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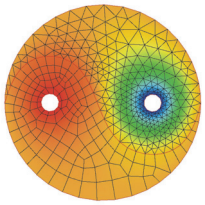

DEVELOPMENT OF NUMERICAL TOOLS FOR THE MULTISCALE MODELLING OF RECRYSTALLISATION IN METALS, BASED ON A DIGITAL MATERIAL FRAMEWORK

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Abstract

This work is currently under development within the framework of an American-European project (Digimat Project). The paper details the development of some numerical tools dedicated to the digital representation of metallic materials structures, to the generation of associated anisotropic meshes and to the finite element modelling of the polycrystalline microstructure deformation under large strains.

The level set method used for the description of the microstructure interfaces is shown to represent a common base to all these developments.

Key words: digital microstructure, polycrystal, anisotropic meshing and remeshing, finite element simulation, level set method

1. INTRODUCTION

The principal purpose of the Digimat project is to model the recrystallization using a multi-scale approach (Rollett, 1997; Kugler & Turk, 2006). The modelling effort is centred on a digital material framework. This framework is based on a digital representation of the material structure (Dawson, 2000; Dawson & al, 2005; Logé & Chastel, 2006), where data coming from different scales can be stored or probed (Cailletaud & al., 2002; Barbe & al., 2001). The digital representation can be converted into finite element meshes, which are then used to model plastic deformation and subsequent recrystallization. The local behaviour of individual microstructure components is computed through models operating at different scales. In particular, grain constitutive models are derived from crystal plasticity concepts, with appropriate hardening/recovery laws which are linked to lower scale approaches at the dislocation level. Grain boundary motion is similarly described by connecting the continuum mechanical and thermal fields to simulations at the atomistic and dislocations levels. A detailed confrontation of the multi-scale approach with experiment will be done at the ESRF synchrotron facility in Grenoble (France).

In this paper, the needed development of numerical tools is presented together with the first finite element simulations. Four main aspects of the numerical developments are described in this paper. Section 2 explains the principles of the Digimat software (dedicated to the concept of digital material) and the philosophy behind it. Section 3 presents

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the numerous advantages of the level set method used to describe the microstructure interfaces. The method represents in fact a cornerstone of the various numerical tools presented here. Section 4 is dedicated to the anisotropic meshing and remeshing strategies used to generate finite element meshes, with appropriate refinement at the grain or subgrain boundaries. Finally, section 5 illustrates the finite element modelling of the polycrystalline microstructure deformation.

Large scale parallel computations are performed using an updated Lagrangian scheme; automatic anisotropic remeshing is needed due to the amount of applied strain. Each section will describe in particular how the numerical developments take advantage of the level set description of the grain boundary network.

2. DEVELOPMENT OF THE DIGIMAT SOFTWARE

The Digital Material framework is being implemented as a software called DIGIMAT. The software must provide the means to construct virtual/digital samples and to probe them after their construction. If the digital features are not in good agreement with the experimental data, an optimization procedure must take place. Once the digital sample has been generated, an output file can be written, which contains all the necessary information for the construction of a corresponding finite element mesh (see section 4), such that digital experiments can be performed on the sample. The digital experiments considered in the Digimat project are mechanical testing (large strains), and heat treatment (recrystallization / grain growth).

Figure 2 illustrates the current development of the Digimat software. The programming work is done in C++, and a friendly user interface is created with graphical display and interactive menus. A recursive Voronoï tessellation algorithm is available and allows to define regions (grains) and subregions (subgrains). The obtained geometrical features can be combined 'manually' according to desired criteria of sizes and shapes. Interaction on the optimization scheme is anticipated with Carnegie Mellon University (USA), based on recently published considerations (Brahme & al., 2006). A sampling algorithm allocates all relevant properties to the different geometries created. Probing algorithms can measure particular instantiations of a microstructure, e.g. grain volume, grain shape distribution, or crystallographic texture. Each individual grain shape is described by a fitting ellipsoid. The microstructure can also be cut along given planes, as illustrated in figure 2. This will allow measuring the digital sample along 2D planes, as it is done experimentally. Grain size and grain shape distributions will therefore be compared with no assumption on the volumetric distribution.

Individual geometries can be converted into coarse meshes, at any scale. The considered scales are so far those of (1) the external shape – a cube in figure 1, (2) the grains – a Voronoi cell in figure 1, and (3) the subgrains, also a sub-Voronoi cell for the moment. The software contains all the tools needed to build a coarse mesh of the microstructure (at any scale) and to visualize it with the software. The output mesh files will make it possible to the user to build easily finer meshes with appropriate meshing tools (Coupez & al, 2000).

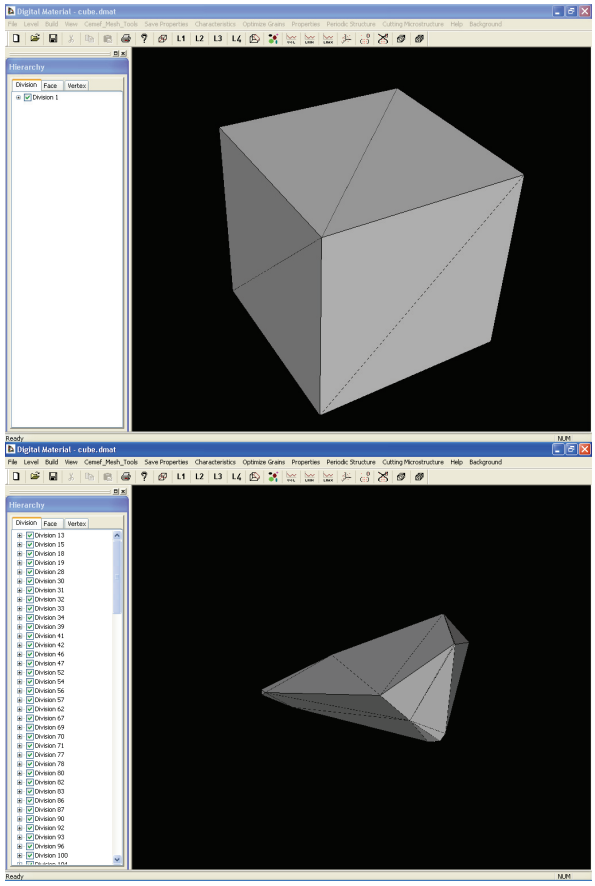

Fig. 1. Coarse mesh of the level one (top) and coarse mesh of one of the grains (bottom).

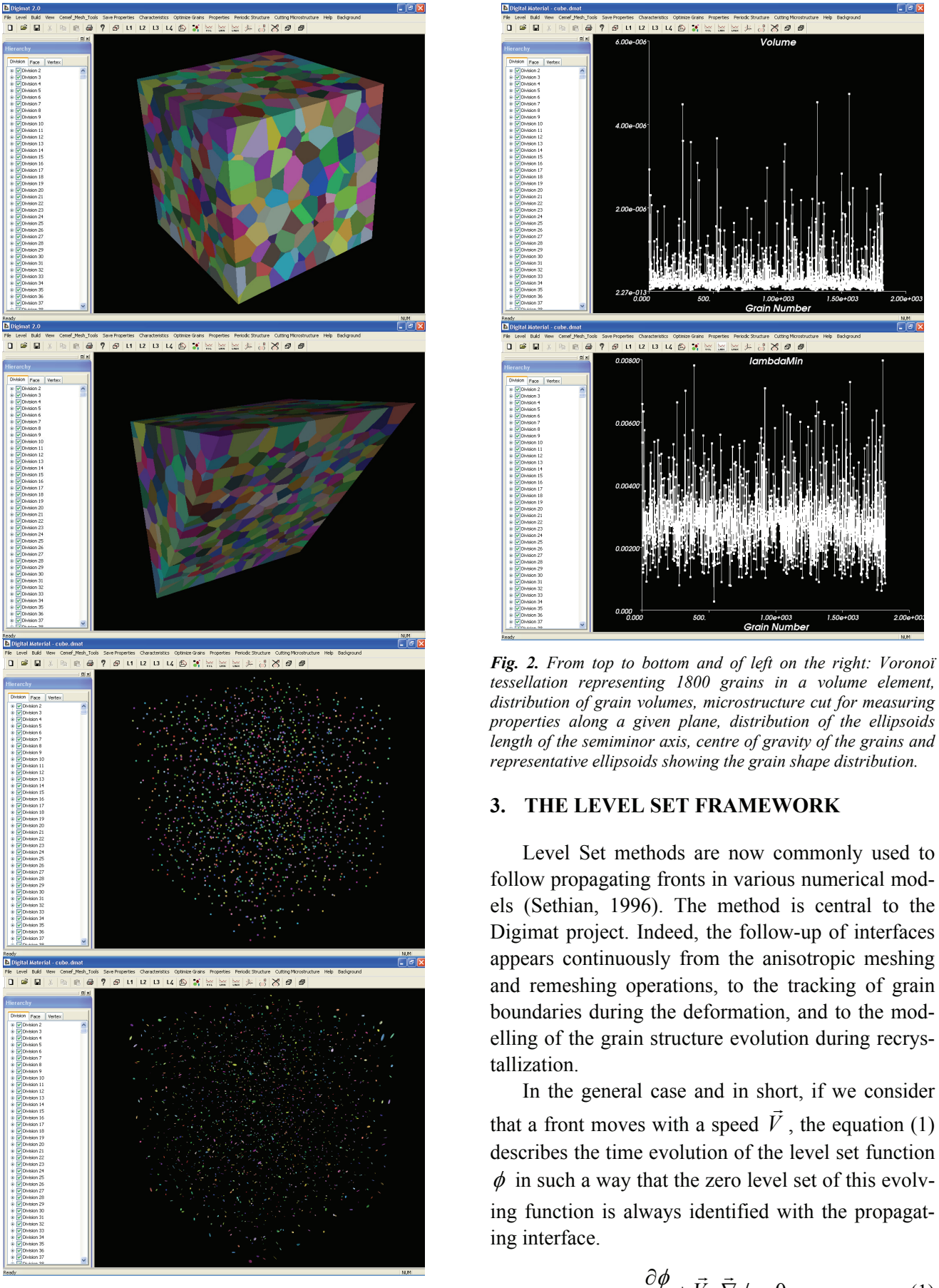

Fig. 2. *From top to bottom and of left on the right: Voronoï tessellation representing 1800 grains in a volume element, distribution of grain volumes, microstructure cut for measuring properties along a given plane, distribution of the ellipsoids length of the semiminor axis, centre of gravity of the grains and representative ellipsoids showing the grain shape distribution.*

3. THE LEVEL SET FRAMEWORK

Level Set methods are now commonly used to follow propagating fronts in various numerical models (Sethian, 1996). The method is central to the Digimat project. Indeed, the follow-up of interfaces appears continuously from the anisotropic meshing and remeshing operations, to the tracking of grain boundaries during the deformation, and to the modelling of the grain structure evolution during recrystallization.

In the general case and in short, if we consider that a front moves with a speed $\vec{V}$, the equation (1) describes the time evolution of the level set function ϕ in such a way that the zero level set of this evolving function is always identified with the propagating interface.

$$\frac{\partial \phi}{\partial t} + \vec{V} \cdot \vec{\nabla} \phi = 0 \,. \qquad (1)$$

In our framework, each individual grain or subgrain is associated to a level set function whose zero

value corresponds to the interface. This description is extremely useful to build an initial anisotropic mesh of the microstructure with appropriate refinement at the grains and subgrains boundaries, as illustrated in figure 4. Indeed, our level set functions can be used as a parameter of our anisotropic mesh generation algorithm (see section 4) because they allow to locate the zones where the mesh needs to be refined, and to define the direction of anisotropy.

Concerning the modeling of the microstructure deformation, the level set function of each grain moves according to the material velocity, which corresponds to the mesh velocity when using a Lagrangian framework. Figure 3 illustrates ten grains of the microstructure built within the Digimat software and their representation by the zero level of ten distinct level set functions. The advantage of such a description of interfaces is that it is fully compatible with automatic remeshing, i.e. the values of ϕ are directly interpolated from the old mesh to the new one. Hence remeshing operations can be anisotropic, exactly like the initial meshing operation.

Concerning the modeling of the microstructure recrystallization after deformation (this point is under development and corresponds to future objectives), the assets of this method are numerous. In fact, for this problem, the convection equation (1) is solved again for each grain, with $\vec{V}$ describing the grain boundary velocity, as defined by a kinetic law for static recrystallization (Kugler & Turk, 2004). The first advantage of this approach comes from the fact that topological changes in the evolving front, contrary to the Lagrangian methods, are handled naturally. We can easily understand the interests of this method to model recrystallization which implies complex topological events such as appearance or disappearance of grains. The second advantage comes from the fact that intrinsic geometric properties of the front are easily determined with this formulation. Indeed, at any point of the front:

$$\vec{n} = \vec{\nabla}\phi / \left\| \vec{\nabla}\phi \right\|, \qquad \kappa = -\vec{\nabla} \cdot \vec{n}\,, \tag{2}$$

with $\vec{n}$ is the unit normal at the interface and indicates the direction of propagation, and κ is the curvature of the front which is also a parameter standardly used in the kinetic law for recrystallization.

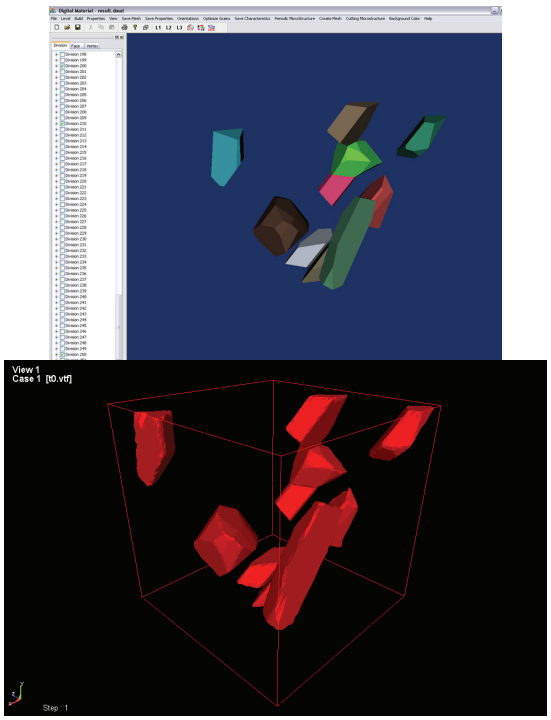

Fig. 3. *Representation of ten grains of the microstructure with Digimat (top) and with level set (bottom).*

4. GENERATION OF FINITE ELEMENT MESHES

The constructed digital microstructures illustrated in Figure 1 must be converted into finite element meshes, with appropriate refinement along the grain or subgrain boundaries. Indeed, this is needed to capture the large strain rate/stress gradients developing across grain boundaries upon deformation of the microstructure, as a result of the heterogeneous mechanical response of neighbouring grains (see next section).

Figure 4 illustrates a 250 grains digital sample created in the Digimat software and the corresponding anisotropic mesh. The mesh is made of tetrahedral elements, whose size and shape are not homogeneous. Anisotropic meshing is used along grain or subgrain boundaries, with a smaller size in the direction perpendicular to the boundary. A corresponding anisotropic metric is defined, while an isotropic metric field is used far from the boundaries. A metric is a symmetric positive tensor that represents a local base which modifies the way to compute a distance, such that:

$$< x, x >_M = {}^t x M x\,. \tag{3}$$

If M is the identity tensor, we are in the general Euclidian space.

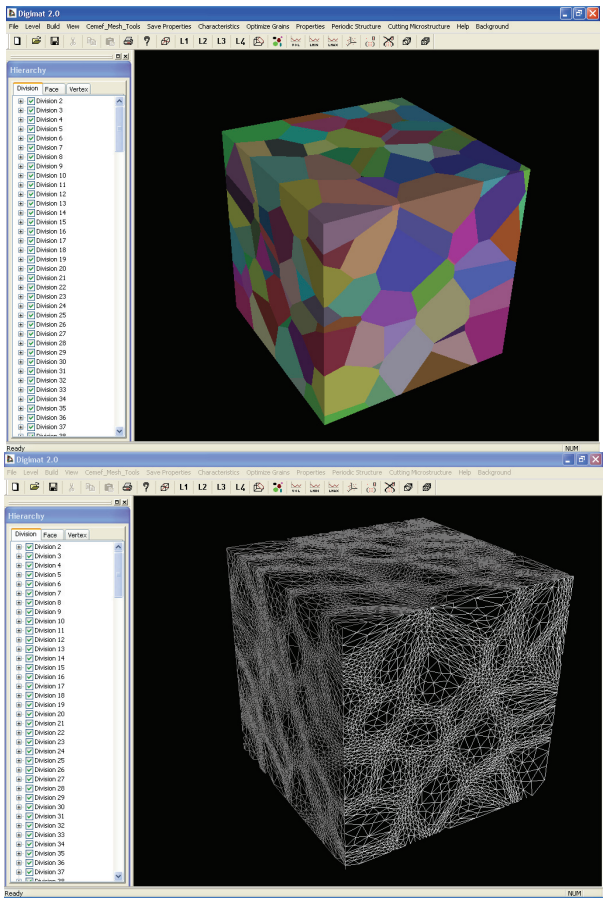

Fig. 4. *Microstructure (top) and fine anisotropic mesh of the microstructure (bottom).*

Anisotropic meshes are built by using the MTC mesher-remesher developed by Coupez (Coupez, 2000; Coupez & al 2000). MTC is a topological mesher that improves a mesh topology by considering the quality of the elements. The quality of an element is defined through a shape factor that gives to equilateral triangles the highest quality, while the worst quality corresponds to a triangle which degenerates into a segment. This quality is normalised within an interval [0,1], and the shape factor is given by

$$c(e) = c_0 \frac{|e|}{l(e)^d}, \tag{4}$$

where c_0 is a normalised coefficient, $|e|$ the volume of the element, $l(e)$ the average length of the element edges and d the space dimension. This shape factor is then modified to take into account the mesh size or the metric we want to use: the volume and the length are defined using equation (3).

The MTC mesher improves the topology of the elements by improving the quality (shape factor) of the elements that define this topology. We now have to define the metric field that gives the variable, anisotropic mesh size close to the grain boundaries. The metric is a tensor with eigenvalues which are linked to the mesh size, with eigenvectors that define the direction in which this mesh size is applied. Let us consider a simple case with only two grains (hence, one interface). The direction of mesh refinement being defined, we need to specify the mesh size in that direction, as well as the zone where the mesh size will be changed. We consequently introduce a characteristic length l_0 which will be used to characterize position, inside a grain or near the grain interface.

$$\begin{cases} |d(x)| < l_0 & \text{near the interface} \\ |d(x)| > l_0 & \text{far from the interface} \end{cases}, \tag{5}$$

with $d(x)$ the distance to the interface. If we are positioned far from the interface, the mesh size will stay at the default value, and near the interface, it will be reduced perpendicularly to this interface. Here, we choose to take advantage of the Level-Set field that is homogenous to a distance. We can therefore make the mesh size h as a function of the Level-Set value.

$$h = f(\phi(x)). \tag{6}$$

A simple example is given by the following function:

$$\begin{cases} |\phi(x)| > l_0 & \Rightarrow \quad h = h_d \\ |\phi(x)| < l_0 & \Rightarrow h = \dfrac{h_d(m-1)}{m l_0}|\phi(x)| + \dfrac{h_d}{m} \end{cases} \tag{7}$$

If x is on the interface the mesh size is minimal and is equal to the default mesh size divided by the parameter m. This mesh size increases with the "distance ϕ" (Level-Set) to the default value h_d at the distance l_0.

In the case study several grains and interfaces exist. The idea is then to repeat the above strategy for each grain, thereby giving a family of normals and distances. As we are only interested in those which are close to the interface (the others do not modify the mesh size), we can reduce the number of coupled variables {normal, distance} to the only ones for which the distance is lower than the defined criteria l_0. At this stage, if we only have one normal left, we are back to the previous case considering only one boundary. If there are more than one normal left, there are two possible situations: (a) all the normals are co-linear, and we keep only one that represents the direction of refinement, and (b) the normals are not co-linear, and we are positioned at an intersection of different grains; this means that

the mesh size must be refined in several directions. In that case, we construct a vector base induced by theses normals, and we refine along these vectors using the different mesh sizes given by the value of the Level-Set function ϕ associated to the vector (see relations (7)).

At the end of this procedure, each node of the mesh is associated to 0 to *d* normals. With 0 normal (no interface) we have an isotropic mesh and use the default mesh size; with *d* normals we have isotropic refinement (the mesh size is refined in all the directions).

Given these normals, we reduce the mesh size only in the direction of the normals, and we keep the default mesh size in the other directions. Figure 5 illustrates our method for two cases of four and ten grains, respectively. Figure 6 illustrates a very complex test case with a one thousand grains microstructure, the mesh (2 125 688 nodes, 12 385 889 elements) was obtained after a twenty six hours parallel calculation on 24 processors of a 96 cores Opteron 280 2,4GHz linux cluster.

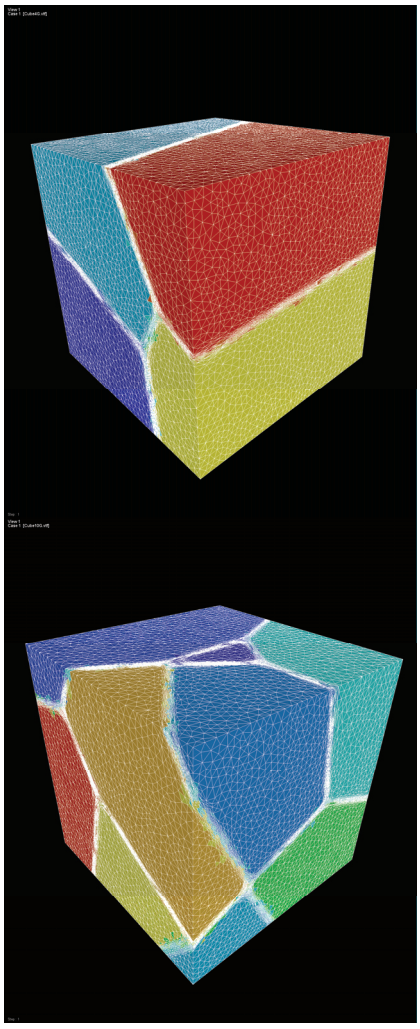

Fig. 5. *Anisotropic mesh for a four grains case (top) and for a ten grains case (bottom).*

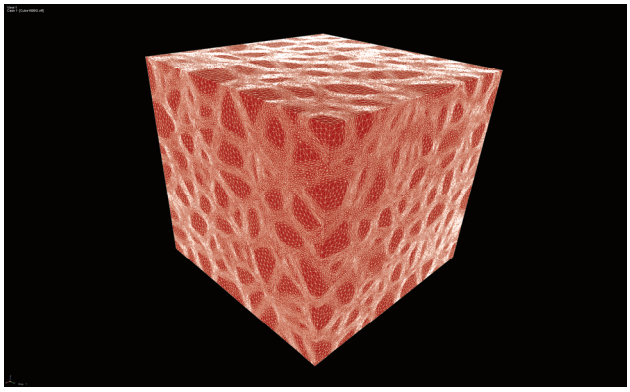

Fig. 6. *Anisotropic mesh for a one thousand grains case (2 125 688 nodes, 12 385 889 elements).*

5. FINITE ELEMENT MODELING OF THE MICROSTRUCTURE DEFORMATION

The objective is to model the large plastic deformation of a polycrystalline volume which can be compared to 3D synchrotron experiments in terms of grain size and shape distributions, crystallographic orientations and stored energy within each grain. Several numerical and modelling efforts are needed to achieve this goal. However, as a first step, our objectives are:

- The modelling of deformation of discretized numerical microstructures using an updated Lagrangian scheme with an elastic-viscoplastic crystal plasticity constitutive law, without remeshing and using a single processor.
- The development of large scale parallel computations describing the deformation of polycrystalline microstructures with automatic remeshing, but using simple viscoplastic constitutive laws (standard macroscopic laws).

In this paper, only the second objective results will be described. The finite element meshes displayed in figure 6 can be used to model plastic deformation under large strains, for example in uniaxial compression. The evolution of the microstructure is illustrated in figure 7. The constitutive law is a viscoplastic power law given by Eq. 8, where $(\boldsymbol{\sigma},\dot{\boldsymbol{\varepsilon}})$ are the Cauchy stress and strain rate tensors, respectively, $\dot{\bar{\varepsilon}}$ is the equivalent strain rate and K is the consistency.

$$\boldsymbol{\sigma} = 2K\left(\sqrt{3}\dot{\bar{\varepsilon}}\right)^{m-1}\dot{\boldsymbol{\varepsilon}}\,. \tag{8}$$

Crystallographic effects are taken into account in Eq. 8 by considering a variable value of K. Regardless of the type of constitutive law, the energy per unit volume dissipated in the material is given by

$$E = \int \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}\, dt\,. \qquad (9)$$

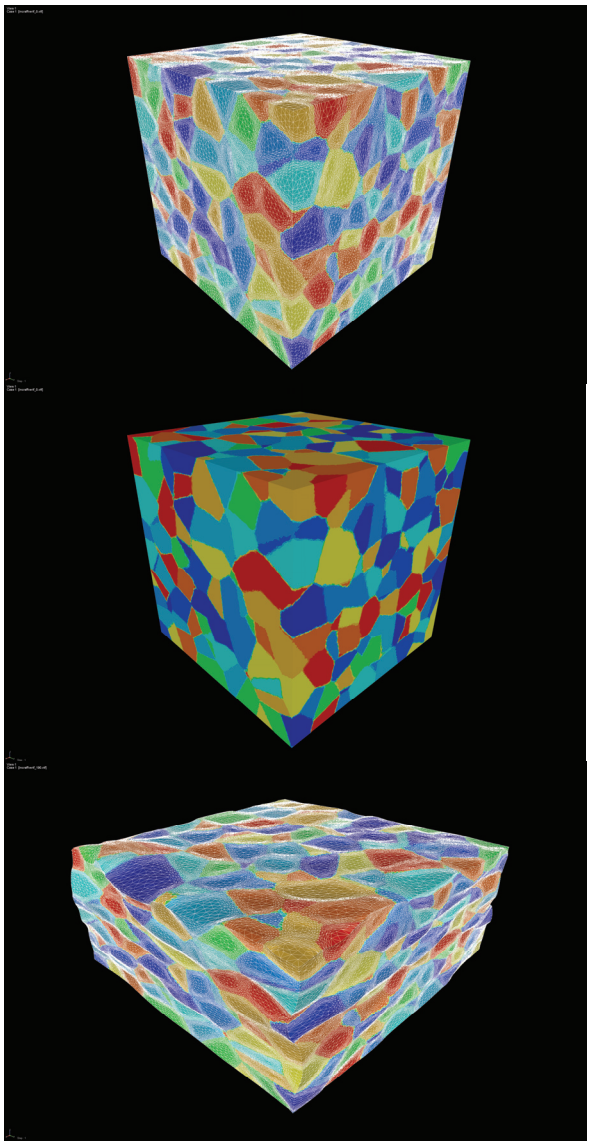

Fig. 7. *Consistency of the microstructure at the initial time with mesh (top), at the initial time without mesh (middle) and after seventy percent of deformation with mesh (bottom).*

A fraction of this energy E is stored in the material into the form of defects, and represents a driving force for subsequent static recrystallization when performing a heat treatment (see for example: Raabe & Becker, 2000; Radhakrishnan & al, 1998). Obviously E varies from one grain to another, and its spatial distribution can be used to predict Strain Induced Grain Boundary Migration (SIBM) phenomena or nucleation/growth processes in primary recrystallization. The configuration of this problem corresponds to a multi-domain Stokes problem. For the resolution, a non-linear solver is used with a Newton-Raphson algorithm. This solver is based on a mixed finite element velocity-pressure formulation and uses the so-called mini-element (P1+/P1). The mini-element is a linear isoparametric tetrahedron (triangle for 2D problems) where a bubble function is added at its center to ensure stability. A penalized slipping bilateral contact is adopted for the contact between the material and the tool used for compression.

Figure 7 illustrates a challenging test case with an engineering strain of 70% and one thousand grains. The initial anisotropic mesh contains more than two millions nodes (figure 6). During the deformation, thirty anisotropic remeshing operations were performed. This parallel test case was simulated in fifty hours on 28 processors of the cluster described in section 4.

These results illustrate the ability to perform very large scale parallel computations describing the deformation of polycrystalline microstructures with automatic anisotropic remeshing. Ongoing work includes the validation of the model using an elastic-viscoplatic crystal plasticity based constitutive law, which can be compared to standard micro-macro models, and to experiments.

6. CONCLUSION

In this paper, the Digimat project philosophy is illustrated and first numerical developments and results are described. The digital material framework started to be implemented within a software which is intended to become a freeware. Conversion of digital formats into finite element meshes is facilitated by the use of a level set description of interfaces. Automatic meshing and remeshing operations rely on the values of level set functions, both for spatial localization of the interfaces and for the definition of appropriate metrics for anisotropic mesh generation. The positioning of the interfaces is updated when large plastic strain of the polycrystalline aggregate is modelled using constitutive laws that vary from one grain to the other. More advanced constitutive laws will allow in future work to compute the stored energy field within the aggregate, which will constitute the starting point for the subsequent modelling of recrystallization. The latter model will again take advantage of the level set description of the grain boundary network, and evolve it according to appropriate kinetic laws based on both grain boundaries geometry and volumetric stored energy.

REFERENCES

Barbe, F. Cailletaud, G., Decker, L., Jeulin, D., 2001, Intergranular and intergranular behavior of polycrystalline aggregates, *Int. J. Plast*., 17, 513-536.

Brahme, A. Alvi, M.H. Saylor, D. Fridy, J. Rollett, A.D., 2006, 3D reconstruction of microstructure in a commercial purity aluminium, *Scripta Mat*., 55, 75-80.

Cailletaud, G., Diard, O., Leclercq, S., Rousselier, G., 2002, Distribution of normal stress at grain boundaries in multicrystals : application to an intergranular damage modelling, *Comp. Mat. Sci*., 25, 73-84.

Coupez, T., 2000, Génération et Adaptation de maillage par optimisation locale, *La Revue Européenne des éléments finis*, 9, 403-423.

Coupez, T., Digonnet, H., Ducloux, R., 2000, Parallel meshing and remeshing by repartitioning, *Appl. Math. Modeling*, 25, 153-175.

Dawson, P.R., 2000, *Int. J. Solids Struct*., 37, 115–130.

Dawson, P.R., Miller, M.P., Han, T.-S., Bernier, J., 2005, *Metall. Mater. Trans*., A, 36A, 1627–1641.

Kugler, G., Turk, R., 2004, Modeling the dynamic recrystallization under multi-stage hot deformation, *Acta Mat*., 52, 4659-4668.

Kugler, G., Turk, R., 2006, Study of the influence of initial microstructure topology on the kinetics of static recrystallization using a cellular automata model, *Comp. Mat. Sci*., 37, (3), 284-291.

Logé, R., Chastel, Y., 2006, Coupling the thermal and mechanical fields to metallurgical evolutions within a finite element description of a forming process, *Comp. Methods Appl. Mech. Engrg*., 195, 6843-6857.

Raabe, D., Becker, R., Modell., 2000, Simulation Mater. Sc. Eng., 8, 445.

Radhakrishnan, B., Sarma, G.B., Zacharia, T., 1998, Modeling the kinetics and microstructural evolution during static recrystallization – Monte Carlo simulation of recrystallization, *Acta Mater*., 46, 4415-4433.

Rollett, A.D., 1997, Overview of modeling and simulation of recrystallization, *Progress in Mat. Sci*., 42, 77-99.

Sethian, J., 1996, *Level Set Methods*, Cambridge University Press.

OPRACOWANIE NUMERYCZNEGO NARZĘDZIA DLA WIELOSKALOWEGO MODELOWANIA REKRYSTALIZACJI W METALACH, W OPARCIU O CYFROWĄ REPREZENTACJĘ MATERIAŁÓW

Streszczenie

Praca jest realizowana w ramach Amerykańsko-Europeskiego projektu (Digimat Project). W artykule opisano rozwój numerycznych narzędzi przeznaczonych do cyfrowej reprezentacji struktur metalicznych oraz do generowania powiązanych siatek anizotropowych dla modelowania metodą elementów skończonych dużych odkształceń polikrystalicznych mikrostruktur. Metoda ustalonych poziomów stosowana do opisu mikrostruktury stanowi wspólną bazę dla wszystkich analizowanych rozwiązań.

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