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# **Towards the simulation of the whole manufacturing chain processes with FORGE®**

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## **Abstract**

Following the metal composition and the microstructure evolution during the whole manufacturing chain is becoming a key point in the metal forming industry to better understand the processes and reach the increasing quality requirements for the parts. Thus, providing a simulation tool able to model the whole chain becomes critical. Physical phenomena occurring during the processes are nowadays better understood, providing always more relevant models for numerical simulation. However, important numerical challenges still exist in order to be able to run those simulations with the required accuracy. This article shows how FORGE® tackles those issues in order to provide highly accurate microstructure and surface treatments simulation features applied on real industrial processes.

## **1 Introduction**

It is quite obvious that final properties of forged parts depend strongly on the main forming processes, but they also depend significantly on all the other processes of the manufacturing chain. As a consequence, the core of a metal forming Finite Element (FE) software is and remains the thermo mechanical computation of the forming processes, with a lot of efforts and innovations delivered to enhance robustness, accuracy and efficiency in this domain (classical and complex rheological behaviours modelling, anisotropic mesh adaptation, bi-mesh methods, multi material simulation, smoothed tools, steady state simulations) [1-8]. However, in order to tackle their daily challenges and better communicate with suppliers and customers, the blacksmith industry will also need a more global software package able to simulate the whole manufacturing chain. Transvalor falls within this approach with the development of FORGE® and our other softwares in order to be able to provide this global metal forming simulation tool.

The knowledge in mechanical and numerical engineering in this domain has been improved a lot in the last decades, but does not permit to fully simulate the manufacturing chain yet. Experimental mechanical engineers are still working hard to enhance our comprehension of the physical phenomena and to describe them in models, as well as numerical mechanical engineers, working to deliver accurate, stable and efficient numerical platforms to run those new models on a wide range of industrial processes simulations.

A brief bibliographic review on the state of the art concerning numerical simulation of the whole manufacturing chain will be presented in the first part of this article. It will

underline both physical challenges, where experimental studies are needed, and numerical challenges, where numerical improvements are needed. Then, as a software editor, we will focus the scope of this article on some points where physical phenomena are at least partially known and already described in generic-enough models, but where the numerical methods are not completely satisfying and could be improved. It will naturally lead us to the following parts of this article, focusing on innovative methods proposed by Transvalor to better address those numerical challenges. Microstructure prediction, induction hardening simulation and nitriding simulation will be detailed and discussed.

## **2 State of the art**

For economic reasons, the metallurgical industry has always looked for reducing the number of steps in the manufacturing chain and in the same time still improving the final parts properties. As the mechanical behaviour is closely linked to the material structure at the micro and nanoscale, a quantitatively correct prediction of the structural state from casting until the final thermal and thermochemical treatments becomes crucial in order to meet both requirements.

### **2.1 Billet history**

The first step of a classic metal forming simulation consists in providing the initial billet properties. Most of the time, the billet history is neglected, and the initial state of the metal is described empirically, using in general constant parameters in the whole part. However, when defects may exist, when initial properties are not uniform, measuring the properties distribution is not straightforward. Simulating the billet history from the mill to predict those parameters would be more convenient than having to perform a complex bunch of experiments.

The numerical answer to this problem consists in connecting an existing casting simulation tool with a metal forming simulation tool. Main metal forming FE software packages have made collaboration with other software editors [9, 10]. TRANSVALOR, unlike its competitors, has interconnected two in-house software packages, THERCAST® and FORGE®, to ensure a maximal flexibility and compatibility. Available physical models allow predicting yet grain structure evolution during solidification, composition of phases in equilibrium, cracks, porosities, macro-segregations distributions and for most of them their evolutions during the whole manufacturing chain [11, 12] (see figure 1). No specific part will be dedicated to this issue in this article.

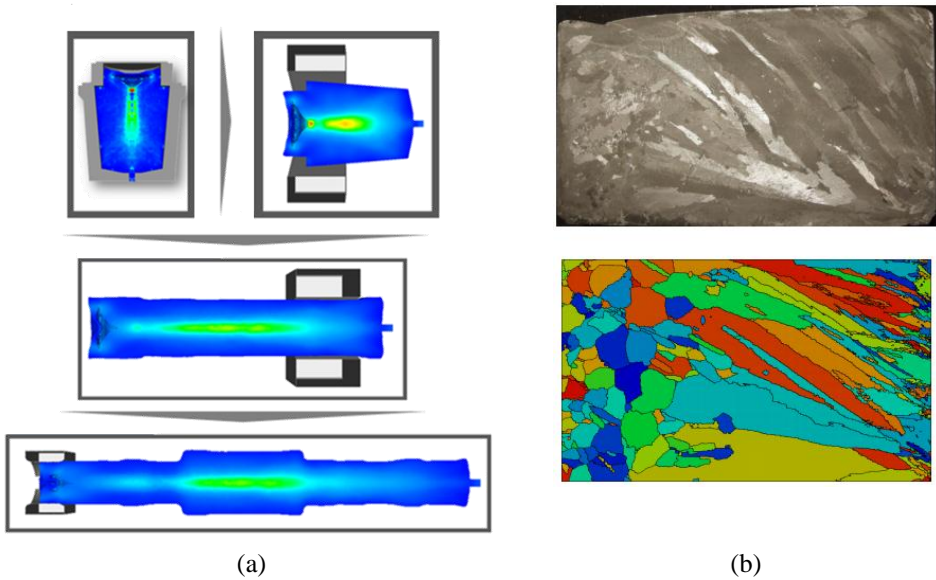


Figure 1: (a) Following porosities from casting to final shape with THERCAST® and FORGE®.  
 (b) Grain structure predicted using CAFE modelling in THERCAST® will be soon importable in FORGE® [12].

## 2.2 Microstructural evolution during forging

In response to the strong demand from the metallurgical industry to reduce characterization campaigns and to introduce more realistic physical behaviour in their simulations, numerous models are proposed today to link chemical composition, microstructural evolution and mechanical behaviour.

Mean field models are generally associated with low computation times making them suitable for full industrial computations. In these approaches, the microstructure is macroscopically described selecting representative material parameters (grain size, inclusions, phase percentage, precipitates, etc.) considered in an average way. The identification of the physical laws governing the evolution of these parameters allows predicting the microstructural evolution and their influence on the mechanical behaviour. Concerning the modelling of recrystallization phenomena, mean field models are becoming years after years more physic, more generic and more accurate [13, 14]. Even if, to our knowledge, no model is generic enough to be easily adapted to a reasonable range of alloys and processes, software editors are also working hard in order to integrate

them in their codes. The main point for the software editor is not to deliver some default models, but to make them easy to modify, and to allow an advanced user to implement new ones. It is possible in FORGE® thanks to the user routines library [15].

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. Therefore, the idea to replace these heavy and expensive experiments by full field simulations on a Representative Volume Element (RVE) is born. Over the last decades, several mesoscale numerical methods have been developed to simulate explicitly the microstructure evolution due to recrystallization during hot forming processes [16-18]. The Center for Material Forming (Cemef Mines ParisTech) has recently proposed a solution based on a FE formulation and a level-set description of phase and grain interfaces to model recrystallization and grain growth phenomena [19, 20] which will soon end up on the first industrial solution DIGI-μ® developed by TRANSVALOR.

## **2.3 Heat treatments**

The control of the structural evolutions occurring during heat treatments of metallic alloys is one of the best ways to confer at the material particular properties adapted to its future industrial application.

Physical models used to predict metallurgical structure evolutions in steels specifically on cooling and quenching are very similar for all main metal forming FE software packages. These models are generally based on the description of the transformation kinetics of austenite during isothermal treatments (represented on TTT diagrams). The anisothermal kinetics can then be calculated using the Johnson-Mehl-Avrami-Kolmogorov (JMAK) formalism [21-25] and the additivity principle [26]. Consideration of the properties (i) of each phase (rheology, thermophysical parameters) and (ii) of each phase transformation (latent heat, crystal structure change) allows predicting parts distortions. More basic semi-empirical models also exist for steel austenitization and annealing simulations.

If the thermomechanical computation and the phase transformations simulation are fully coupled one to the other, thermal computation in case of heat treatments remains challenging on the numerical point of view.

First, very local phenomena occur at the part boundaries and an accurate simulation is possible only if the mesh size is adapted to the problem. The use of isotropic or

anisotropic mesh adaptation is then critical. Moreover, modelling of heat supply for furnace or blowtorch heating and bath or spray cooling is generally quite well approximated with well-defined boundary conditions. However, in the case of induction heating and hardening, the electromagnetic computation of the eddy current in the part is necessary to deduce the heating rate distribution. The problem is driven by the well known Maxwell equations, and the challenge is now on the numerical side. The common approach, based on connection elements between the inductor and the part, is well suited for 2D computations. However, 3D computations are almost impossible because of the big band width, which means bad convergence, high computation times and bad parallel scalability [27, 28]. The other approach, chosen by TRANSVALOR, consists in discretizing the whole domain in one single mesh (parts, inductors, air) [29-35]. This method is perfectly adapted to 3D computations and is easily parallelizable, with a much smaller band width. The work to extend it to parallel computation and to processes with complex relative motions of the part and the inductor will be presented in section 5 of this article.

## **2.4 Thermochemical treatments**

The difference between a pure heat treatment and a thermochemical treatment is that in the second one, at least one physical element is diffused toward the metal.

In the case of carburizing, only carbon is diffused in the matrix, which can be simulated by most of the main metal forming simulation software packages. Diffusion properties and boundary conditions are quite well known and not really problematic. As for heat treatment, mesh adaptation is here the key numerical feature to obtain both efficiency and accuracy in the computations. The subsequent quenching can then be simulated taking into account the shift of the phase transformations kinetics due to the modification of the local carbon rate in the material.

Nitriding is a more complex process. First, on the numerical side, two elements are diffused in the metal (Nitrogen and Carbon), which cannot be simulated by all software packages. Secondly, on the physical side, several precipitates can appear and dissolve themselves, and the boundary conditions through the white layer are not yet well understood. Experimental studies start to obtain encouraging results on some alloys, and have traduced them into 1D dedicated simulation tools [36, 37]. Thermodynamical calculations provided for example by JMatPro® or ThermoCalc® can predict phases and

precipitates composition at equilibrium depending on the local chemical composition and temperature for different alloys. Gathering all this available information in user routines library, nitriding simulations have been performed with FORGE®, with results in pretty good agreement with experiments and 1D dedicated academic simulation software, as we will see in section 5 of this article.

### 3 Microstructure evolution modelling during hot forging

#### 3.1 Principle

Metal forming modelling can be predictive only if the strain rate, strain and temperature dependency of the flow behavior is correctly described. The mechanical properties and behavior 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 and phase transformation.

#### 3.2 Models description

##### 3.2.1 Semi-empirical JMAK approach

The analytical modelling of recrystallization phenomena very often uses modified versions of the JMAK equation. For isothermal and steady state conditions, the different recrystallized volume fractions  $X$  and recrystallized grain sizes  $d$  evolutions were established as a function of initial grain size  $d_0$  and processing variables such as equivalent strain rate  $\dot{\bar{\epsilon}}$ , temperature  $T$  and equivalent strain  $\bar{\epsilon}$ . An overview of well known relations is given in Table 1.

Dynamic recrystallization	Static recrystallization
$X_{d_{rx}} = 1 - \exp\left(-0.693 \cdot \left(\frac{\bar{\epsilon} - \epsilon_c}{\epsilon_{0.5} - \epsilon_c}\right)^{n_{d_{rx}}}\right)$	$X_{srx} = 1 - \exp\left(-0.693 \left(\frac{t}{t_{0.5}}\right)^{n_{srx}}\right)$
$\epsilon_c = A_1 \cdot d_0^{\alpha_1} \cdot \dot{\bar{\epsilon}}^{m_1} \exp\left(\frac{Q_1}{RT}\right)$	$t_{0.5} = A_4 \cdot d_0^{\alpha_4} \cdot \bar{\epsilon}^{n_4} \cdot \dot{\bar{\epsilon}}_f^{m_4} \exp\left(\frac{Q_4}{RT}\right)$
$\epsilon_{0.5} = A_2 \cdot d_0^{\alpha_2} \cdot \dot{\bar{\epsilon}}^{m_2} \exp\left(\frac{Q_2}{RT}\right)$	$d_{srx} = A_5 \cdot d_0^{\alpha_5} \cdot \bar{\epsilon}^{n_5} \cdot \dot{\bar{\epsilon}}_f^{m_5} \exp\left(\frac{Q_5}{RT}\right) \cdot X_{srx}^{a_{srx}}$
$d_{d_{rx}} = A_3 \cdot d_0^{\alpha_3} \cdot \dot{\bar{\epsilon}}^{m_3} \exp\left(\frac{Q_3}{RT}\right) \cdot X_{d_{rx}}^{a_{d_{rx}}}$	

Table 1: Example of equations describing (i) the kinetics of dynamic and static recrystallization and (ii) the evolution of the recrystallized grain sizes.

With an extremely low CPU time, this approach is well-suited for computations at each integration point of a finite element mesh. Implemented in the FORGE® user routines library, the model has undergone several modifications in order to be used with any thermo-mechanical local loading and to take into account multiple recrystallization steps that can be encountered during multi-pass processes [38]. Comparison between simulation and experimental results for Inconel718 in figure 2 illustrates the good agreement obtained as soon as the parameter values are correctly calibrated.

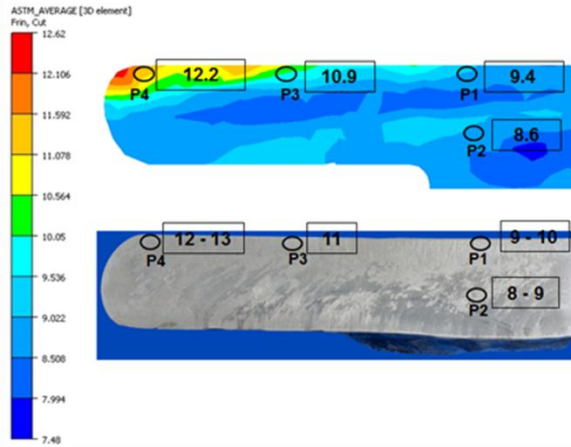


Figure 2: Comparison of simulated and measured average ASTM grain sizes on an Inconel718 part after a rotary forging process (courtesy Tecnalía, ES).

### 3.2.2 Physically based approach, mean field model

The JMAK based model requires a significant experimental effort and the parameters are difficult to interpret physically. In order to have predictive capabilities in complex industrial conditions, physically based models have emerged to link the metallurgical principles.

First of all, the microstructure is described by a set of internal averaged variables representative of the material (average dislocation density and equivalent grain size for the recrystallized and non recrystallized grains). The microstructural evolution is then directly given by the modelling of the physical laws governing the evolution of these parameters.

During a deformation step for example, the evolution of the dislocation density depends on two competing processes namely work-hardening and dynamic recovery softening and is often described by the Kocks-Mecking model:

$$\frac{d\rho}{d\varepsilon} = K_1\sqrt{\rho} - K_2\rho \quad \text{eq. 1}$$

Where the term  $K_1\sqrt{\rho}$  represents the dislocation density storage and  $K_2$  is the softening parameter. Dynamic recrystallization modelling necessitates (i) the modelling of the nucleation rate of the recrystallized grains and (ii) the modelling of the grains growth kinetics. The mean dislocation density  $\rho_m$  can then be calculated by:

$$\rho_m = (1 - X_{rx}) \cdot \rho_d + X_{rx} \cdot \rho_{rx} \quad \text{eq. 2}$$

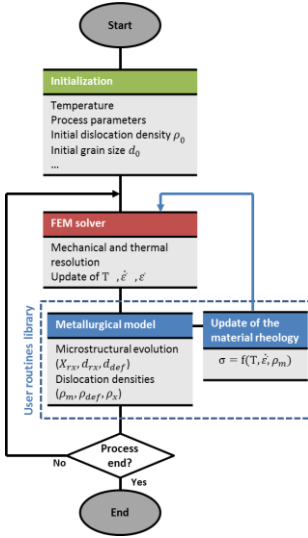
Where  $\rho_d$  is the dislocation density of the deformed matrix,  $\rho_{rx}$  is the dislocation density of the recrystallized grains and  $X_{rx}$  is the recrystallized volume fraction.

Since the metal behaviour depends on the dislocation density, such approach allows a direct coupling with the rheological behavior of the material. As an example, the Taylor equation hereafter defines the flow stress  $\sigma$  from the dislocation density by:

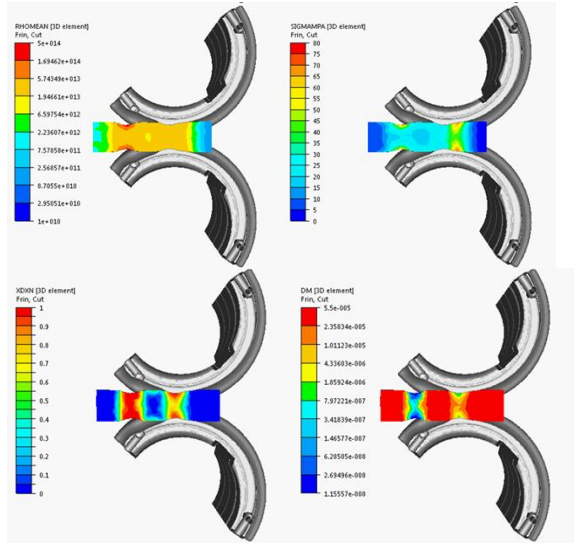
$$\sigma = \sigma_0 + M\alpha\mu b\sqrt{\rho_m} \quad \text{eq. 3}$$

With  $\mu$  the shear modulus,  $b$  the Burgers vector,  $M$  the Taylor factor,  $\sigma_0$  a “dislocation free” yield stress and  $\alpha$  a constant [13, 39].

The user routines structure proposed in FORGE® allows implementing or modifying easily such kind of models with the possibility to couple the material rheology with the metallurgical evolution (see figure 3a). These mean field approaches are generally associated with low CPU times, making them suitable for macroscale computations over a whole part (see figure 3b).



(a)



(b)

Figure 3: (a) Simplified FORGE®'s organisation chart. (b) Microstructural evolution calculated with a mean field model during a reducer-rolling simulation

### 3.2.3 Full field approach

The idea behind these approaches is that morphology and topology play a non-negligible role in the evolution of the microstructure, which is difficult to capture with other models. Microstructures are explicitly represented and simulations are performed on a Representative Volume Element (RVE) at the mesoscopic scale. The polycrystal is constructed respecting the topological characteristics of the grains and the metallurgical properties [40, 41]. This approach is based on a level set (LS) description of interfaces in a finite-element context: for each individual grain, a signed distance function  $\phi$ , gives at any point the distance to the grain boundary. Thus the interface is given by the level 0 of the function  $\phi$ . This method has the advantage of avoiding the difficult problem of tracking interfaces.

The model works in 2D and in 3D and computational cost is reduced thanks to an anisotropic mesh adaptation around the interfaces (see figure 4). As the interface moves, periodic remeshing is performed such that the refinement zone always coincides with the interface position.

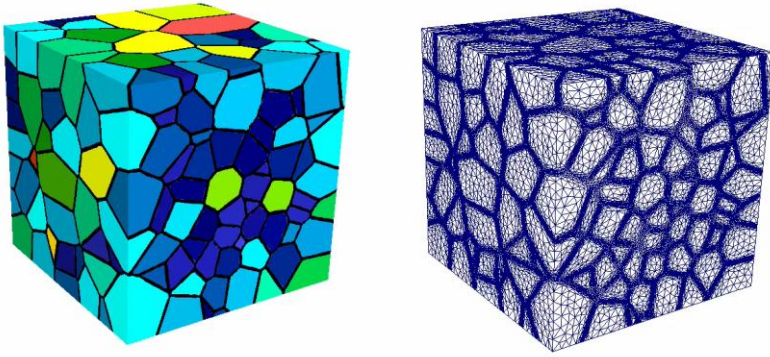


Figure 4: Polycrystal description in 3D with finite element mesh (anisotropic meshing near grain boundaries)

This approach has been introduced to model primary recrystallization, including the nucleation stage and has been extended to take into account the grain growth stage [19, 20, 41]. Moreover in this LS context, Zener pinning phenomenon can be taken into account in a natural way [42]. Thus this aspect will be considered in the development of the DIGI- $\mu$ ® software. In primary recrystallization, the kinetics of interface motion is directly linked to the state variables stored in the mesh, related to the stored strain energy. In the case of pure grain growth, the curvature of the grain boundaries pilots the interface motion (see figure 5 and 6).

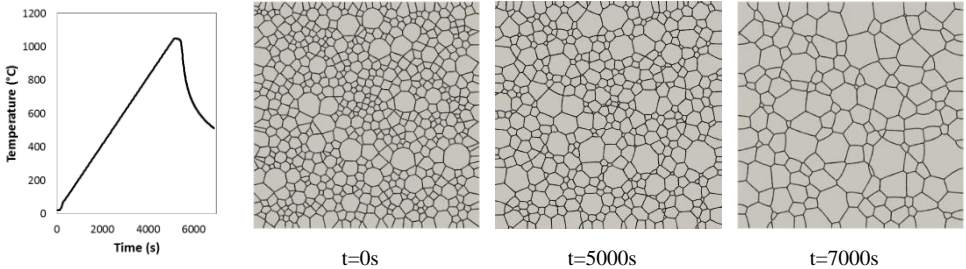


Figure 5: Microstructure evolution of a 304L stainless steel undergoing the heat treatment cycle defined on the left (pure grain growth evolution). Initial configuration with a mean grain diameter of  $90\mu\text{m}$

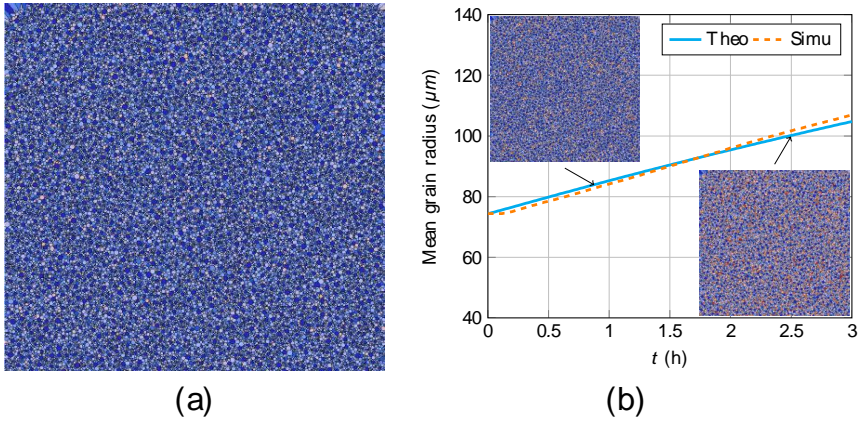


Figure 6: Microstructure evolution of a 304L stainless steel (50000 grains) during an isothermal heat treatment (1050°C) obtained with the DIGI- $\mu$ ® software: (a) initial microstructure and (b) time evolution - comparison with the Burke and Turnbull model [43, 44]

### 3.3 Conclusion

Three approaches are proposed to predict metallurgical evolutions occurring during thermo-mechanical processes. The two first approaches are based on mean field models. Well-suited for large-scale simulations, they have been implemented into FORGE® software package through the user routines library. The third approach simulates the microstructural evolution at the mesoscopic scale where the microstructure components are fully modeled. Modelling at this 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 cannot be directly integrated in a macroscale finite element computation, but they are much closer to physical phenomena and allow describing in a natural way the materials in terms of microstructural features.

## 4 Induction hardening

### 4.1 Principle

Induction heating and more precisely induction hardening are nowadays widely used. Those processes allow a quick and local heating, but predicting the temperature distribution without the use of numerical simulation in real 3D configurations is quite complex. FORGE® proposes a unique formulation for metal forming FE software,

enabling the full 3D computation of the electromagnetic field in the whole domain (air, workpiece, surrounding parts, inductors), coupled to the standard FORGE® computation.

## 4.2 Finite element formulation

The problem consists in solving Maxwell equations system in order to deduce the heat power created by the circulations of the eddy currents in the part. Several simplifications can however be applied to Maxwell equations system in the case of induction heating. First, due to the dimensions of industrial induction heating installations and the current frequencies used in the inductor, from about 50 Hz to 1MHz, the magneto-quasi-static hypothesis can be done.

The problem is then written in a single non-linear equation thanks to the A-V formulation [29] described in the first line of eq. 4.  $\vec{A}$  represents the magnetic vector potential,  $V$  the electric scalar potential,  $\rho$  the electrical resistivity and  $\mu$  the magnetic permeability. In order to have a unique solution, we have to add the two divergence free gauges corresponding to the second and third line of eq. 4.

$$\left\{ \begin{array}{l} \frac{1}{\rho} \frac{\partial \vec{A}}{\partial t} + \vec{\nabla} \times \left( \frac{1}{\mu} \vec{\nabla} \times \vec{A} \right) + \frac{1}{\rho} \vec{\nabla} V = 0 \\ \vec{\nabla} \cdot \vec{A} = 0 \\ \text{div} \left( \frac{1}{\rho} \vec{\nabla} V \right) = 0 \end{array} \right. \quad \text{eq. 4}$$

The magnetic field  $\vec{B}$  and the electric field  $\vec{E}$  are linked to  $\vec{A}$  and  $V$  by:

$$\left\{ \begin{array}{l} \vec{B} = \vec{\nabla} \times \vec{A} \\ \vec{E} = - \frac{\partial \vec{A}}{\partial t} - \vec{\nabla} V \end{array} \right. \quad \text{eq. 5}$$

This equation is discretized in space on the whole domain (inductors, air, parts, and concentrators) using Nedelec edge elements [45]. This equation is solved over a few electric current periods until the periodic state is reached (in general three periods are reasonable). Then, the mean local heating rate on the last electric period is computed and used as a heat source term in the standard thermo mechanical computation of FORGE®.

The thermo mechanical time step used in FORGE® can of course be several orders of magnitude bigger than the current period in the inductor. It is however reasonable to compute several thermo mechanical time steps with the same heat source term. A new electromagnetic computation is done only when the computation configuration has undergone significant enough changes (temperature changes, making  $\rho$  and  $\mu$  evolve, or relative motions of the parts and the inductors).

This electromagnetic formulation, in comparison with the boundary element approach, presents the advantages to generate symmetric numerical problems with small bandwidth, which ensure a good performance for sequential and parallel resolutions (Single Program Multiple Data paradigm) with iterative solvers [46, 47].

### 4.3 Results

This formulation enables the computation of full 3D complex geometries for the workpieces and the inductors. We will see in the following example local induction hardening on a crankshaft's crankpin's journal with an adapted inductor (see figure 7), with both motions of the crankshaft and of the inductor (see figure 8). After this local heating, the part is quenched in polymer and water.



Figure 7: Geometry of the part of the crankshaft and of the inductor used for local induction hardening.

During the process, the crankshaft turns around its main axis at 60 rpm. The inductor also turns around the main axis of the crankshaft at 60rpm, but also around the axis of the crankpin's journal at -60 rpm.

The austenization rate prediction during heating on a cutting plane in the crankpin’s journal can be seen in figure 8.

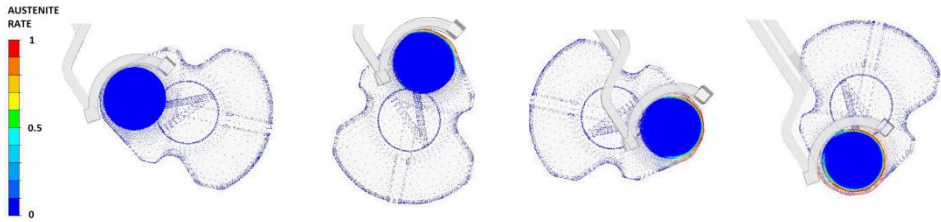


Figure 8: Austenite rate on a cutting plane in the crankpin’s journal during the first second of the induction heating process.

A precise distribution of phases during the heating and the following quenching process can be computed. Final hardness and residual stresses can be predicted by the solver (see figure 9). We can see in this example that the martensite rate is not homogeneous on the crankpin’s journal, which is indeed what is observed in the real process. The use of magnetic field concentrators should be studied in order to improve the process.

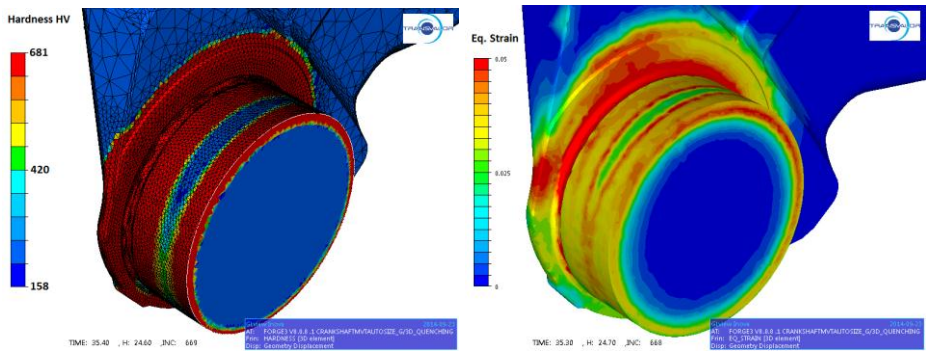


Figure 9: Hardness (HV) and equivalent strain distribution in the crankshaft’s journal after quenching.

#### 4.4 Conclusion

The technical choices made by FORGE® enable to perform with high accuracy a very wide range of induction heating simulations, with complex 3D geometries and even complex motions between the inductor and the part. Those computations are fully parallelizable, with a good parallel efficiency. Thanks to the parallel version, complex

induction heating calculations with relative motions between the part and the inductor can be done in a reasonable time on parallel cluster machine. The features presented here will be available in the next commercial release of FORGE®.

## 5 Nitriding

### 5.1 Principle

Nitriding can be applied on various metals under various conditions. It consists most commonly in diffusing nitrogen into the surface of a steel part at about 550°C to harden the surface and improve its mechanical properties. This process has a lot of advantages in terms of fatigue life, wear, friction, corrosion and a relatively good predictiveness of the induced distortions. However, it remains very long and then expensive, with about 100 hours for treating less than 1 mm of depth.

Directly at the surface, a thin white layer from 0 to 30 microns composed of nitride  $\epsilon$  and nitride  $\gamma'$  is formed. Then nitrogen will diffuse from this layer in a solid solution of ferrite to form what is called the diffusion layer, which is about 0.1mm to 1mm thick (see figure 10). Some of this freely diffusing nitrogen will precipitates with various elements of the alloy, included carbon. This is the reason why carbon diffusion can play an important role, even without carbon enrichment of the part: the gradient created in the freely diffusing carbon because of nitrogen and carbon precipitates will also engender a diffusion of the dissolved carbon, and then can modify the composition at equilibrium of the alloy. The presence of the nitrogen precipitations is the main cause of hardening and of the creation of compressive stresses.



Figure 10: Micrograph showing the white layer and the diffusion layer after nitriding (Arts et Metiers ParisTech Aix-en-Provence)

## 5.2 Finite element formulation

Our task during the DEFINIT project consisted in adapting the dedicated 1D nitriding simulation tool, developed at Arts et Metiers ParisTech in Aix-en-Provence, to full industrial 3D simulations, and confront it to the industrial partners' results [36, 37]. In our finite element simulation, the problem is described by adding several variables at each element: the rate of free nitrogen, free carbon (free means here dissolved, free to diffuse), and the rate of phases and precipitates. First, the evolution of free carbon and nitrogen rates is computed at each node by solving two diffusion problems, described by the following equation.  $C$  represents here the chemical element concentration free to diffuse, and  $D$  the diffusivity.

$$\frac{\partial C}{\partial t} = \text{div} \left( D \overrightarrow{\text{grad}}(C) \right) \quad \text{eq. 6}$$

Then, the composition of the metal in the element is computed depending on temperature (which is in general constant), carbon rates and nitrogen rates. Precipitates can be formed or dissolved, also modifying the free carbon and nitrogen rate. All data needed to compute the metal evolution can be obtained with the software JMatPro or Matcalc. The composition computed at each element enables local volume variation computation and hardness estimations.

Of course, such a computation only makes sense if the mesh is fine enough at the boundaries to model the phenomenon, which means that the mesh size must at all cost be smaller than 0.2 mm for a 1mm diffusion layer, or even smaller.

## 5.3 Results

We have the privilege to present here some results we obtained on a fully nitrided gear, provided with courtesy of Airbus Helicopters, one of the partners of the DEFINIT project (see figure 11).

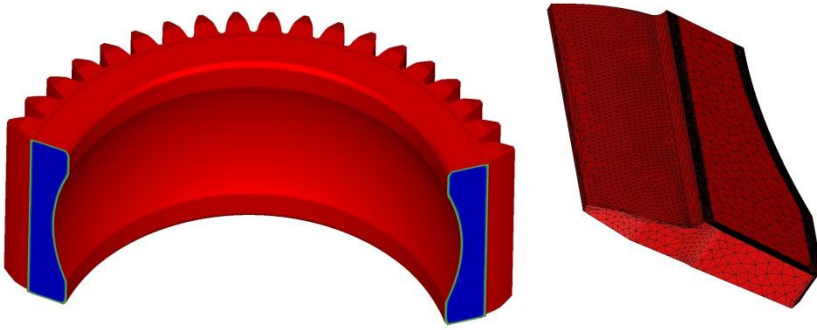


Figure 11: Geometry of the gear provided by Airbus Helicopters (the blue zone is not affected by the nitriding process), and the corresponding anisotropic mesh used to the finite element simulation (a fourth of a tooth).

The use of anisotropic mesh is here of first importance in order to describe the phenomenon occurring in the diffusion layer, but on a fourth of a tooth. We can obtain a mesh size equal to 0.05mm at the boundaries with only 22000 nodes in the mesh. In comparison, we would have needed 1.5 millions of nodes with an adapted isotropic mesh to obtain the same precision (see figure 12).

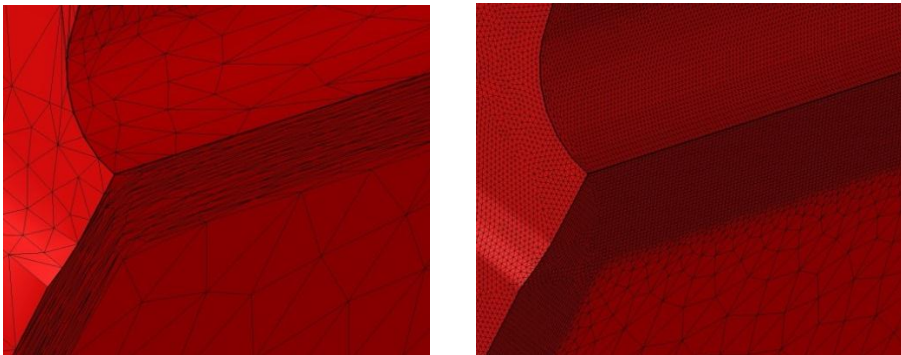


Figure 12: Comparison between an anisotropic (22000 nodes) and an isotropic mesh (1.5 millions of nodes) providing the same accuracy for nitriding simulations.

Using material data provided by JMatPro® and the results of the free carbon and free nitrogen diffusion in the material, it is possible to compute the composition of the metal and the presence of precipitates in the diffusion layer. As illustrated in figure 13, we can

obtain the characteristic carbon, nitrogen and precipitates rate in function of depth [36, 37].

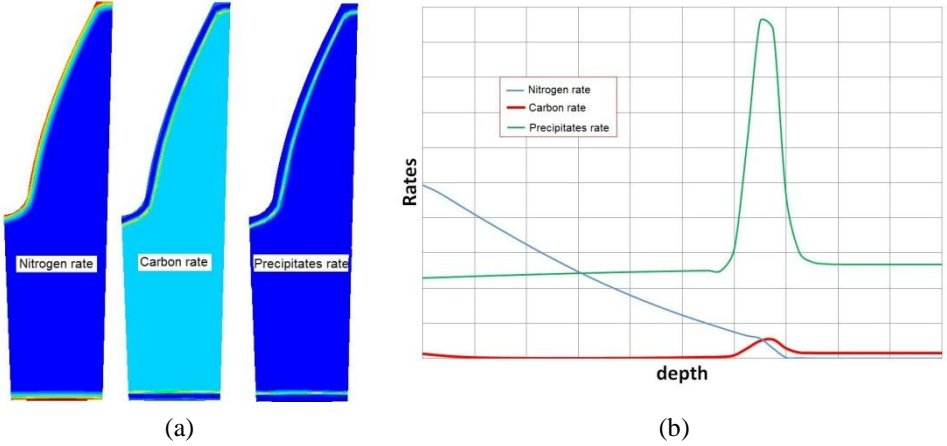


Figure 13: (a) Overview of the composition of the diffusion layer predicted by FORGE® on the gear provided by Airbus Helicopters using 2D distributions on the medial plane of the gear. (b) Corresponding 1D curves in function of the depth. No scales for confidentiality issues.

## 5.4 Conclusion

With those simulations, FORGE® has opened the doors of full 3D simulation of nitriding on industrial parts. First results are encouraging. Thanks to anisotropic meshing, accurate predictions can be obtained in the diffusion layer of a full industrial part. Parameters data files can be provided by JMatPro® or ThermoCalc® for first approximation simulations, allowing the user to easily predict phase and precipitates distribution, and then deducing hardness, residual stresses and distortion thanks to the full thermo mechanical simulation. We will carry on this ongoing work to provide you as soon as possible an advanced industrialized nitriding simulation tool in the commercial version of FORGE®.

## 6 Conclusion

In order to match the increasing quality requirements for the mechanical parts, a better understanding of the effect of the manufacturing processes on metal composition and microstructure evolution is needed. In the last decades, a lot of experimental work has been carried out to study the different physical phenomena at work, and build models.

Those models have been implemented in FE software packages and have democratized microstructure computations.

The main issue from the experimental point of view is not only to describe the phenomena occurring in the different processes but also to obtain the material parameters for the models. This long term work requires high technical and scientific knowledge as well as advanced laboratory devices. Our historic and on-going links with Cemef Mines ParisTech and our collaborations with renowned customers and academic research laboratories allow us enriching our software packages with the most relevant models and corresponding associated data.

From the numerical point of view, this article has shown that the main issues for microstructure and surface treatments simulations were not so different than those encountered in usual metal forming simulations. The key is to provide a performing simulation tool able to run those models on complex industrial workpieces, to catch local phenomena with always more accuracy, and everything in a reasonable computation time.

In order to describe with accuracy the microstructure evolution in a component, with mean field models, during induction hardening or nitriding, or even more to follow grain topology on a representative volume element, the first requirement is to discretize the domain finely enough. Isotropic and anisotropic mesh adaptation is the first answer in order to reduce as much as possible the number of degrees of freedom. However, when it is not anymore possible to reduce it, parallel and massive parallel computations must be used. For that reason, each TRANSVALOR's software package is based on a full parallel approach, which allows obtaining very high parallel efficiency and very high speedups. To complete that, an open data structure based on user routine concept allows the user to adapt those models to its particular needs and then to improve the predictions provided by the simulation.

In order to make sure that any user will obtain with FORGE® and any other TRANSVALOR's software packages the best accuracy cost ratio for his advanced physical model applied to industrial configurations, those lines of work will remain in the future among Transvalor's highest priorities.

## Literature

- |     |  |   |
|-----|--|---|
| /1/ | Revil-Baudard, B.<br>Massoni, E.   | Simulation of the anisotropic behavior of titanium alloys during sheet metal forming<br>In: International Journal of Material Forming, vol.2 (2009) pp.73-76  |
| /2/ | Demurger, J.<br>Forestier, R.<br>Kieber, B.<br>Lasne, P.                     | Deep rolling process simulation : impact of kinematic hardening on residual stresses<br>In: ESAFORM – April 2006 – Glasgow, U.K.  |
| /3/ | Cao, T.-S<br>Montmitonnet, P.<br>Bouchard, P.-O                              | A detailed description of the Gurson–Tvergaard–Needleman model within a mixed velocity–pressure finite element formulation<br>In: International Journal for Numerical Methods in Engineering, vol. 96 (2013) pp.561–583 |
| /4/ | Perchat, E.<br>Francois, G.<br>Coupez, T.                                    | Multi criteria anisotropic adaptive remeshing for sheet metal forming in FORGE®<br>In: NUMISHEET 2014 – January 2014 – Melbourne, Australia   |
| /5/ | De Micheli, P.<br>Perchat, E.<br>Ducloux, R.<br>Digonnet, H.<br>Fourment, L. | Dramatic speed-up in FEM simulations of various incremental forming processes thanks to multi-mesh implementation in FORGE®<br>In: NEMU – June 2013 – Fellbach, GERMANY   |
| /6/ | Chenot, J.-L.<br>Beraudo, C.<br>Bernacki, M.<br>Fourment, L.                 | Finite element simulation of multi material metal forming<br>In: Procedia Engineering 10/2014, issue 81, pp 2427-2432   |
| /7/ | Hachani, M.<br>Fourment, L.  | A smoothing procedure based on quasi-C1 interpolation for 3D contact mechanics with applications to metal forming<br>In: Computers & Structures 01/2013, issue 128, pp 1-13   |
| /8/ | Ripert, U.<br>Fourment, L.   | Efficient numerical simulation of steady-state metal forming processes by an iterative surface calculation<br>In: METALFORMING 2014 – sept. 2014 – Palermo,   |

## ITALIA

- /9/ Hahn, I. Sequential Casting/Forging Simulations Aid Forged Steel Quality  
Schneider, M. In: FORGE – June 2014  
Schafstall H. [http://digital.bnpmedia.com/article/Sequential\\_Casting-Forging\\_Simulations\\_Aid\\_Forged\\_Steel\\_Quality/1723314/211542/article.html](http://digital.bnpmedia.com/article/Sequential_Casting-Forging_Simulations_Aid_Forged_Steel_Quality/1723314/211542/article.html)  
Barth, C.
- /10/ Skripalenko, M.M. Computer Modeling of Chain Processes in the Manufacture of Metallurgical Products  
Bazhenov, V.E. In: Metallurgist, May 2014, Volume 58, Issue 1-2, pp 86-90  
Romantsev, B.A.  
Skripalenko, M.N.  
Koltygin, A.V.  
Sidorov, A.A.
- /11/ Jaouen, O. From hollow ingot to shell with a powerful numerical simulation software tool  
Costes, F. In: iFM 2014 - 11th International Conference on Integrated Formal Methods - sept. 2014, Bertinoro, Italy  
Lasne, P.  
Barbelet, M.
- /12/ Carozzani, T. 3D CAFE modeling of grain structures: application to primary dendritic and secondary eutectic solidification  
Digonnet, H. In: Modelling Simul. Mater. Sci. Eng. 20 (2012) 19 p.  
Gandin, Ch-A.
- /13/ Bernard, P. A two-site mean field model of discontinuous dynamic recrystallization  
Bag, S. In: Materials Science and Engineering: A, Vol. 528 (2011) pp 7357-7367  
Huang, K.  
Logé, R.E.
- /14/ Mukherjee, M. Modelling of microstructure and flow stress evolution during hot forging  
Prahl, U. In: Steel Research Int. 81 (2010) pp.1102-1116  
Bleck, W.
- /15/ FORGE® NxT Reference documentation
- /16/ Rollett, A.D. A hybrid model for mesoscopic simulation of recrystallization  
Raabe, D. In: Comput. Mater. Sci. 21 (2001) pp. 69-78
- /17/ Piekos, K. Generalized vertex model-Study of Recrystallization in copper  
Tarasiuk, J.

- Wierzbowski, K. In: Recrystallization and Grain Growth III Proc. (Jeju Island, Korea) (2007) pp. 1157-1162
- /18/ Bacroix, B. Phase-field models for microstructure evolution  
In: Ann. Rev. Mater. Res. 32 (2002) pp. 113-140
- /19/ Bernacki, M. Finite element model of primary recrystallization in  
Resk, H. polycrystalline aggregates using a level set framework  
Coupez, T. In: Modelling Simul. Mater. Sci. Eng. 17 (2009) 22 p.  
Logé, R.E.
- /20/ Bernacki, M. Level set framework for the finite-element modelling of  
Logé, R.E. recrystallization and grain growth in polycrystalline  
Coupez, T. materials  
In: Scripta Materialia 64 (2011) pp 525-528
- /21/ Johnson, W. Reaction kinetics in processes of nucleation and growth  
Mehl, R. In: Trans. Am. Inst. Min. Metall. Eng., vol. 135 (1939) pp.  
416-458
- /22/ Avrami, M. Kinetics of phase change, I. General theory  
In: Journal of Chemical Physics, vol. 7 (1939) pp. 1103-  
1112
- /23/ Avrami, M. Kinetics of phase change, II. Transformation-time relations  
for random distribution of nuclei  
In: Journal of Chemical Physics, vol. 8 (1940) pp. 212-224
- /24/ Avrami, M. Kinetics of phase change, III. Granulation, phase change  
and microstructure  
In: Journal of Chemical Physics, vol. 9 (1941) pp. 177-184
- /25/ Kolmogorov, A.N. Statistical theory of crystallization of metals  
In: Bull. Acad. Sci. USSR Mat Ser. 1, vol. 24 (1937) pp.  
355-359
- /26/ Cahn, J.W. Transformation kinetics during continuous cooling  
In: Acta Metall. 4(6) (1956) pp.572-575
- /27/ L'Eplattenier, P. An MPP version of the Electromagnetism module in LS-  
Ashcraft, C. DYNA for 3D coupled Mechanical-Thermal  
Ulacia, I. Electromagnetic simulations,  
In: International Conference on High Speed Forming –

- march 2010, Columbus, Ohio, USA
- /28/ L'Eplattenier, P. LS-DYNA® R7: Update on the electromagnetism module  
Caldichoury, I. (EM)  
Anton, J. In: 9th European LS-DYNA Conference 2013
- /29/ Cardinaux, D. A coupled multi-physics model for induction heat  
Bay, F. treatment processes.  
Chastel, Y. In: Computer Methods in Materials Science 2010, issue  
10(4), p307
- /30/ Bay, F. Numerical Analysis and Optimisation of Multiphysics  
Cardinaux, D. Problems Involving Electromagnetic Couplings.  
Naar, R. In: proceedings of the seventh international conference on  
engineering computational technology, No. 26, Chapter-8,  
sep. 2010, Valencia, Spain.
- /31/ Naar, R. Numerical optimisation for induction heat treatment  
Bay, F. processes  
In: Applied Mathematical Modelling 37 (2013), pp 2074-  
2085
- /32/ Bay, F. A numerical model for induction heating processes  
Labbe, V. coupling  
Favennec, Y. electromagnetism and thermomechanics  
Chenot, J.-L. In: International journal for numerical methods in  
engineering 2003, issue 28, pp839-867
- /33/ Bay, F. Computational modelling for electromagnetic forming  
Zapata, J.A. processes.  
In: Proceedings of the International Scientific Colloquium  
Modelling for Electromagnetic Processing, pp.259-264 -  
ISBN 978-3-00-046736-3, Sep 2014, Hannover, Germany.
- /34/ Zapata, J.A. Magnetic Pulse Forming: Simulation and Experiments for  
Bay, F. high-speed forming processes.  
In: Proceedings of the Advances in Materials & Processing  
Technology Conference, Nov 2014, Dubaï, United Arab  
Emirates.
- /35/ Internet site of software package "Flux" :

- <http://www.cedrat.com/en/software/flux.html>
- /36/ Jegou, S. Phase transformations and induced volume changes in a  
Barrallier, L. nitrided ternary Fe-3%Cr-0.345%C alloy  
Kubler, R. In: Acta Materialia 2010, issue 58(7) pp2666-2676
  - /37/ Jegou, S. Evolution of residual stress in diffusion zone of a model  
Barrallier, L. Fe-Cr-C alloy during nitriding. HTM  
Kubler, R. In: Journal of Heat Treatment and Materials 2011, issue  
Sonnens, M.A.J. 66(3), pp 135-142.
  - /38/ Teodorescu, M. Modeling recrystallization for 3D multi-pass forming  
Lasne, P. processes  
Logé, R. In: Materials Science Forum Vols. 558-559 (2007) pp  
1201-1206
  - /39/ Montheillet, F. A grain scale approach for modeling steady-state  
Lurdos, O. discontinuous dynamic recrystallization  
Damamme, G. Acta materialia, vol. 57, no. 5 (2009) pp. 1602-1612
  - /40/ Cruz-Fabiano, A.- Assessment of simplified 2D grain growth models from  
L. numerical experiments based on a level set framework  
Logé, R. In: Computational Materials Science, 92 (2014 ) pp.305–  
Bernacki, M. 312
  - /41/ Hitti, K. Precise generation of complex statistical representative  
Laure, P. volume elements (RVEs) in a finite element context  
Coupez, T. In: Computational Materials Science, 61(2012) pp.224–238  
Silva, L.  
Bernacki, M.
  - /42/ Agnoli, A. Development of a level set methodology to simulate grain  
Bozzolo, N. growth in the presence of real secondary phase particles  
Logé, R. and stored energy– application to a nickel-base superalloy  
Franchet, J.-M. In: Computational Materials Science, 89 (2014) pp.233–  
Laigo, J. 241  
Bernacki, M.
  - /43/ Burke, J. E. Recrystallization and grain growth  
Turnbull, D. In: Progress in Metal Physics, vol. 3 (1952) pp. 220-292
  - /44/ Scholtes, B. Advances in level-set modelling of recrystallization at the

- Shakoor, M.                    microscopic scale – development of the Digi- $\mu$  software  
 Bozzolo, N.                    In: ESAFORM 2015, Graz, Austria, April 15-17 2015  
 Bouchard, P.-O.  
 Settefrati, A.  
 Bernacki, M.
- /45/    Nédélec, J. C.                A New Family of Mixed Finite Elements in  $R^3$   
    In: Numer. Math, vol. 50, pp.57–81, 1986.
- /46/    Coupez, T.                    Parallel simulation of 3D forming processes  
    In: Proceedings of the International EUROSIM Conference  
    pp. 221-228, june 1996, Delft, The Netherlands.
- /47/    Coupez, T.                    From a Direct Solver To a Parallel Iterative Solver in 3-d  
    Forming Simulation.  
    In: International Journal of High Performance Computing  
    Applications, dec. 1997, 11: 277-285,  
    doi:10.1177/109434209701100402