Part I
Materials Modeling and Simulation: Crystal Plasticity, Deformation, and Recrystallization

Microstructural Design of Advanced Engineering Materials, First Edition. Edited by Dmitri A. Molodov.

1
Through-Process Modeling of Materials Fabrication: Philosophy, Current State, and Future Directions

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1.1
Introduction

Mathematical modeling of physical phenomena is not new science or a recent development but a fundamental ingredient of physical sciences. In fact, mathematics is the language of natural sciences, and it is the objective of physical research to extract from observed phenomena the general behavior in terms of mathematical relations that will allow making quantitative predictions. Physical phenomena are usually described in terms of respective equations of state (thermodynamic considerations) and equations of motion (kinetic considerations). Both types of relations are typically expressed in terms of differential equations, mostly partial differential equations (PDEs). The solution of these equations for usually complex boundary conditions can most commonly not be obtained in closed form, and therefore, the behavior of respective thermodynamic or kinetic systems can only be determined for very special conditions, for example, at the limits of time and space. Forty years ago, owing to the lack of easy to handle closed form solutions particularly engineers refrained from utilizing physics-based concepts, but instead they developed empirical models by fitting simple mathematical functions to obtained data, mostly power law relations for monotonic dependencies, since a power law could still be handled by a slide rule, the typical personal computational tool at that time. Such empirical approaches were actually very accurate as long as the same material was processed the same way, but beyond measured regimes they lacked any predictive power.

With the advent of powerful computers, the situation changed dramatically. Besides the fact that complicated PDEs and complex boundary conditions could now be solved numerically, simulation tools became available to probe virtual materials behavior at any length and time scale. On the macroscopic scale the finite element method (FEM) became the predominant numerical tool for engineers; on the mesoscopic level, the phase-field theory besides Monte Carlo (MC) methods, cellular automata (CA), and front tracking algorithms such as vertex models or level-set methods advanced to established modeling approaches for microstructural evolution of materials. On the atomistic level molecular dynamics

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(MD) simulations enabled a large variety of atomistic phenomena to be explored, and eventually density functional theory allowed *ab-initio* quantum mechanical studies of complex atomistic configurations, to name only the most popular approaches. With these computational tools at hand, one does not generate new physics, since the models and tools essentially reflect our understanding of physical phenomena and the underlying mechanisms. Instead, available computational power allows us to address complex phenomena, mutual interaction of different physical processes, and nonsteady-state behavior of physical systems. If we confine our consideration to materials, in particular to crystalline solids, specifically commercial metallic materials, we have now the option to utilize computer power, sophisticated simulation approaches, and advanced numerical algorithms for the prediction of material properties and therefore, for an optimization of materials processing and materials performance in service, in other words we are now able to put 50 years of physical metallurgy to work.

To make reliable predictions of materials behavior one has to understand that, contrary to common believe of engineers, the properties of a material are not controlled by the processing conditions but by chemical composition and microstructure. In other words, there are no processing–property relationships that can be utilized for the prediction of material properties; rather the only state variable of properties is, besides the unchanged overall composition, the microstructure, which is liable to change by thermal and mechanical processing (Figure 1.1). Hence, the prediction of final properties of a material requires to pursue the development of microstructure along the entire processing chain, in principle from solidification through the semifinished product and eventually to a part in service. The simulation of microstructure evolution and therefore of materials properties along the processing chain is referred to as through-process modeling (TPM) in Europe or, more

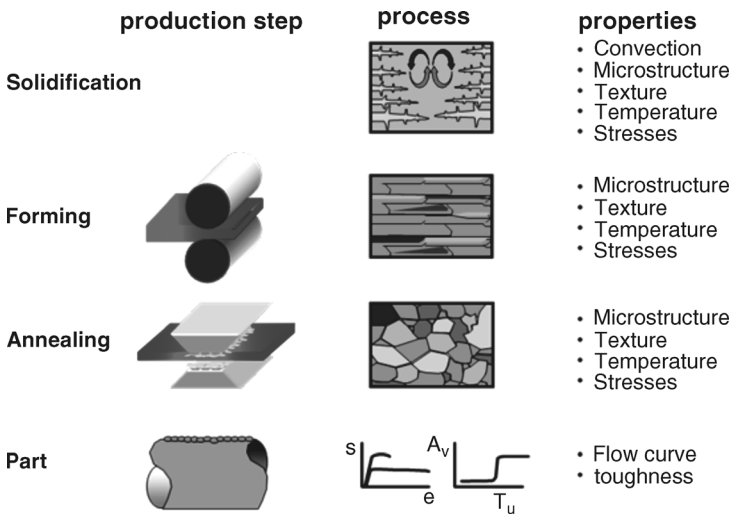


Figure 1.1 Microstructural change along the process chain of tube fabrication.

recently, integrated computational materials engineering (ICME) in the United States. In the following, we will use throughout the term TPM, keeping the identity with ICME in mind.

1.2 Microstructure Evolution

In view of the observed microstructural complexity in commercial materials the prediction of microstructure evolution during processing seems to be an intractable problem. Hence, it seems surprising at first glance that physical metallurgy research of the past 80 years has shown that there are only three processes involved that have to be considered for microstructural change, that is, crystal plasticity, recrystallization and related processes, and phase transformations. Admittedly each of these three microstructural processes is very complex and their mutual interaction can lead to widely different microstructures; the principles have been laid out by metal physics research in the recent past and mathematical concepts exist to address microstructure evolution quantitatively. Also, specific relations have been derived that associate microstructure with material properties.

Most of concepts of microstructural phenomena are formulated in a continuum approach on the mesoscopic level, which is typically of the order of micrometer (Figure 1.2).

The underlying mechanisms proceed on an atomistic level and determine continuum properties like diffusivities, mobilities, and enthalpies. The mesoscopic approach is attached to the macroscopic world by microstructure–property relationships that can be used in FEM simulations of materials processing. The most germane approach to TPM is therefore modeling of microstructure on a mesoscopic scale under processing conditions delivered by FEM simulations. On demand, atomistic simulations are engaged to generate intrinsic material data that are needed in the mesoscopic approach. In the following, we will shortly introduce the essentials of current modeling approaches of respective microstructural processes.

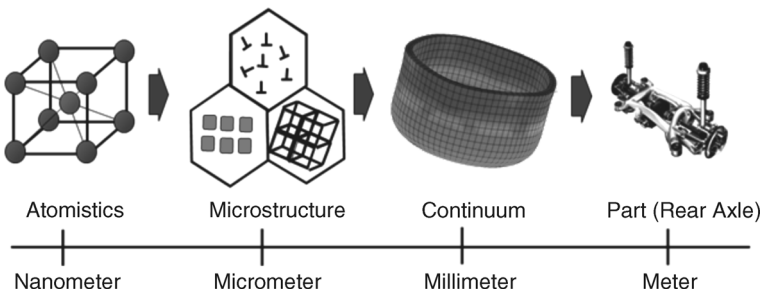


Figure 1.2 Multiscale modeling, macroscopic properties, microstructure, and atomistic processes are defined on different length scales.

1.3 Microstructural Processes

Crystalline solids can deform plastically by crystallographic slip, mechanical twinning, diffusion controlled plasticity, or transformation plasticity. The dominant mechanism of *crystal plasticity* in most commercial materials is crystallographic slip by dislocation motion. During deformation a material undergoes work hardening, that is, dislocation storage, and a change of crystal orientation, that is, texture [1]. The introduced dislocation structure is the microstructural variable of the mechanical properties of the material after deformation, for example, strength. The orientation change leads to the formation of a nonrandom orientation distribution. Whereas modeling of deformation texture is already well advanced and yields reasonable predictions that compare well with experiments, modeling of the deformation microstructure is much more complicated. Even if we neglect the microstructural inhomogeneities that usually accompany cold forming, a prediction of large strain work hardening and dislocation arrangement on the basis of 3D discrete dislocation dynamics is not yet feasible. More powerful in this context are statistical deformation models such as the Kocks–Mecking approach [2] with the total dislocation density as single microstructural state parameter or the 3IVM+ with three internal variables [3] (Figure 1.3).

The latter considers the evolution (production + and reduction −) of dislocation density ρ or even several (n) types of dislocation densities ρ_i with strain ε:

$$d\rho_i = d\rho_i^+ + d\rho_i \qquad (i = 1, n) \tag{1.1}$$

and utilize the classical kinetic equation of state for dislocation plasticity (Orowan equation)

$$\dot{\varepsilon} = \rho_m b v \tag{1.2}$$

where $\dot{\varepsilon}$ is the strain rate, ρ_m is the mobile dislocation density, b is the Burgers vector, and v is the dislocation velocity.

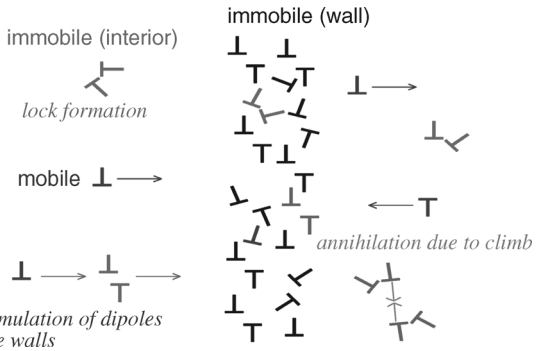


Figure 1.3 The 3IVM+ work hardening model distinguishes three different dislocation densities and their mutual interaction.

The strength σ is then obtained via the Taylor equation

$$\sigma = \alpha G b \sum f_i \sqrt{\rho_i} \tag{1.3}$$

f_i represents the respective volume fraction associated with the dislocation density ρ_i.

Respective models can approximate the measured flow curves quite well and are able to make reasonable predictions for different deformation conditions and changing alloy composition after optimizing a significant number of unknown physical parameters. While this development is promising, more detailed investigations are necessary to make the models easier to handle and to anticipate the model parameters by theoretical concepts.

Crystallographic slip by dislocation motion proceeds by pure shear and therefore is accompanied by a rotation, that is, a change of crystallographic texture of a polycrystal. The respective orientation changes in a polycrystal can be calculated by a variety of methods, notably by the Taylor approach [4], where it is assumed that each crystal undergoes the same deformation as the macroscopic specimen. More refined models take also the interaction of the grains into account, for example, the Lamel code [5], viscoplastic self-consistent approaches [6] or the grain interaction model (GIA) [7,8]. In the latter, an eight grain aggregate is considered that has grain boundaries in all three spatial directions (Figure 1.4). The entire cluster is forced to comply with the Taylor conditions but the grains in the cluster are allowed to deform freely and impose shears on next neighbor grains across these internal boundaries; however, this incompatibility has to be compensated for by the introduction of geometrically necessary dislocations. An energy minimization yields the activated slip systems and the respective shears. These models effectively reproduce the experimentally obtained crystallographic textures.

Softening phenomena are caused by *recovery*, *recrystallization*, and *grain growth* [1]. Whereas *recovery* and related phenomena such as continuous recrystallization or recrystallization *in situ* are simply dislocation controlled processes and can be addressed by means of crystal plasticity concepts outlined earlier, recrystallization and grain growth require different modeling approaches.

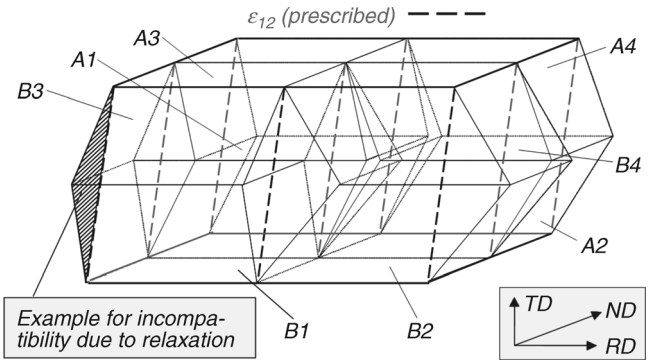


Figure 1.4 The grain cluster model GIA considers an arrangement of eight grains and allows for interaction across their boundaries.

Recrystallization proceeds during annealing of deformed crystals and consists of the nucleation of strain free grains and their growth into the deformed matrix until the entire deformed volume has been consumed. The growth process can be modeled reasonably well with a variety of mesoscopic simulation tools, like Monte Carlo simulations, cellular automata, or phase field methods. The crucial issue in recrystallization modeling is a physical approach of nucleation and, correspondingly, the prediction of nucleus locations and orientations and nucleation kinetics. The latter determines incubation time and nucleation frequency. Owing to the dramatic change of microstructure and thus properties of a material during recrystallization, an inaccuracy in the selection of nucleation kinetics and/or mechanisms is liable to engender a totally wrong prediction of the state of the material during processing. Therefore, substantial efforts have been dedicated to this problem with obvious success but far from a satisfactory solution. While for specific alloys, a prediction of distinct properties such as texture or grain size can be accomplished, it is still beyond our capabilities to predict the recrystallization behavior of a new and untested alloy. For real time and real-space simulations, deterministic modeling tools like cellular automata are most appropriate if modified to accommodate the specific circumstances of recrystallization. For this purpose, the sample volume is discretized and each volume elements can assume discrete states depending on the local environment; with regard to recrystallization the state can switch from "deformed" to "recrystallized." The transformation occurs when a volume element in a deformed state is touched by the grain boundary of a growing recrystallization nucleus, so that the speed of transformation is determined by the growth rate of a grain, that is, the grain boundary velocity

$$v = mp \tag{1.4}$$

where m is the grain boundary mobility that will depend on misorientation, local chemistry, temperature, and so on, and p is the local driving force, essentially the local stored dislocation energy. To accommodate a locally varying growth rate, advanced CA codes like the smart cellular automata code CORe [9] are capable of adapting its grid size to the local and temporal environment and are also referred to as cellular operators (Figure 1.5).

Like all recrystallization simulation tools CORe is a pure growth model that has to be merged with a nucleation model like the ReNuc [10] code that has recently been

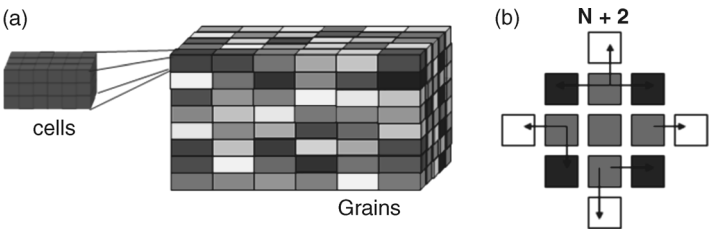


Figure 1.5 Cellular automata modeling of recrystallization; a grain in a polycrystal is subdivided into volume elements (a) that can change their state once touched by a growth front (b).

developed for aluminum alloys to output nucleation rates for typical nucleation mechanisms such as recrystallization at grain boundaries, transition bands, shear bands or at large particles [11]. Given the nucleation frequency and nucleus texture the kinetics of recrystallization, grain size distribution and texture development can be computed.

Recrystallization is succeeded by *grain growth*, which is observed by a coarsening of the grain structure. It is driven by grain boundary curvature and proceeds by grain boundary motion with local migration rate

$$v = m\frac{2\gamma}{R} \tag{1.5}$$

where γ is the specific grain boundary energy and R is the local radius of the boundary curvature [1].

Grain growth can be simulated by a variety of methods such as the phase field method, cellular automata, Monte Carlo simulations, or front-tracking algorithms like the network models. The latter have the advantage that they are deterministic and simulate grain growth in real time and real space [12]. Moreover, they most closely reflect the physical nature of the process in terms of curvature-driven grain boundary motion. A typical vertex model discretizes the grain boundary network into linear segments (2D) or triangular elements (3D) that are bound by virtual vertices (on the boundaries and triple lines in 3D) or real vertices (quadruple points in 3D) for which the displacement in a specific time increment is computed according to Eq. (1.5).

This setup allows flexibility in driving force p and mobility m assignment to the various constituents of a grain boundary network in a polycrystal (Figure 1.6), namely grain boundaries (p_b, m_b), triple lines (p_t, m_t), and quadruple points (p_q, m_q). Since only the boundaries are considered whereas the grain interior remains unconsidered, respective codes are very fast and allow us to address systems of substantial size and thus, cover an essential change of microstructure during grain growth. An example is the 3D virtual vertex model developed at the Institute of Physical Metallurgy and Metal Physics (IMM) of RWTH Aachen University.

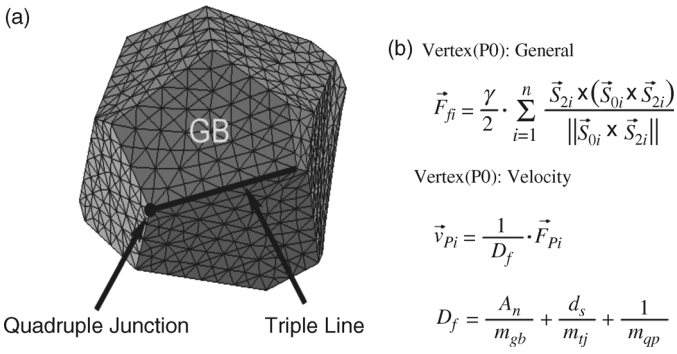
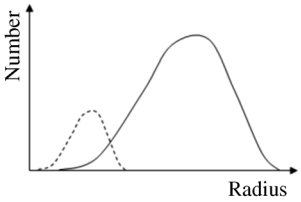


Figure 1.6 Three-dimensional vertex modeling of grain growth; grain boundaries (GB), triple lines, and quadruple points are discretized by vertices (a) that are displaced according to the equation of motion (b) under local conditions.

Nucleation energy: $\Delta G(r_c) = \frac{4}{3} \cdot \pi \cdot r_c^2 \cdot \sigma$

Critical radius: $r_c = \frac{2 \cdot \sigma}{\Delta g_T}$

Growth rate (Zener): $\frac{dr}{dt} = \frac{c(t) - c^{\alpha}(r)}{c^{\beta} - c^{\alpha}(r)} \cdot 0.5 \cdot \left| \frac{c(t) - c^{\alpha}(r)}{c^{\beta} - c(t)} \right| \frac{D}{r}$



Nucleation rate (Becker/Döring): $\dot{N} = N_0 \cdot Z \cdot \beta \cdot \exp\left(-\frac{\Delta G(r_c)}{k_B \cdot T}\right)$

$$\frac{\partial f(r,t)}{\partial t} + \frac{\partial}{\partial r}\left(\frac{dr}{dt} \cdot f(r,t)\right) = \dot{N}$$

Figure 1.7 Fundamental relations of the ClaNG model; the grain size distribution $f(r,t)$ obeys the continuity equation.

Phase transformations like the α–γ-transformation in steels or precipitation and dissolution phenomena in aluminum alloys are most adequately addressed by the phase field method. However, this method is computationally demanding and requires substantial computer power with long computation times. Moreover, for many, in particular industrial applications, there is no need to obtain highly detailed information on space resolved microstructure evolution, since the relations between microstructure and properties are generally based on statistical average values that can be obtained from much simpler approaches. For instance, precipitation, particle coarsening, or dissolution in aluminum alloys can be addressed successfully by classical nucleation and growth theory as laid out by Becker and Döring 80 years ago. Coupled to a thermodynamic database for a computation of the equilibrium phase diagram and supplemented by the Kampmann–Wagner approach for the evolution of particle size distribution, it renders solute content, particle size, and particle volume fractions as function of annealing time for a given temperature or temperature profile. An example is the ClaNG code [13] (Figure 1.7) that can be readily interfaced to Calphad databases, and its fast computation speed lends itself for interfacing with concurrent processes such as recrystallization and grain growth.[1)]

Work hardening, recrystallization, and related phenomena and phase transformations constitute the basis for following and predicting microstructure evolution during materials processing, if connected to a process model that is capable of predicting temporally and locally temperature and strain as usually provided by FEM.

1.4 Through-Process Modeling

In the following, we shall present an example of through-process modeling for the fabrication of the aluminum sheet [14,15]. To begin with, one has to specify which particular property or properties are to be determined. In this example, we want to

1) All the models outlined in this text have been published and respective codes are accessible through SimWeb on the IMM homepage (www.imm.rwth-aachen.de).

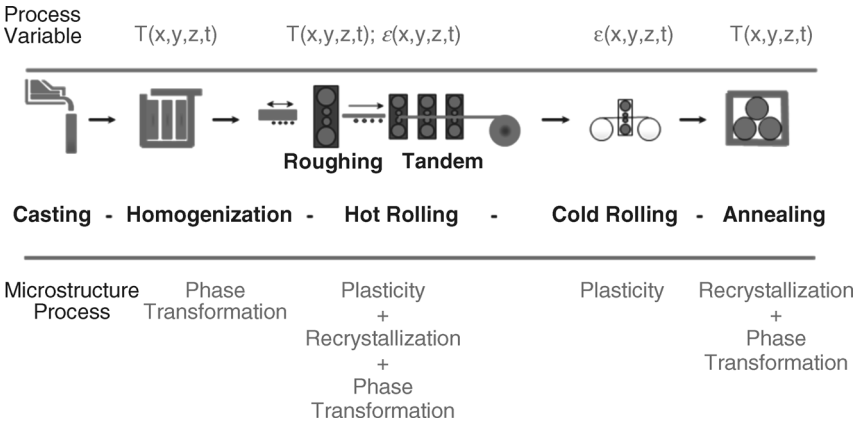


Figure 1.8 Through-process modeling of aluminum sheet fabrication; the process variables are obtained by FEM simulations, the microstructure undergoes changes by three microstructural processes.

predict the earing behavior during deep drawing of a processed sheet. For this, one needs to know the microstructure of the rolled and annealed sheet in terms of crystallographic texture and dislocation structure to predict the behavior during sheet forming. We start out with the cast and homogenized ingot, and the process chain consists of hot rolling, coiling, and multiple cold rolling and annealing until the final sheet thickness is obtained (Figure 1.8).

The process data are given by streamlines from FEM simulations of deformation and temperature for select characteristic sheet locations such as center plane and surface. With the temperature and displacement gradient known as function of time and space along the entire process chain, microstructure evolution in each volume element can be simulated by considering deformation, recrystallization, and precipitation–dissolution in a given volume element for each time increment (Figure 1.9).

During hot rolling the material will undergo deformation in the rolls as well as recrystallization and precipitation during interstand times and during coiling. It is stressed that deformation and recrystallization will impact texture so that texture evolution needs to be followed along the processing chain. During cold rolling work hardening and deformation texture development will occur and subsequent annealing will cause recrystallization and potentially precipitation, particle coarsening, or dissolution that will also affect texture. Eventually, after the last annealing step the final texture and dislocation structure are established.

This information can then serve as input to compute the in-plane strength anisotropy and yield surface as needed for simulation of the deep drawing process. For the aluminum alloy AA5182, this exercise was conducted in cooperation with the Institute of Metal Forming (IBF) of RWTH Aachen University and industrial partners, notably Hydro Aluminium Germany [16]. At defined processing steps,

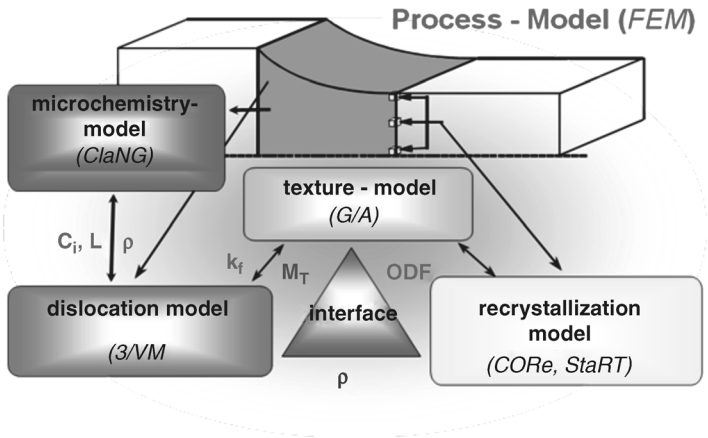


Figure 1.9 In each increment of time, the change of state of an FEM volume element has to be updated with respect to its microstructural changes.

samples could be taken to compare predictions and experimental results. It is emphasized that in this study the computational prediction was made prior to the measurements in order to evaluate the true predictive power of the simulation tools. The results are given in terms of the volume fractions of the major texture components (Figure 1.10).

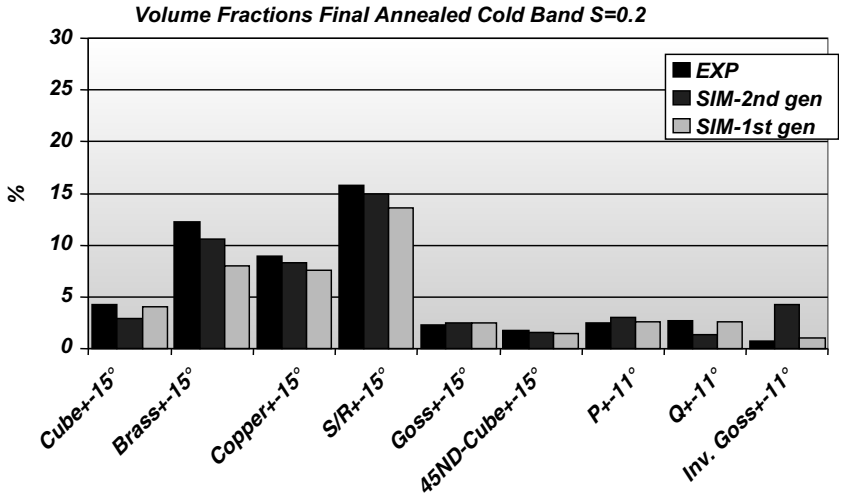


Figure 1.10 Volume fractions of major texture components in the center plane of finally annealed AA5182 sheet after 13 processing steps. Predictions prior to measurements (light gray), refined predictions with experimental results known (dark grey), and experimental results (black).

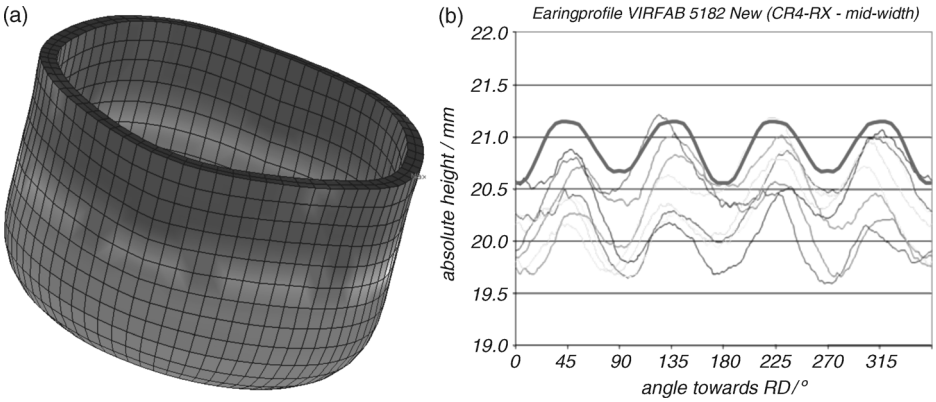


Figure 1.11 Result of FEM simulation of deep drawn cup (a) measured on several samples (thin lines) and computed (bold line) earing profiles of AA5182 sheet. (courtesy IBF)

Apparently, the predictions after 13 processing steps are quite reasonable, although a second simulation, after the experimental results were known, allowed to even better optimize the parameters and rendered some quantitative improvement.

If the computed final texture is input in a subsequent sheet forming FEM simulation, the experimentally observed earing behavior can apparently be predicted with acceptable accuracy (Figure 1.11).

At this point, it is important to realize how the predictive power or the accuracy of a simulation has to be evaluated. Typically, the quality of a simulation is obtained by benchmarking with experimental results, so that the experiment always constitutes the reference. However, one should be aware that also experimental measurements and in particular industrial processes are subject to a certain scatter that has to be taken into account for an assessment of the quality and reliability of a model. In principle, an optimized simulation tool does not lend itself to an error analysis, since the prediction is made exactly according to the assumptions implemented in the code. However, the used fit parameters may be subject to scatter and frequently a multivariate regression analysis of a multiparameter model may yield more than a single set of optimum parameters, which however may render different predictions for different conditions. With respect to the predictive power of the work hardening model 3IVM+, the variance of the predicted flow curve was compared to the expected fluctuation of temperature in an industrial hot rolling process. As obvious from Figure 1.12, the potential variation of the predicted work hardening curve is still within the accepted inaccuracy due to temperature fluctuations, which means that the predictions are in an acceptable range. Of course, for multistep through-process modeling it is important to know, how the permissible deviations in each step affect the final result, but this analysis has always to be related to the potential variations of the simulated industrial process that will still generate an acceptable final product.

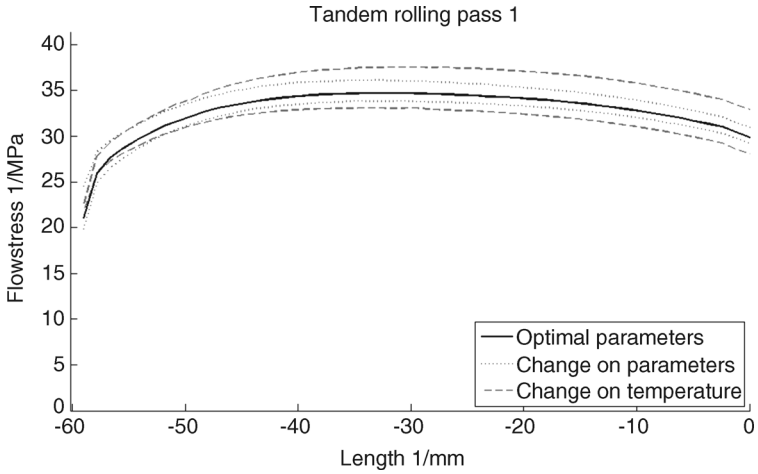


Figure 1.12 Scatter of predicted flow curve (three center curves) and variation due to acceptable temperature fluctuations (top and bottom curve) (courtesy IBF).

1.5 Future Directions

Although the results of the simulation trial were very promising, there is still a long way to go, if more complex processing schemes or more advanced alloys are to be addressed. To correctly predict work hardening with strength contributions of various alloying elements and several constitutive components in an alloy is still a challenge. The effect of particles, on both nucleation of recrystallization and nucleus growth, the problem of orientation-dependent recovery and thus, incubation time of recrystallization, and local fluctuations of Zener drag, need to be refined by respective theoretical concepts to obtain better predictions of recrystallization kinetics and texture.

Most importantly, one should not underrate that all models rely on the knowledge of specific material properties, such as elastic constants, diffusivities, boundary mobilities and boundary energies, and so on that are difficult to obtain experimentally and are likely to depend sensitively on composition since they are known to be seriously affected by alloying elements and misorientation distribution. It is very unlikely that such data can be generated experimentally so that in the future it will be indispensable to employ atomistic simulations for providing these data. While *ab-initio* simulations are promising for computing elastic properties and for providing energetic information [17], today's predictions of grain boundary mobility by MD are still orders of magnitude different from experimental results [18,19]. The same is true for diffusivities, in particular for interdiffusion in multicomponent alloys.

For commercial applications, it is also necessary to develop adaptive interfaces for automation of the computational procedure and for the handling of more complex microstructural features, for example, partially recrystallized microstructures or concurrent precipitation and recrystallization [20].

Finally, it is mentioned that computation times are still by far too long to address large and complex systems. Despite of the availability of seemingly ever increasing computer power simulations that mimic real world conditions take too long. Correspondingly, the developed simulation tools will have only limited acceptance in an industrial environment. While they lend themselves for alloy development in a research laboratory, for process control one would need orders of magnitude higher computational speed. In this context, it is helpful to remember that virtually most of the simulation tools have been designed for single CPU operations. The future of high-performance computing, however, calls for codes that can make use of massive parallel computer architectures. It is also not of much gain to optimize a serial code for parallel computation. If really a quantum leap in computational speed is to be obtained it will be necessary to redevelop basic physical models and to utilize modern mathematical tools to completely separate individual computational procedures and still extract from the separately obtained output the desired physical information.

It is important to realize that through-process modeling is designed to predict material development and the terminal state of a material for a given process chain. This is highly valuable information since computer simulations do speed up alloy and process development and are much more cost-effective than traditional empirical approaches. However, true materials design calls for the inversion of the procedure, that is, poses the question: What material and process one has to choose for obtaining a material for optimum performance for a specific application? This so-called inverse modeling is certainly much more difficult to perform than the current – already highly demanding – through-process modeling activities. However, there is no time and reason to wait until all open questions of microstructure evolution and through-process modeling have been solved, since substantial efforts for a development of inverse simulation approaches and adequate mathematical tools will be necessary to take the next step.

Computer simulations have long faced skepticism and criticism of scientists who prefer the classical approach of analytical modeling. It is certainly true that one cannot generate new physics on the computer since the computer can only work in the frame of the encoded physical models. Computational materials science however, means that one can handle complexity that cannot be addressed analytically. This is the true benefit of computer simulation of materials, and with increasing computational modeling power there is hope and expectation that we shall be able to make virtual materials design and virtual materials engineering eventually come true.

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