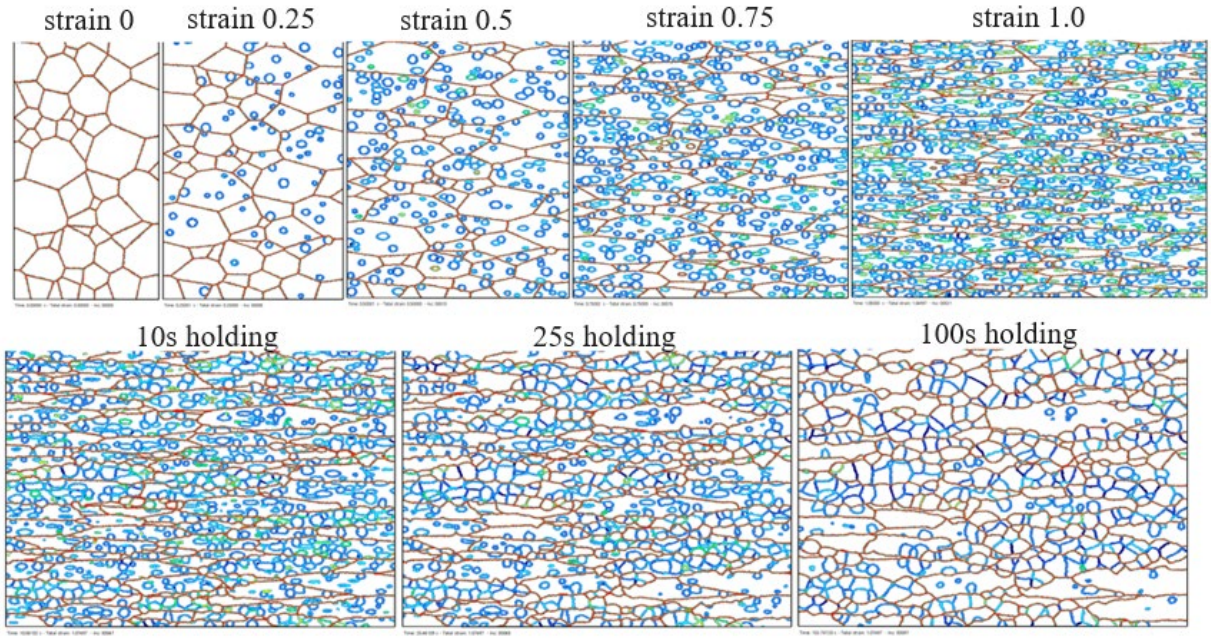

Fig. 2: Creation and evolution of sub-grains in Zircaloy-4 during CDRX and PDRX simulations (compression and maintain). Color is related to the grain boundaries energy. HAGB are in red, other ones are LAGB, more or less disoriented.

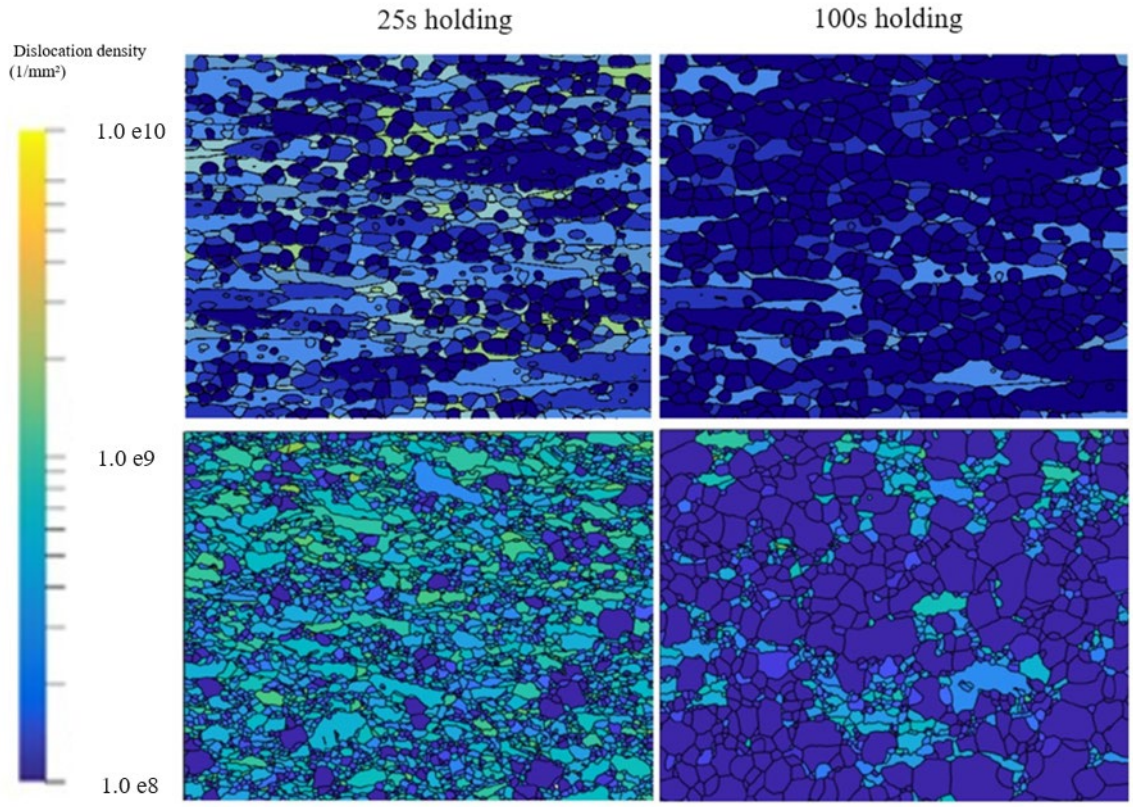

Fig. 3: Comparison between simulated (up) and experimental (down) dislocation densities evolutions after 25s (left) and 100s (right) of heat treatment.

Simulate CDRX with an evolutive population of SPP

Zirconium alloys can present some precipitation, with a solvus temperature close to the recrystallization temperatures. Precipitates are present in the microstructure and can evolve during post-dynamic phase. In the previous example, this precipitation has been neglected. The idea here is to see if it could be possible to couple the two previous models in order to present a CDRX-PDRX simulation coupled with particles dissolution, on a process similar to the one presented in the previous chapter.

In experiments, precipitates are present in the material since the beginning of the compression and conserve their equiaxed shape during it. This is one of the limits of our approach, where the SPP are simply deformed with the matrix. Furthermore, the presence of a dense SPP population in the polycrystal may modify the behavior of sub-grain generation, reducing the space available for their nucleation. This should be considered during the CDRX parameters identification, which was not the case here. For those two reasons, the presence of the precipitates during the CDRX simulation step is disturbing. Happily, during the short time of compression, the consequences of Zener pinning are rather small, as sub boundaries mainly appear and disorient, but do not have a lot of time to evolve. For those three reasons, it was decided to insert the particles only at the end of the deformation, with a quick nucleation process of a few tenths of seconds, until the desired fraction of precipitates fraction was reached. SPP are then only present in the PDRX phase, when their effect is the most important. Afterwards, a simple constant dissolution velocity is applied to the boundaries of the precipitates, leading to a complete disappearance in 180s.

Simulation results are presented in Fig. 4. The initial state of precipitation is visible in the first image, just after CDRX. After 40 seconds of PDRX, it is clearly visible that the remaining particles have bent the boundaries and sub boundaries. After 180s, all the particles have disappeared, and the microstructure is already well recrystallized. In this case, it was not clear that the presence of

the SPP has really slowed down the recrystallization process, or even modified the final grain size, which confirms the hypothesis made in the previous paragraph and by Grand et al. [18,19,27]. However, the feasibility of such simulations is proven, and further simulations will be done on different initial material configurations, and different materials.

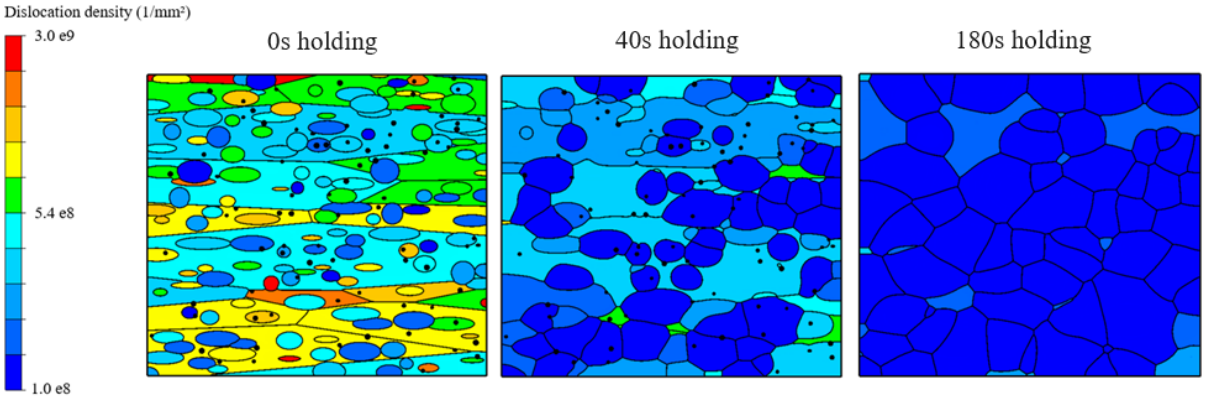

Fig. 4: Evolution of Grain and sub-grain boundaries and dislocation densities after CDRX for Zircaloy-4, with simultaneous dissolution of precipitates (black dots).

Conclusion

DIGIMU® has proven these last years to be an efficient and convenient tool to predict and better understand microstructural evolutions in industrial processes and heat treatments, simulating grain growth, Smith-Zener pinning and recrystallization. Very recently, two interesting features have been developed, enabling the simulations of SPP evolution, sub grain evolutions and a first CDRX model.

This article deals with the combination of those two features to simulate CDRX in high stacking fault materials presenting precipitates population whose solvus temperature is close to the recrystallization temperature. Even if the model presents some important approximations, such as the insertion of the sub boundaries as closed circular sub grains, it converges rapidly to realistic microstructures, enabling relevant simulations. It is possible to couple those two models together. In this case, we however preferred to insert the particles after the compression step to avoid their deformation and to not disturb the sub grain nucleation model, identified without the presence of particles. Even if the simulation with precipitates has not been strictly compared to experimental results, the Smith-Zener pinning effect is clearly visible. In this configuration, no global effect on final grain size or recrystallized fraction evolution was predicted, in accordance with Framatome observations.

The actual work will consist in confronting the model to other industrial cases, concerning zirconium alloys first, but also aluminum alloys and ferritic stainless steels, to determine its capabilities and limits in a wider range of material and processes.

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