# The newest benefits of simulation for heat treatment & microstructure prediction

# A practical overview of recent developments in process modelling for heat treatment operations and microstructure prediction

Dipl.-Ing **Olivier Krafft,** Transvalor SA, Mougins (Frankreich) Dr. **Amico Settefrati,** Transvalor SA, Mougins (Frankreich) Dipl.-Ing **Patrice Lasne,** Transvalor SA, Mougins (Frankreich)

# Kurzfassung

Unser Vortrag stellt die Vorteile in der Simulation der Wärmebehandlung und der Vorhersage der Mikrostruktur vor. In den letzten Jahren wurden viele Entwicklungen in numerischen Methoden und Material-Modellen implementiert, um die Software zu verbessern. Die meisten Wärmebehandlungen in der Materialumformung wie z.B. Austenetisierung, Aufkohlung, Härten und Nitrierung von Stahl können heutzutage mit FORGE® simuliert werden. Wir zeigen weitere Verbesserungen in der Vorhersage der Induktionserwärmung und des Induktionshärtens. Weiterhin beschäftigen wir uns mit der Mikrostruktur und setzen den Schwerpunkt auf die Phasenänderungen bei Titanlegierungen in der Warmumformung. Zum Ende zeigen wir laufende Entwicklungen, die von einfachen makroskaligen Modellen zu zukünftigen mesoskaligen Modellen führen sollen und so eine Simulation polykristalliner Mikrostruktur ermöglichen werden

# Abstract (optional)

This article aims at promoting process simulation in the forging industry by presenting the newest opportunities available in Transvalor simulation software so-called FORGE®. The topics covered include heat treatment simulations among those autenitization, quenching, carburizing and nitriding. Focus is also given to the software novelties related to induction forge heating and induction heat treating for surface hardening. In a second part, recent work related to the modelling of phase transformation for titanium alloys is highlighted allowing the prediction of  $\beta$  phase and of every  $\alpha$  phases during the forming cycle. Finally, leading edge modelling based on full field approach introduces grain size prediction at mesoscale level and its implementation into the new so-called DIGIMU® software.

#### 1. Introduction

For almost three decades, Transvalor has been involved into process modelling and is supporting the forging industry with robust and reliable simulation software in order to improve the quality of the forged components, shorten the time-to-market and reduce the cost. However, the ambition has changed over the time and forging designers are nowadays focusing on the entire manufacturing process chain. Therefore, the simulation objectives are no longer targeting only on the forging sequence itself, but on questions related to the metallurgy, the heat treatment operations and the prediction of in-use properties. In this matter, this paper is presenting a global overview of the simulation benefits applied to heat treatment & metallurgy together with an introduction to the most recent developments implemented into FORGE® software in the field of induction heating and microstructure prediction.

#### 2. Review of Heat Treatment Capabilities

Several heat treatments and thermochemical treatments are used in the metal forming industry to give the desired material properties before and after the forming stages.

For hot forming processes, the billet is heated to become more ductile and therefore reach great deformation rate with reasonable press force. The heating part can be achieved thanks to two main ways: furnace or induction heating. Furnace heating is used for all kinds of parts: from small parts to huge ingots in open die forging. Induction heating is used on small to medium parts and can focus the heat on specific areas. The material heating induces changes of microstructure which are very important for the coming forming stages.

In case of furnace heating; the engineers optimise the heating cycle to guarantee correct microstructure with the shortest cycle to avoid loss of time and gas. Small parts can be heated in few minutes whereas ingots used in open die forging requires several hours.

In case of induction heating, the electromagnetic effects are very complex to predict. Therefore simulation is a key tool to understand and master this process.

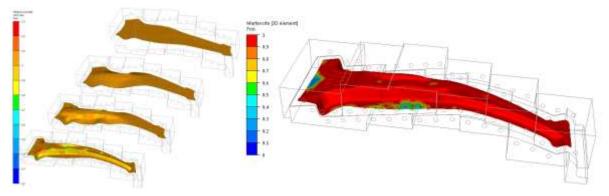
Changes of temperature during heating processes lead to a microstructural evolution. In case of low-alloy steels, the metallurgical phases present at room temperature will transform in austenite as soon as the temperature is high enough: this is called austenitization. At low heating rates, these transformations start at a given temperature (A1) and complete austenitization is reached at higher temperature (A3). A1 and A3 are thermodynamic values depending on chemical composition. For higher heating rates, phase transformations are shifted towards higher temperatures. It is therefore necessary to be able to propose models

taking into account phase transformation kinetics in order to predict the various eventualities. Four austenitization models have been developed into FORGE® software:

- Thermodynamic equilibrium model: the simplest model concerning the slowest heating rates, valid for a large range of FORGE® applications.
- JMA model with isothermal TTA: requiring the isothermal TTA diagram, this model predicts the austenite formation kinetic. It can be used for both slow and rapid heating.
- Continuous TTA: requiring the continuous TTA diagram, this model can also be used for both slow and rapid heating.
- Simplified Leblond and Devaux model: model particularly adapted to extreme heating rates.

Once the material has the proper microstructure and temperature for the forming stages; the heat treatment can be done during or after the forming stages. The heat treatment consists generally in a more or less strong cooling to reach the desired microstructure: air cooling or quenching in a liquid medium (water, oil or polymer).

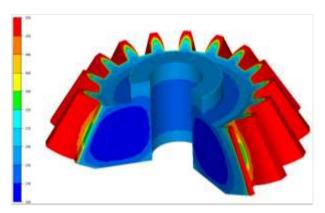
If the dies are cooled down thanks to a temperature regulation device; the desired microstructure can be achieved at the end of the forming stages. This process is mainly used in case of hot sheet metal forming. A coupled model between the thermal, mechanical and microstructural aspects is thus necessary. FORGE® is able to merge and couple the forming data and the heat treatment data to perform such a simulation. In addition to the classical flow curves and thermophysical properties, heat treatment simulations require specific material data like for example phase transformation kinetics.



Picture1: B-Pillar - Thickness evolution and micro-structure prediction after the forming and controlled cooling

Metallurgical models used to predict metallurgical structure evolutions in steels on cooling and quenching are very similar in all major FEM software. These models are generally based on the description of the transformation kinetics of austenite during isothermal treatments (represented on TTT diagrams) using the Johnson-Mehl-Avrami-Kolmogorov (JMAK) formalism [1-5]. The anisothermal kinetics can then be calculated by considering the additivity of the transformations. Consideration of the properties of each phase (rheology, thermophysical parameters) and of each phase transformation (latent heat, crystal structure change) allows predicting parts distortions.

To perform accurate simulations we need material data including transformation kinetics, rheological and thermomechanical properties. FORGE® software has been interfaced with external material database like JMatPro® from Sente-Software. A Transvalor tool has been also developed to compute a TTT diagram from the chemical composition and grain size of the steel grade. Another possibility of this tool is the conversion of a given CCT diagram into a TTT diagram used in our model.

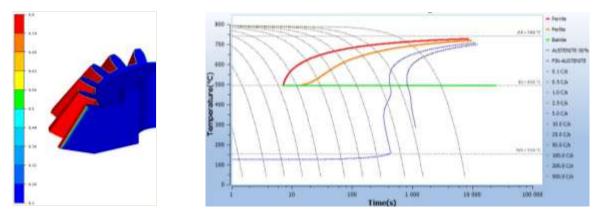


Picture2: Vickers hardness simulation map on a bevel gear after quenching.

This typical bevel gear will have to sustain continuous loading and unloading cycles generated by contact with another part. To avoid both damage of the surface and fatigue cracks, hardness on the surface and ductility in the core of the material are required. A possible solution to this dilemma is to use different carbon content on a different area of the part. This is achieved through the carburizing process. Carburizing is a surface treatment where carbon diffuses from the surface in contact with the carburizing atmosphere into the part, leading to a carbon rate gradient from the surface to the core. The higher the carbon rate, the higher the steel quenchability, and thus the easier to form martensite on quenching

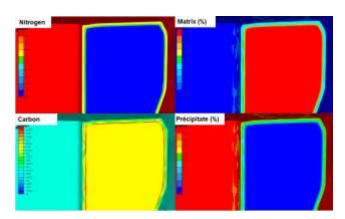
(indeed higher carbon rates shift the transformation of austenite into ferrite, pearlite and bainite towards longer times).

FORGE® is able to simulate the carburizing process and the subsequent quenching operation taking automatically into account the modification of the phase transformations kinetics according to the local carbon rate.



Picture 3: Carbon rate after carburizing simulation and corresponding TTT diagram for the highest carbon rate on the part (0.8%)

Nitriding is a more complex process: in this case, the ambient atmosphere brings nitrogen to diffuse through the metal surface. This process has many advantages for fatigue, wear, friction, corrosion, and a relatively good assessment of the induced distortions. On the physical side, several precipitates can appear and dissolve leading to a complex diffusion path of the nitrogen atoms but also of the carbon atoms initially present in the steel. 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.

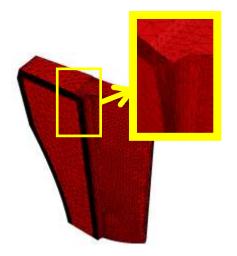


Picture 4: Results of a nitriding simulation (nitrogen & carbon & precipitate rate)

As mentioned earlier, good quality simulation for heat treatment applications significantly depends on the thermo-mechanical-metallurgical models and the input material data.

Notwithstanding, there are two additional key-points: heat transfer coefficient and mesh quality. Heat transfer coefficient (HTC) and emissivity are driving the heat exchanges by convection and radiation between the parts and the surrounding area. Values for several treating conditions are easily available from the literature.

Secondly, the mesh size is critical. During heat treatment, the part is subject to very important thermal shock. In order to well capture the change of temperature at the part/medium interface, the mesh size must be adapted. Usual mesh size computed from the physical properties and thermal shock leads to not acceptable computation times for industrial applications. FORGE® is able to generate an anisotropic mesh with a smaller mesh size from the surface to the core on a given depth. The mesh size in the other directions remains normal. It allows having a very fine mesh in the direction of the huge temperature gradient and a normal mesh in the direction with smaller temperature gradient. This feature allows an accurate simulation of the process with reasonable computation time.

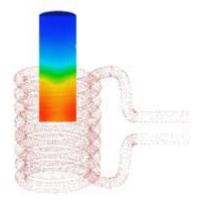


Picture 5: Example of anisotropic mesh

# 3. Simulating Induction Forge Heating & Induction Heat Treating

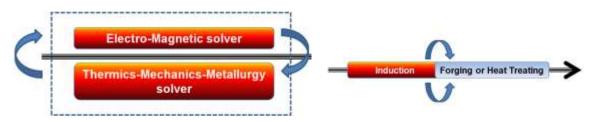
Induction heating is a very common operation carried out either for a global heating of a billet before forging, or either for a local heating of a forged component prior to surface hardening. In case of induction forge heating, one of the challenges consists in controlling the temperature build-up into the billet to get a uniform distribution. When applied to induction heat treating, it is important to master the depth of the so-called heat affected zone (HAZ) and to regulate the metallurgical changes which can occur.

Simulation enables to try out the influence of various process parameters among those current intensity & frequency and nominal power. Multiple design alternatives can be tested including the coil design and the location of magnetic field concentrators.



Picture 6: Temperature distribution into a steel billet partially located into a copper inductor

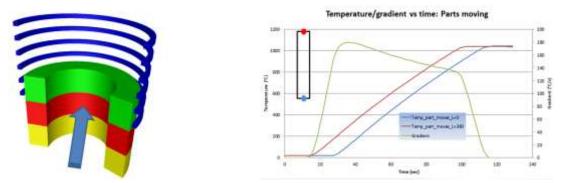
The simulation of the induction process is governed by a coupling between electromagnetic & thermo-mechanical phenomena. FORGE® software integrates the two kinds of resolution into a single loop, such as the heat source generated by the electromagnetic calculation is applied to the thermal-mechanical-metallurgical solver in order to calculate temperature evolution and metallurgical variations. As the material (steel grade for instance) may have thermo-dependent electromagnetic properties, it is crucial to loop back to the electromagnetic calculation and update these properties. FORGE® software automatically links together the 'induction' simulation with the following 'forging' or 'heat treating' simulation. The results are directly transferred from 'induction' to 'forging/heat treating' avoiding any sort of tedious manual transfer of data between stages.



Picture 7: Coupling electro-magnetic solver & thermo mechanical-metallurgical solver and associated chain of simulations with automatic data results transfer

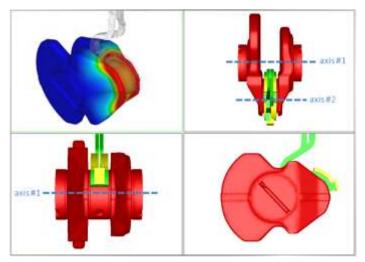
Regarding induction forge heating, Transvalor has recently introduced the possibility to simulate not only a static billet located into a coil, but also one or several billets travelling inside the heating tunnel. Therefore, it is possible to evaluate the efficiency of the induction

equipment and to study the influence of process parameters such as the line speed and the power supply frequency. As a matter of example, the modelling results can illustrate the axial temperature gradient observed between the front & rear face of the billet while it is moving along the tunnel.



Picture 8: Billet heating into induction tunnel (left: three rings moves across the coil; right: temperature evolution on front end and rear end of the billet)

Regarding induction heat treating, the same concept of mobility is also implemented into FORGE® software to take into account the motion of coil or concentrator. This is particularly useful for the induction heat treatment of crankshafts which is among the most impressive technique. The inductors and concentrators must keep rotating together with the crankpin according to two combined rotations.

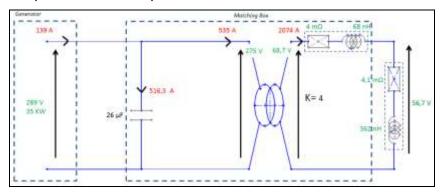


Picture 9: simulation of induction heat treating on a crankpin with moving coil & concentrator (courtesy of PSA Group & EFD Induction)

Hence, it is now possible to simulate precisely a very localized heating applied in a specific area followed by a sudden spray quenching aiming at increasing the surface hardness.

Designers are getting full benefits from the modelling as they can obtain an accurate prediction of the heat affected zone and they can access to a reliable representation of the steel phase transformation.

Recent research work conducted with a major automotive supplier have demonstrated that considering standard input data such as inductor current and frequency is not enough to get the most accurate results. Indeed the behavior of the induction generator itself is neglected leading to imperfect results on the heat affected zone or on metallurgical changes. FORGE® software includes a dedicated model in which the generator is power-driven. As the electrical properties of the part are changing with respect to the temperature, the generator's electrical circuit is taken into account. Hence, the frequency and the current intensity are automatically deduced from the RLC components. Therefore, the frequency and the current intensity are no longer constant; they are adapted during the FEM calculation in order to deliver a nearly constant nominal power to the workpiece.

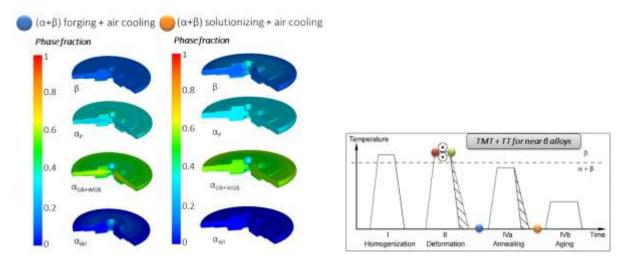


Picture 10: schematic representation of the generator with the RLC circuit (courtesy of NTN-SNR)

# 4. Prediction of Phase Transformations in Titanium Alloys

With respect to the ultimate goal of predicting the in-use properties of a forged component, the modelling of phase transformations is among the primary concerns for engineering people. Controlling the microstructure and its evolution during the entire process manufacturing chain is essential to deliver the best quality products. Today's state-of-the-art of FEM simulation includes the modelling of recrystallization and grain growth phenomena using macroscopic models which are essentially JMAK-based. For alloyed steels, phase transformation phenomena are easily calculated assuming proper material data such as TTT or CCT diagrams. Consequently, for a given complete forging sequence, FORGE® software can calculate the static, meta-dynamic and dynamic recrystallization occurring during the heating, forming and resting phases and can predict the final grain size as well.

More recent challenges focused on phase transformations prediction for titanium alloys. These materials combine great mechanical properties, low density and a good resistance to corrosion. However these properties highly depend on the process which affects the microstructure including the phase composition and the phase topology (morphology, size, spatial arrangement). In this spirit, macro-scale models have been implemented into the latest release of FORGE® software. These models allow the prediction of the phase transformation kinetics and the fraction of  $\alpha$  and  $\beta$  morphologies. In this matter, simulations of a complete forming cycle have been conducted on a jet engine compressor disk with two titanium alloys (Ti17 and Ti-6AI-4V). Hence, the evolution of the  $\beta$  phase and every  $\alpha$  phase ( $\alpha_{p}$ ,  $\alpha_{gb+wb}$ ,  $\alpha_{wi}$ ) has been carried out by the simulation from the initial temperature homogenization through the forging stages until the final annealing (or aging) stage.



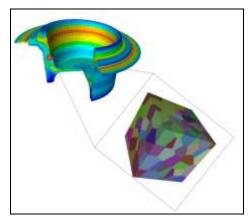
Picture 11: prediction of the different  $\alpha$  morphologies in compressor disk after forging & solutionizing

#### 5. From Macroscale to Full Field Approaches for Microstructure Evolution

As opposed to the macro-scale model, Transvalor promotes alternative multi-scale approaches and consequently has closely developed 'mean field' and 'full field' models. These more sophisticated models aim at considering the physical phenomena such as density dislocations and grain boundary migrations. The main output results are grain size, recrystallized fractions, nucleation rate and the evolution of the dislocation density. As the rheology of the material is coupled with the microstructure, the models imply an impact on the flow stresses. Elaborated in association with the German RWTH Aachen University and the French research center CEMEF from Mines ParisTech, the most recent 'mean field'

models are now introduced into FORGE® software with the opportunity to get material behaviors depending on microstructural evolution.

Nevertheless, if this mean field framework is quite convenient, it can lead to a large amount of experiments to calibrate these models. Moreover, the homogenization of the microstructure is not relevant to capture the very local phenomena. With the 'full-field' model, one moves to mesoscale level where the scale of analysis shifts to the grain or cluster of grains. It is not realistic today to conduct such approach on the entire part as the number of grains would be nearly infinite. So, the analysis has to be performed on specific areas of the forged component. The 'full field' model considers the topology and the morphology of the grain using an innovative RVE (Representative Volume Element). The study is conducted on a polycrystal and allows the modelling of primary recrystallization including the nucleation stage. Moreover, the Smith-Zener pinning (SZP) phenomenon can be taken into account in a natural way Transvalor has fully implemented this approach in its newest software named DIGIMU®.



Picture 12: Full field approach at grain level with representative volume element (RVE)

# 6. Conclusions

Process manufacturing simulation software effectively leverages innovations in the forging industry and today's scope is not limited anymore to the traditional targets (e.g. metal flow & tooling failure prediction). FORGE® software offers one of the largest ranges of capabilities to simulate heat treatment & induction processes and to predict microstructure evolutions for steel & titanium alloys. No doubt that virtual manufacturing is and will remain a major breakthrough bringing multiple benefits to intensify your process development cycle, to supply parts with proven in-use properties and to differentiate your products from the competition.