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Edited by Georg J. Schmitz and Ulrich Prahl

Handbook of Software Solutions for ICME

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Preface

Integrated Computational Materials Engineering: Past, Present, and Future

The present *Handbook on Software Solutions for Integrated Computational Materials Engineering* is probably best introduced by giving a look back onto the roots and by providing an outlook into the future. Based on the editor's own professional experience, we have a quick look at the situations ±30 years from now.

1986: The Historical Ground

Materials were often characterized by optical microscopy and respective microstructures were recorded on black and white glossy prints. These were collected in microstructure catalogs. First personal computers with 80 286 processors and a Windows 3.1 operating system entered into the research practice of noncomputer experts. Floppy disks had a storage capability of a few hundred kilobytes, and a 10 MB hard disk was already considered as advanced equipment. The Internet was in the early nascent state. Digitizing the glossy prints at that time was the first step to automatic image processing and to subsequent statistical evaluation of microstructures. Finite element method (FEM) modeling of entire components on large computers filling a whole room entered into applications. The foundations for computational thermodynamics were already laid. Materials processing, however, could still be considered rather as a skill or as an art than as a science at that time.

2016: The Present Status

The evolution of computational capabilities during the last decades has triggered a tremendous progress. The development of simulation models proceeded on all time and length scales, and a huge variety of simulation tools being nowadays available has been compiled in this book. Even complex simulations may sometimes be developed and be run on a standard multicore laptop computer. Data storage in the terabyte region is usual even in private use. Microstructure features increasingly are digitally recorded in 3D and sometimes even in 4D. FEM modeling has replaced experimental efforts to a large extent and often only final validation proceeds "physically," for example, in crash tests. Computational thermodynamics have further matured into a spatially resolved description of phase transformations based on the phase-field concept, which nowadays allows the simulation of microstructure evolution even in complex technical alloy systems. Materials engineering thus has transformed from being skill-based toward being a science. The complex interplay of atomistic processes, thermodynamics, processing conditions, microstructure evolution, materials and component properties, component functionality, and component performance has been identified to be only accessible via a combination of different simulation tools in an ICME-type, holistic approach. The current major challenge seems to facilitate communication between the different model worlds and communities.

2046: The Future Vision

All software tools and experimental devices in the area of ICME have a common communication standard similar to jpeg formats for pictures in 2016. 3D and 4D simulation data with highest spatial resolution can easily be exchanged. Metadata will collect all information about origin, precision, validation, and many other aspects of the data. Data will be stored in the cloud or on powerful exabyte local devices. Simulations running for weeks in 2016 will run in hours. Well-calibrated surrogate models with a lower precision will run within seconds and provide assistance in business decisions. Models will be available to simultaneously describe all known phenomena affecting the properties of any material. Individual results can easily be integrated into suitable common data structures and can easily be retrieved. A new community of holistically educated "ICME engineers" has entered their professional life and takes responsibility in leading positions.

The design of new materials and components will essentially be based on simulations. It will be optimized with respect to a desired functionality and performance obeying constraints given, for example, by their manufacturing processes, ecological footprint, and economic impact. The prediction of materials and component properties will be possible along their entire production and service life cycle. Simulations will bridge interfaces between inorganic, organic, and biological materials and even encompass human tissue. The morphogenesis in complex biological systems can be tackled by simulations.

The editors are eager to contribute to further shaping the necessary developments, and they are also curious to see whether their vision might really come true by 2046.

Editing this book has been performed within the ICMEg project and has received funding from the European Union Seventh Framework Programme

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Our thanks also go to 93 authors from 15 countries, who volunteered and contributed their expertise and took quite an effort to make this book real. We do hope that it will become a valuable documentation for anybody – whether "process engineer" or "simulation guy" – seeking a holistic view on things.

Aachen,
January 2016

Georg J. Schmitz and Ulrich Prahl

1
Introduction

Georg J. Schmitz and Ulrich Prahl

1.1
Motivation

Integrated Computational Materials Engineering (ICME) – by its name and its nature – draws on the combination and the simultaneous or consecutive use of a variety of software and modeling tools. This simple phrase immediately raises a number of further questions:

How to combine tools?
How to select suitable tools?
How to decide on a specific tool?
And many more ….

Eventually, before answering these questions, some even more direct issues arise:

Which tools are available at all?
How to become aware about suitable tools?

Thus, there is obviously a need for something like the "yellow pages of software solutions for ICME" or a similar "one-stop shop" like institution. Such kind of yellow pages listing – even if being very comprehensive – would be quite boring to read (and also to write …) and probably would even be outdated after a short time in view of new codes emerging and old codes being discontinued.

The ICMEg project partners [1] therefore decided to extend the scope of this book beyond the "yellow pages" and to include also a general introduction and overviews to the different fields, models, and software tools. The book content thus eventually evolved into an "overview" of overviews. All contributions are as generic as possible and references are mainly limited to "further reading" and refer to textbooks and tutorials for the different fields and review articles. The book also provides an "overview" of tutorials, reviews, and textbooks for the different fields.

Major scope, however, is to "name" phenomena, models, descriptors, and other terms and to arrange them in an overall context structure. Looking up the details

Handbook of Software Solutions for ICME, First Edition. Edited by Georg J. Schmitz and Ulrich Prahl.

Figure 1.1 A large variety of simulation tools is available around the globe. Not all codes in general have their own websites and logos. There is an even bigger number of particularly academic tools that are hidden and waiting to be exploited.

behind the different "names" is left to the reader and nowadays can often best be achieved by drawing on the Internet.

In summary, the ultimate motivation for the authors to write this book is that it could become a standard tutorial for future ICME engineers, which by nature of ICME need to have a holistic education, a general background, and a "bird's eye view" on things.

The motivation for this book is making the first steps toward providing a thematically structured directory of the huge and heterogeneous variety of state-of-the-art models (Figure 1.1). It is thus also particularly suited for young scientists and engineers seeking an overview of modern simulation tools in the area of Computational Materials Science and ICME.

1.2
What is ICME?

"Integrated computational materials engineering (ICME) as an emerging discipline aiming to integrate computational materials science tools into a holistic system will accelerate materials development, transform the engineering design optimization process, and unify design and manufacturing" [2].

Looking at the names, a definition of ICME has been attempted in a previous book [3] based on the analysis of the ingredients I, C, M, and E. An ambiguity has been identified with respect to the term "E" – engineering – which is applied to a product/component in Computational Engineering/Integrated Computational Engineering (CE/ICE) and to a specific material in Computational Materials/Computational Materials Engineering (CM/CME). This ambiguity can be resolved by putting the focus of ICME on:

> *Engineering the properties of a component as a function of*
> *the local properties of the material inside the component*
> *and along its entire production and service life cycle*

"I" in this context especially means integrating along the process chain (time, history), integrating across the scales (space, structures), integrating several models/tools, and integrating real and virtual worlds. "E" refers to engineering of technical alloy systems, engineering under industrial boundary conditions, and engineering of materials in components during manufacture and under operational load.

Technically, ICME is an approach for solving advanced engineering problems related to the design of new materials, processes, and products by combining individual materials and process models. Is ICME just a synonym for the coupling/linking of simulation tools by data exchange? From a systems point of view, the coupling of individual models and/or software codes across length scales and along material processing chains leads to highly complex metamodels.

ICME thus is more than just linking/coupling tools. The global optimum of a process chain might – and actually will – differ from a chain of individually optimized process steps (Figure 1.2).

ICME is also not only about exchange of some data between different simulation tools but further requires information contingency in view of subsequent processes downstream the value chain (Figure 1.3).

ICME currently is already known to combine, to address, and to exploit "processing–microstructure" relationships and "microstructure–property" relationships. An emerging area is the "microstructure–processing" relationship, which investigates how processing is affected by the initial microstructure or how the microstructure affects the robustness of a process – in other words, how the history of a component affects its response to processing and how it defines its properties for operation.

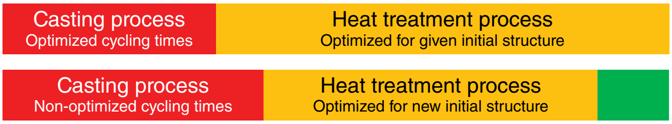


Figure 1.2 Example for a global optimum. Slightly suboptimal casting cycles with samples remaining at higher temperature for some more time may allow for shorter heat treatment times and thus result in an overall shorter production cycle.

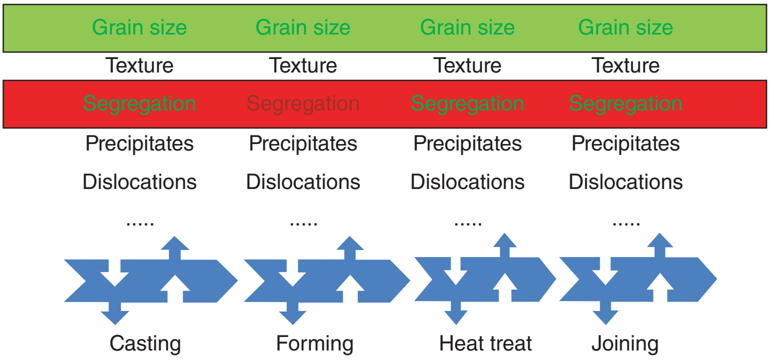


Figure 1.3 The importance of information contingency for the example of a process chain. While, for example, the grain size is simulated in all tools, the segregation of alloy elements is not modeled in the "forming" step. Segregation however becomes important again in subsequent processes.

In summary, ICME is an emerging discipline spanning various disciplines from materials technology, mechanical engineering, chemical and physical science, information technology, and numerical and mathematical science, for which a generic structural framework has to be elaborated, established, and maintained.

1.3
Industrial Needs for ICME

When discussing the industrial needs for ICME, two perspectives have to be differentiated. On the one hand, there are the commercial software providers trying to provide their software solutions to as many customers as possible. On the other hand, any industrial user of software tools is interested in exploiting software solutions to design new materials and production processes for components with tailored performance. The interests and needs of these two communities have to be discussed independently.

The interests of commercial software providers in ICME essentially relate to providing software solutions, to continuously developing new functionalities, to providing data along with their models, to making models faster and/or more robust, to making reliable/predictive models, and eventually to earning money by selling their software solutions and/or their simulation-based consulting competence.

Commercial software industry needs to identify, meet, and anticipate the needs of industrial users of their models and codes. This especially includes anticipating the potential needs not even yet being identified by these users themselves. The situation somehow corresponds to a fire brigade, which in general is not needed but anybody is happy to have it in case of a fire. The better the software provider meets the industrial user's needs for specific application tasks, the higher the user's motivation will be to further use (and thus to pay for …) the provider's software solution.

Even before any type of simulation was available, people were already able to construct airplanes. Nowadays – using simulations – they can do it faster, cheaper, better, and also with less ecologic impact. Currently, however, materials data entering respective finite element method (FEM) simulations are still often estimates based on similar materials, being isotropic and often revealing no temperature dependency. Large safety margins thus have still to be considered making the airplane heavier than needed. Better understanding and knowledge of materials and their processing will open pathways to new designs and even lighter airplanes.

From the application point of view, the industrial user of ICME is interested in solutions to his actual, real problems in ongoing production processes. He aims at optimizing current production sequences and the value of his products or at obtaining an improved understanding and control of materials and processes along the production chain. He aims at improving his products and processes in terms of cost and time and to increase the planning quality toward predictability of process chains to decrease waste and recycling material. Additionally he will develop new materials, new processes, and new products and will exploit emerging new options and applications. Eventually, simulation shall support a faster time to market of new material and process solutions by minimizing risks. This especially holds for "first-time-right" products where a classical trial-and-error approach bears unacceptable financial risks. Additional benefit of ICME can be generated for industrial users by using simulation results originating from their suppliers to improve their own processes or by providing a simulation history as an added value of products to their customers.

Industrial users of ICME are interested in designing their product as efficient as possible. ICME will be applied to reduce the design effort for new products/processes/materials in terms of costs and time. A specific requirement during modern simulation tasks within industrial design process concerns the configurable combination of different tools from different providers instead of monolithic solutions. A "plug-and-play"-type combination of tools in workflows and open simulation platforms is the key vision of future ICME. A future standardized data exchange will drastically decrease the efforts of software providers with respect to providing and maintaining a large number of import and export functionalities for their tools.

Though the benefits of using advanced material simulations are widely accepted, the application of the ICME approach within industrial settings still is a challenge in terms of complexity, capacity, and specific knowledge needed. Analyzing the needs of industry for ICME the following general conclusions can be drawn:

Conclusion 1

Cheap, fast, readily available, and reliable solutions are needed to tackle complex topics of technical interest.

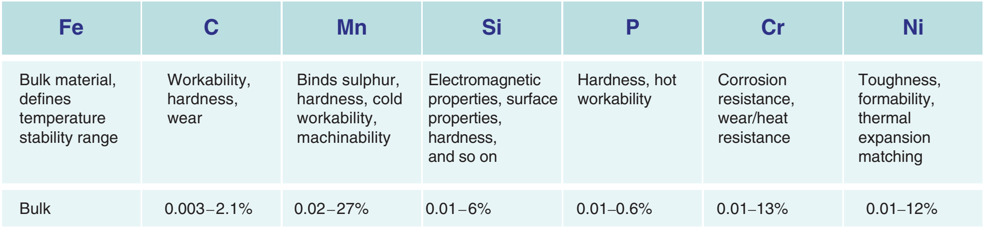
Future markets will not relate to *products* and their *properties* but rather to *functionalities* and *performance*. An airplane manufacturer – or the airline as its final customer – is not really interested in the turbine but in procuring and having “a propulsion *functionality*” performing best for an estimated operational scenario. Best *performance* could, for example, be a long operational period with a minimum of interrupts in operation or a low price with a minimum of operational costs (fuel), meeting environmental constraints and laws and many other conditions.

Topics and materials of interest are exemplarily depicted for processing and properties of bulk materials/components essentially being made from metallic alloys. Typical customers for metallic alloys are the aerospace industry (superalloys, light materials), the steel industry (steel), power utilities and respective industry (superalloys, steels, etc.), automotive industry (steels, Al alloys, and Mg alloys), electronics industry (solders, semiconductors, solar silicon), biomedical devices (Ti alloys), and other industrial branches. The alloys of interest, in general, comprise a large number of alloy elements each of them purposely added in a well-defined amount to fulfill a specific functionality (Figure 1.4). The specification of the exact amounts of alloy elements by now is a long-lasting and expensive – in terms of both time and money – task. The development and qualification of new materials and their processing in the past took years to decades. These development cycles will be drastically shortened by future ICME-type approaches.

In other areas, the relevance of treating numerous chemical elements results from the small size of components being at the scale of the diffusion length such as in electronic solder configuration, where the composition of the solder joint is determined by both the solder composition comprising, for example, some melting point depressants, and the coatings on the components to be joined (Figure 1.5):

Conclusion 2

Models and tools are needed for complex multicomponent and multiphase materials and their processing.



Fe	C	Mn	Si	P	Cr	Ni
Bulk material, defines temperature stability range	Workability, hardness, wear	Binds sulphur, hardness, cold workability, machinability	Electromagnetic properties, surface properties, hardness, and so on	Hardness, hot workability	Corrosion resistance, wear/heat resistance	Toughness, formability, thermal expansion matching
Bulk	0.003–2.1%	0.02–27%	0.01–6%	0.01–0.6%	0.01–13%	0.01–12%

Figure 1.4 The technical metallic alloy steel consists of numerous alloying elements with very different amounts and specific contribution to the overall performance and processing of the material.

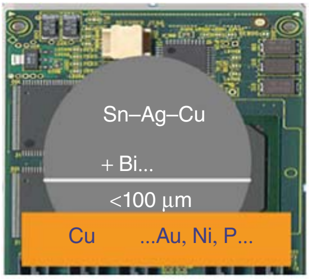
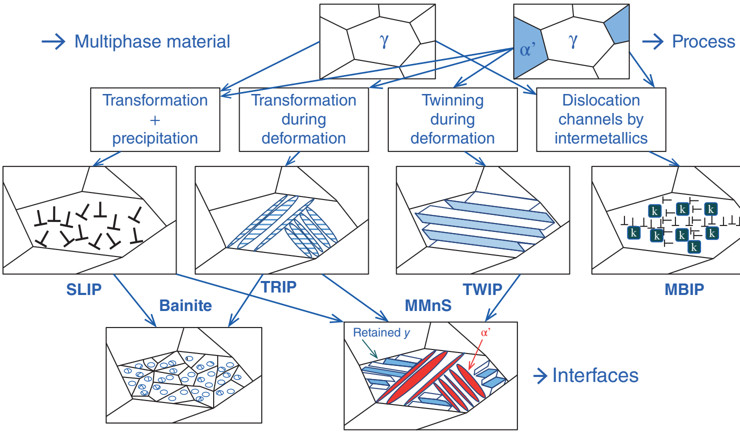


Figure 1.5 Steadily increasing miniaturization requires consideration of the effects of boundaries dissolving their chemical elements, for example, into a solder ball. A ternary Sn–Ag–Cu solder ball thus rapidly turns into a complex multicomponent, multiphase alloy system.

Advanced technical materials are not only a composition of various ingredients (alloy composition) but also consist of various phases of different crystallographic nature and/or local chemical composition. In steels and also in aluminum alloys, hard and brittle precipitates and inclusions are embedded in a more ductile matrix controlling the dislocation mobility. For example, steel may consist of two or more crystalline phases (e.g., ferrite, martensite, and austenite in parallel) being present in specific size, shape, and orientation. Recent developments aim at decreasing the structural length of single components (nanosized microstructures) and at exploiting metastable phases revealing complex deformation mechanisms during loading (e.g., transformation-induced phase transformation or inhomogeneous dislocation gliding) (Figure 1.6).

The costs of components are determined by the raw material, the production costs, and the costs arising during service life including repair and recycling. It is not only about the alloy composition. The *processing history* plays a decisive role in achieving the desired properties. During production, the material undergoes various process steps like casting and solidification, hot or cold forming, annealing, machining, joining, and coating. Each process during the entire production



SLIP: Dislocation slip or gliding (homogeneous or inhomogeneous)

TRIP: Transformation-induced plasticity

TWIP: Twinning-induced plasticity

MBIP: Microband-induced plasticity

MMnS: Medium Mn steels

Figure 1.6 Modern steel development aims at tailored properties by adjusting a multiphase microstructure by applying deformation mechanisms based on metastable phases and by decreasing the structural length scale of microstructural components.

chain affects the microstructure and thus the properties of the material. Also, the process itself is affected by the properties being controlled by the microstructure. Thus, there is a strong dependence between processing and properties during the production and also during the final operation of the component. It should be mentioned that the macroscopic properties of the component in general are determined by mechanisms occurring at the length scale of nanometers or even below.

Damascus steel can be considered as a thousand-year-old nanomaterial although nobody really knew about "nano" at that time. Knowledge about the process parameters for the repeated and well-defined application of numerous individual forming and heat-treatment steps eventually leading to the superior properties of Damascus steel took generations to evolve on the basis of trial-and-error approaches.

Conclusion 3

Models are needed to track the evolution of materials and components along their entire production and service life cycle.

Modern simulation techniques will drastically shorten the development times for new materials and their processing. Respective developments will become much more targeted. However, the vision of "materials design out of the computer" by now is still only in reach for few examples. Nevertheless, it is widely accepted that simulating processes and materials evolution during processes significantly supports the design process. Some modern materials and components can only be produced using quantitative simulations of their microstructure, their processing, and their performance.

Eventually, simulation results have to be validated against measurements, existing data, and real – sometimes even financial – arguments increasing the confidence into the model, in its predictive capabilities and in its commercial value. Such validation can be based on data provided and shared by companies and academia alike. This validation includes information about the quality of calculated results including the uncertainty to be expected due to the use of nonexact input parameters and also due to the limits of the models. In particular, any user has to be aware of such uncertainties and limitations if he is applying models for situations or questions that are not within the – hopefully well-defined – input parameter space.

Conclusion 4

Validation is needed requiring improved interaction between virtual and real worlds.

Validation does not only include proving that models are able to predict materials properties correctly in a quantitative manner. The modeling-based design approach itself has to be validated respectively has to be evaluated against a traditional design approach based on trial and error combined with tailored experiments. Thus, it is mandatory to know the quantitative predictability of models and to balance the benefit against the simulation costs. Only if modeling costs and efforts can be turned into an added value, for example, by improved production results, industry will continue to invest into simulations. To decrease simulation costs, it will be necessary to integrate all modeling components into a single work flow in a way that all tools are independent, but mutually connected.

This financial validation is a major industrial requirement. All industrial applications of ICME will focus on the delivery of the outcome. The following four key questions have to be discussed: (i) What is the outcome and the contribution of simulated results to the design or optimization process? (ii) How much does a specific tool and its application cost? (iii) How much does a specific calculation cost? (iv) What is the risk associated with feeding the virtual simulation results into real production?

Quantifying the “risk” becomes a priority, especially for SME use. A desirable output would be a predictive tool running hypothetical scenarios, which include both the technical and the market inputs into a holistic decision-making process by optimizing component performance and cost efficiency in parallel.

Conclusion 5

Multicriteria optimization of the workflow is needed to balance all business.

Improving the knowledge about processes and materials is not the final aim of an industrial ICME user. Eventually, simulations shall support the industrial user in making his business decisions and in optimizing his products. Simulations are an investment for a company in terms of software tools, IT infrastructure, and a highly skilled work force.

In terms of business decisions, the optimal solution from a technical point of view may not be the most effective solution from an economic point of view. The same holds for simulations during the design process. The perfect, quantitative, and predictive simulation approach is not always needed. Often simpler approaches offering a sufficient depth of understanding in a shorter response time are more appropriate to meet a specific design objective. This implies the need for nonmonolithic software solutions and for an effective adaptation of various software tools into a single simulation workflow. Different types of software solutions have to be available to tackle the same topic with different degrees of accuracy. These may reach from fast solutions providing quick estimates for decision making up to highly precise approaches requiring substantial simulation times for complex trouble shooting.

1.4
Present ICME

A major target of ICME is a holistic simulation approach comprising entire process chains for engineering components. ICME addresses not only the macroscopic component and the process scale, but also the local material properties of individual components on the microscopic scale. ICME not only encompasses

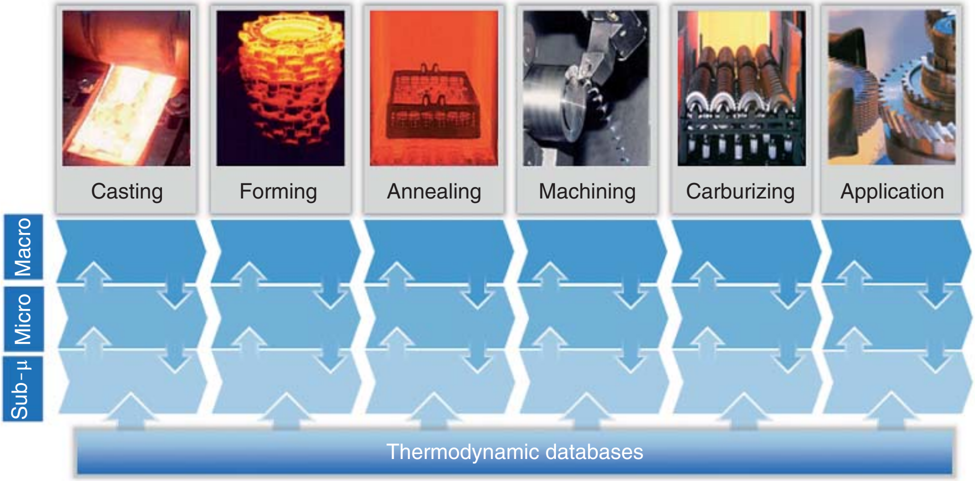


Figure 1.7 ICME aims to combine multiscale and through-process simulation toward a thorough description of all mechanisms being relevant for the production and performance of technical materials.

the material state for a given time at various length scales, but it also integrates the evolution of local material properties along the entire manufacturing process and eventually during service life (Figure 1.7). This concept promises better predictions and control of performance and service time of individual components or component assemblies. In this context, material microstructures and their evolution represent central issues in ICME as the microstructure is the carrier of the material properties.

Currently, numerous software solutions have reached a level allowing for valuable contributions to modern engineering tasks within knowledge-driven production models.

Simulations on the macroscopic scale of the manufacturing processes already are widely accepted and successfully used in industry on a Technology Readiness Level (TRL, according to the European Commission definition) of 8–9. Microstructure evolution codes and even more detailed electronic, atomistic, and mesoscopic models by now have reached a TRL of approximately 4–5 or even less. Respective approaches thus essentially are used in very specialized laboratories. However, the benefits of respective simulation tools and especially the needs for their mutual coupling and linking are widely accepted. The need for describing and simulating materials in more detail and at higher resolution is clearly formulated from an industrial perspective.

A major gap has especially been identified between continuum mesoscale models and world of discrete models (electronic/atomistic/mesoscopic). The usability, compatibility, and interoperability between these two model worlds have been formulated to be one of the major challenges for future ICME.

In spite of ICME currently emerging as a new and powerful discipline, coupling of different software tools is, however, still in its infancy and represents an issue consuming significant effort in terms of time and workforce if a coupling is realized at all. The combination of models by now is mainly achieved by manual transformation of the output of a simulation to form the input to a subsequent one. This subsequent simulation is either performed at a different length scale or constitutes a subsequent step along the process chain. Concerning the return of investment, the industry still complains on the significant amount of engineering efforts spent in data conversion and result management at the interfaces between different heterogeneous software tools. And indeed, there are several serious hindering factors: the missing of general standards for data format and platforms (in particular, the user friendliness of lower scale models is limited in most cases), the limited simulation knowledge at user side, expensive IT capacities, and no license schemes for short term but challenging calculation projects have to be mentioned.

1.5
Scope of this Book

The book covers essentially process chain for metals and alloys and to some extent also plastics, composites, and bulk components for structural applications (including coatings). These specific process chains could be composed based on the experience of the contributing authors. The developed concepts and descriptions, however, are all meant to be generic and may in future be extended to other fields actually not yet being covered, for example, pharmaceuticals, smart or functional materials, electronic or optical materials, textiles, and human tissue.

The book does not address (at least not explicitly):

- Hardware requirements
- Processing of nanoparticles, powder, molecules, and so on
- Subsystems of ICME like ICE not comprising materials as a central ingredient
- ICME politics

Scopes of this book are to:

1) *Serve as a tutorial for ICME engineers and scientists*
   Currently, there are only few educational schemes of "ICME engineers and scientists". ICME by now, in general, is performed by "self-learning" by people who recognized the importance of combining models and tools to achieve better performance of their materials, processes/products, and software tools. There is a need to at least basically acquaint engineers and scientists in a specific field with the basic concepts, problems, and solutions of all other field downstream or upstream the production chain. This handbook shall allow skilled engineers and scientists to get such an overview of adjacent fields. It shall create awareness about the possibilities and the needs/requirements of the other fields and possible limitations.

This overview shall further encompass the phenomena, models, and tools across all length scales relevant for the production process and for the properties of the materials and eventually the final product.

2) *Provide an introduction to different processes along the production chain including the lifetime of components*
For each of the process steps along the value chain like casting, forming, heat treatment, coating, joining, machining, corrosion, and recycling, an introduction is given even substructuring the particular field (e.g., casting: continuous casting, die casting, investment casting, etc.) and highlighting the relevant phenomena for each of these process steps. For each of these fields, current trends and actual developments are also shortly highlighted.
3) *Provide a general overview about concepts, methods, models, and tools across all scales*
The book addresses different concepts and methodologies like numerical methods, pre- and postprocessing of simulation results, thermodynamics, electronics, atomistics, mesoscopic, and discrete models as well as continuum models for both microstructure and processing scales.
4) *Provide references for further reading*
For each field, a number of references like review articles are provided for further reading, which themselves may be considered as "standard handbooks" or tutorials, reviews, or key publications for the field.
5) *Provide a structured directory of some prominent software tools in the different fields*
This book provides a directory of globally available software tools in the area of ICME. However, it does not simply draw on an alphabetic list-type directory. In contrast, it provides a structured compilation of these tools. The structure in this context is provided by the processes along the value chain during the production of a component.
6) *Discuss the origin of different data, initial conditions, and boundary conditions necessary to run the tools*
This discussion allows the identification of possible interactions between different models, for example, by providing data by one model for another model at the same or at a different scale. A similar strategy is applied for data on initial and boundary conditions. Further needs for new models to create required data may emerge from this discussion. Another topic under this discussion is the harmonization of information exchange between real and virtual worlds.
7) *Discuss current concepts to combine simulation tools in platform-type approaches*
The identified simulation tools are further discussed with respect to their integration into simulation platforms and ICME types of operation. This discussion especially focuses on interfaces and data formats being provided for import/export of information and also covers aspects of workflow management.

8) *Identify missing tools and functionalities and formulate suggestion for further development*
   In view of covering an entire life cycle of a component by simulations, also "missing tools" and "missing functionalities" are identified and suggestions for their development are outlined.

1.6
Structure of the Book

The structure of this book is "top-down" instead of "bottom-up" and thus follows the philosophy of "starting from the outcome." This outcome may be a certain consumer-desirable property of a specific product or of a specific component. Based on the respective requirements the physical, processing, and additional requirements allowing meeting the objective and tools for their simulation can be identified. Based on the identified requirements at each length scale, models at smaller scales eventually are either needed or allow for refining "down to the atoms" wherever this seems necessary or beneficial. This strategy is based on the conclusion that processing and properties cannot be treated independently but are strongly correlated. Materials cannot be tailored without considering their processing, and processes can only be optimized if materials behavior during processing is well understood in a quantitative manner.

A future strategy in ICME may be to investigate and consider only those scales contributing relevant information for understanding the given problem – a strategy of scale hopping instead of multiscale modeling. Even at a specific length scale, a fast and robust model providing estimates might be given preference over a sophisticated and very detailed model. This choice eventually will depend on the risks associated with the given task and the time and capacity being available to tackle it.

This chapter provides an introduction to the field and the motivation for future readers. Following an overview on "Integrated Computational Materials Engineering (ICME)," the potential benefits to industrial users are shortly highlighted. A section on industrial needs for ICME is followed by a short review of the current status on ICME. The introduction concludes with an outline of the book.

Chapter 2 details the variety of processes, simulations, models, tools, and phenomena occurring at the scale of component and being relevant to its production and its use. Following a short overview over a typical process chain, this chapter starts from primary shaping processes, for example, by solidification of a melt and then follows the entire manufacturing cycle, comprising the fundamental processes of forming, heat treatment, joining, coating, and machining. Eventually, this chapter also addresses the service life cycle in terms of corrosion, fatigue, and recycling.

Understanding of component behavior during processing or operation often requires understanding the microstructures of the materials building up the component. The evolution of microstructures is not only affected by the process conditions but by phenomena at all length scales.

Chapter 3 summarizes different models and tools to describe the evolution of microstructures. Following an overview and a specification of the term microstructure, a categorization is provided to describe microstructures at different levels of detail. Subsequent to the identification of the major phenomena affecting microstructure evolution, an overview of the different modeling approaches is provided. A section on nucleation modeling is followed by sections on models/methods describing diffusion/reaction processes and precipitation phenomena. Models and methods for the description of the spatiotemporal evolution of microstructures based on cell, lattice, or field representations are outlined. These include cellular automata and Potts Hamiltonian lattice models solved by Monte Carlo methods, as well as phase-field and multiphase-field models, phase-field crystal models, and crystal plasticity models. The chapter concludes with a structured list of software tools, specifically comprising tools for the analysis of 3D digital experimental microstructures.

Major requirements for any type of microstructure simulation are thermodynamic data and kinetic data as well as other parameters/properties of the phases present in the microstructure. Also the properties of the interfaces play a significant role. Respective data can be obtained from thermodynamic/kinetic databases and calculations as depicted in Chapter 4 or from electronic/atomistic/mesoscopic models as described in Chapter 5.

Chapter 4 provides an overview and an introduction to thermodynamics and thermodynamic modeling. Following a discussion on the role of thermodynamic modeling in ICME, the CALPHAD approach is explained. Based on its history and the minimization of the Gibbs energy as theoretical basis, the crystallography and models of phases, the development of CALPHAD databases, their formats, and future extensions are highlighted. The chapter concludes with sections on “use of thermodynamics at larger scales” and on “deriving thermodynamics/materials properties from small scale models.” This section addresses the future of determination of effective properties in ICME where first principles’ DFT methods are used to predict, for example, thermoelastic properties of materials.

Chapter 5 focuses on mesoscopic, atomistic, and electronic models following the overall “top-down” structure of the book. Following an overview on discrete and semidiscrete mesoscopic models in materials science, the specification of some definitions and an introduction to atomistic simulations like kinetic Monte Carlo and molecular dynamics is provided. A section on electronic structure methods addresses Hartree–Fock theory and post-Hartree–Fock methods and density functional theory (DFT) in its different approximations (local density approximation, “LDA,” generalized gradient approach, GGA). Further sections address actual developments like meta-GGA methods, hybrid DFT–Hartree–Fock approaches, and van der Waals-corrected DFT. In addition to providing a structured overview of approximately 80 different simulation tools in the area of electronic, atomistic, and mesoscopic simulations, the chapter further provides a number of links to online sources for potentials, force fields, and effective cluster interactions.

Chapter 6 goes back to larger scales and is devoted to the determination of effective properties and provides an overview of different approaches like finite-element-based homogenization methods, mean-field homogenization methods, and virtual testing approaches. Finite-element-based homogenization methods apply the method of homogenization on the continuum description of the microstructure of the material – resulting, for example, from phase-field models – being discretized into a finite element description. Details of this approach such as sensitivity of the obtained properties to the underlying microstructure and to numerical influences, for example, size of representative volume elements (RVEs), mesh density, and element type are highlighted and discussed on the basis of examples. Mean-field homogenization methods are explained based on example(s) for fiber-reinforced materials and address especially nonlinear and evolving material properties. A section on screening and virtual testing of material properties highlights the potential of usage of computationally derived effective properties to obtain tailor-made materials from the virtual stage and is presented for an application to a polycrystalline material and cover the subsequent usage for different microstructures.

Chapter 7 deals with numerical methods for the computational simulation of a wide range of multiphysics and multiscale problems within an ICME framework. Following an overview on preprocess and space discretization methods, a large section provides an overview of different kinematic descriptions, solution methods for coupled problems, and numerical methods for the solution of a wide variety of engineering problems such as the finite difference method (FDM), FEM, boundary element method (BEM), discrete element method (DEM), mesh-free methods (MFMs), particle finite element method (PFEM), extended finite element method (XFEM), isogeometric analysis (IGA) method, and model order reduction (MOR) methods. This overview is followed by a description of numerical methods for contact problems, such as Lagrange multipliers, penalty and augmented Lagrangian, direct elimination, mortar, and IGA methods. Further sections address postprocessing and visualization methods, and numerical methods for mapping and data transfer in the FEM simulation of multiphysics/multiscale problems using either Lagrangian or arbitrary Lagrangian–Eulerian (ALE) formalisms. Data transfer algorithms are discussed for the numerical simulation of a single process using Lagrangian or ALE formalisms and requiring remeshing operations. Sections on reduced-order models and on different issues related to high-performance computing (HPC) and parallelization precede a list of software tools for pre- and postprocessing.

Chapter 8 addresses "software platforms" and "software integration," which in industry currently essentially correspond to integrating continuum models. Respective developments are dominated by structural mechanics or computational fluid dynamics tools based on finite elements or finite volume numerical schemes as part of product life management or computer-aided engineering (PLM/CAE) environments. However, advances in nanotechnology require descriptions of processes occurring on the smaller scales, which can be provided by electronic, atomistic, and mesoscopic models and continuum models applied to the mesoscale. This demand requires extending the tools and approaches of ICME to include tools on the smaller scales as well and to make this variety of tools "interoperable." Following an overview of different integration approaches (object-oriented, component-based, service-oriented, data-centric, model-based, and ontology-based approaches), existing standards for integration and different available approaches to coupling and linking are briefly highlighted.

Chapter 9 discusses the needs for future developments required toward the objective of covering an entire life cycle of a component by simulations. In view of covering an entire life cycle of a component by simulations, also "missing tools" and "missing functionalities" and needs for interoperability are identified and some suggestions for future developments into these directions are outlined.

This book eventually provides a *directory of globally available software tools* in the area of ICME. However, it does not simply draw on an alphabetic list-type directory. In contrast, it provides a structured compilation of relevant models and tools. The structure in this context is provided by the processes along the value chain during the production of a component from a given material as depicted in the individual chapters. Almost all chapters identify the most relevant simulation tools and discuss them with respect to their underlying models, the origin of the required data, the necessary initial and boundary conditions, and eventually with respect to their integration into simulation platforms and ICME types of interoperation. A structured table of software solutions for each field marks the end of each chapter.

These tables are based on and compiled from a survey of modeling tools in a number of resources:

- Precompiled lists of software codes, for example, the TMS [4], or a recent Japanese activity [5]
- A list of software tools being used in research project funded by the European Commission with a focus on electronic/atomistic/mesoscopic models [6]
- Software repositories such as GitHub [7], nanoHub [8], or SourceForge [9]
- Software identified during the 1st International Workshop on Software Solutions for ICME
- Software companies in different fields being compiled on the basis of personal acquaintance and by Internet search
- A private homepage [10] providing a survey of public domain and commercial mesh generators
- The NIST Materials Data Digital Library [11]
- Two TMS studies on ICME [12, 13].

The resulting list – eventually comprising approximately 350 different software tools – was then further complemented by the knowledge of the authors of the individual chapters. Each of the almost 70 authors from at least 12 countries in 3 continents is a renowned scientist or engineer in his/her field making their comments on the different tools a highly valuable piece of information and advice.

The focus of the book definitely is on structural mechanics applications. In other areas, for example, electronic design automation, the Technology CAD (Technology computer-aided design or TCAD) is an ICME-type approach of modeling semiconductor fabrication and semiconductor device operation. The modeling of the fabrication is termed Process TCAD, while the modeling of the device operation is termed Device TCAD. The software tools available in this field are widely documented in [14]. Some thematic overlap between structural and electronic materials processing already occurs in the domains of crystal growth and thin-film deposition.

In the end, the book has actually become what it was originally intended to be: "the yellow pages for software solutions for ICME." But the book has evolved even further into something the editors and authors would like it to become: "a tutorial for young students in the emerging field of ICME" and a handbook for scientists and engineer wanting to get a quick but sound impression on adjacent fields of expertise.

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2

Modeling at the Process and Component Scales

Handbook of Software Solutions for ICME, First Edition. Edited by Georg J. Schmitz and Ulrich Prahl.

2.1
Overview of Processing Methods and Process Chains

Ralph Bernhardt and Georg J. Schmitz

The processing of materials and their targeted shape and property modification have a long-standing tradition in human history. Entire historical eras are named after a material, whose production and processing dominated a time period and determined technological advancement – examples are the “Stone Age” or the “Iron Age.” In general, many of the ensuing principles and approaches discussed in this book can be applied to technologically relevant engineering materials for solids. Whether for glass, plastic, concrete, wood, or metal, each material class has a specialized subdivision in materials sciences, materials engineering, and manufacturing technology. What they all have in common is mankind’s ongoing search for the most suitable method and approach to efficiently manufacture products made from the different materials, tailored to the individual requirements.

Today, the field of materials sciences and materials engineering already stands for new innovations in socially relevant, cutting-edge fields such as energy, climate and environmental protection, resource optimization, and mobility as well as the health sector, security, and communication. Current studies underline the exceptional direct or indirect dependency of all technological innovations on materials. Materials science and materials engineering belong – next to information technology – to the key technologies of the twenty-first century [1].

The insights gained in materials science enable the manufacture of high-tech materials with new or improved properties and also the improvement of existing and the development of new processes. The material selection, the structural design, the manufacturing process, and the workload and operational conditions influence a component’s properties. This encompasses the entire life cycle of a component up to recycling or material recovery, including the development of entirely new manufacturing processes.

Covering all possible material classes in this chapter would hardly be possible and also not serious. This particular chapter thus focuses on essential fundamental principles and approaches to the production, processing, and treatment of metallic materials as well as their modeling at the process scale, representative for all other relevant types of engineering materials.

Handbook of Software Solutions for ICME, First Edition. Edited by Georg J. Schmitz and Ulrich Prahl.

This introductory chapter briefly depicts the history of primary shaping and forming technologies of different metals. A second historical excursion relates to the development of modeling of manufacturing processes.

To widen the readers' view and to demonstrate the generic nature of the concepts being discussed in this book, the appendix of this introductory chapter discusses a very special process chain for a very special nonmetallic product: asparagus.

2.1.1
History of Metalworking

The beginnings of metalworking can be traced all the way back to the fifth century B.C. Depending on the historical source, either Persia (now Iraq) or the Mediterranean region is identified as its origin. It is proven that during the "Copper Age," gold, silver, and copper were already melted, cast, and cold-hammered. Craftsmen of that time already discovered that alloying copper with, for example, arsenic increases the material hardness, making it more suitable for the manufacture of weapons. About 3000 B.C., the first alloy system was established with the discovery of bronze. In the wake of this discovery, sheet pressing tools were introduced, the marking stamp was invented, and needles or rather profiled wires were manufactured. The spread of forming technology over the course of the Iron Age and throughout the Roman Empire – until about the thirteenth century – led to the first heyday of metalworking between the fourteenth and eighteenth centuries. Hydropower was increasingly used as a power unit driving forging hammers; the first presses and rolling mills found their way into manufacturing.

The great significance of metal tools and commodities is reflected in the contents and definition of the "Artes Mechanicae" of the seven mechanical arts of the Middle Ages [2, 3].

Further milestones on the way to mechanized and automated mass production of metal products were the invention of the steam engine by James Watt and the improvement of steel quality through new processing methods in the middle of the nineteenth century. Only these new advancements in steel production could supply the durable tools required for metalworking. With them, the technologies still relevant today such as die forging or rolling were able to gain their industrial and economic importance. After the 1960s, the industrial era was succeeded by the information age of today. Also known as the "silicon era," modern important advancements have occurred in the field of computer-aided modeling of technological processes. Next to metallic materials (ferrous and nonferrous metals), silicon has gained a particular importance as a metalloid. Metallic materials and iron-based materials such as steel continue to be of immense value as engineering materials. Around 1.6 billion tons of raw steel were produced in the year 2014. For 2015 alone, 1.5 billion tons of finished steel products (excluding nonferrous metals) were projected (see [2–6]).

2.1.2
History of Modeling of Manufacturing Processes

For centuries, the production and processing of materials was marked by empirical and heuristic approaches. Exploiting observed or accidentally discovered phenomena and effects was predominant. For example, the hardening of steel, a 3000-year-old technology, was "long enveloped by superstition and a mystery even to experienced masters" [7].

First systematic approaches to explain and to model materials already existed in the form of the particle model by Demokrit (around 400 B.C.) in old Greece. Similar to the works of Leonardo da Vinci (1452 – 1519) and Galileo Galilei (1564 – 1642) about determining and analyzing hardness on metal wire and structures, these discoveries were not systematically used to proactively develop new technologies. The book of metallurgy *De re metallica libri XII*, published in 1556 by Georgius Agricola, provided a substantial compilation of "recipes," yet this approach to the contemporary technologies was of a more descriptive and heuristic character (Figure 2.1.1).

During the seventeenth and eighteenth centuries, the philosophers of nature began to address the subject. They catalyzed the breakthrough of the old Greek concept of atomic structure of matter and discovered "crystallinity." With the transition from alchemy to chemistry and from metaphysics to physics at the end of the eighteenth century, the foundations for the systematic, mathematical – physical description of material properties and material processing were laid. The beginnings, for example, of the plasticity theory were born. Names such as Coulomb, Tresca, Levy, Huber, von Mises, Hencky, Poisson, Cauchy, Lamé, Green, Young,

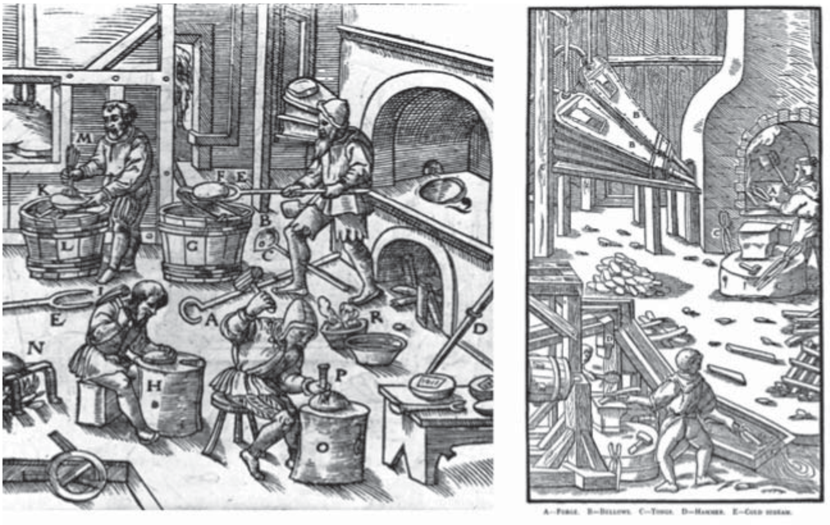


Figure 2.1.1 Steelmaking and blacksmithing in the Middle Ages – woodcuts from the book *De re metallica libri XII* (Georgius Agricola) – showing the interior view of workshops with men at various stages of the metallurgical process. (Wikimedia-commons.)

and many others stand for some of the groundbreaking models and theories still supported today. A good overview of the historic evolution of the theory of plasticity can be found in [8].

The development of mathematical methods and algorithms for solving complex equations and systems of equations in particular for partial differential equations enabled an increasing depth and importance of modeling results. Numerical methods became an indispensable tool for scientists as a supportive branch of mathematics. The importance of numerics was raised to new heights along with the invention of the computer in the 1930s. Computers and numerics provided the two basic ingredients for the introduction of the finite element method (FEM) in the 1940s. Today, FEM is one of the most internationally widespread software methodologies for numerically solving partial differential equations in almost all engineering fields, in both research and industrial applications.

Solving problems with the help of the FEM can boast a 70-year tradition today. Limited to linear elastic problems in the beginning, the still valid concept of a stiffness matrix and element assembly to also solve nonlinear problems has established itself since the 1960s – more precisely with the introduction of NASTRAN in 1965 by John Davidson. While the development of elaborate and complex models was reserved for an elite circle of highly specialized computer experts in the early days, the method now has been established as a commercial tool in the manufacturing industry since the mid-1980s. While the first applications were limited to 2D problems and rather simple geometries, nowadays even complex 3D applications with a high level of detail can be calculated on conventional desktop computers.

The digital revolution and along with it the development of measuring and characterization technologies down to the individual atoms have made tremendous progress during the last decades. They are nowadays both prerequisites and driving forces for increasingly more detailed modeling of industrial manufacturing processes. Respective simulations have made the much quoted “lightweight design” possible in the first place. Integrated Computational Materials Engineering (ICME) is emerging as a main pillar of this overall concept as this integrated model approach not only integrates different length and timescales but also simulation and experiment and fundamental research with applications.

Crucial for the significant improvement and innovation in functionality, reliability, life span, and business efficiency of products is the integral approach, meaning the interlinking of information from different length scales and tracking of evolution of material properties over several process steps. A number of mechanisms influence and therefore determine material responses to workloads. ICME is the method of choice to quantitatively describe the relationships between process steps, material microstructure, material properties, and component behavior.

Future ICME will achieve the continuous cross-linking of production and application-related mechanisms, which the materials undergo on different length and timescales. Thus, changes in the material properties can be tracked and numerically described throughout the entire component manufacturing process. Based on these observations, weak spots in the process chain as well as during the lifetime can be determined and eliminated.

2.1.3
Overview of Processing Methods

A first rough classification of manufacturing processes following the German Standard DIN 8580 [9] is depicted in Figure 2.1.2. Similar classifications can also be found in [10]. Manufacturing processes are defined as processes in which products (outputs) are generated from other goods (inputs). Manufacturing technology defines manufacturing processes as processes for the production of geometrically defined solid bodies. This includes semifinished products or components of technical structures.

In general, several manufacturing processes have to be combined to proceed from raw parts to semifinished products and eventually to finished products such as machines, devices, tools, vehicles, and other single- or multipart objects/components and systems. The aforementioned DIN standard comprises – besides the geometric form – also the targeted modification of the properties of the manufactured product. The manufacturing sequence of a product is illustrated for the example of a vise in Figure 2.1.3.

Modern sustainable economies have to take into account not only the manufacture of a product but also its efficient and economic use during lifetime operation and eventually its recycling. Recycling is the process of reusing wastes/waste materials to generate secondary raw materials. Recycling is defined as "every recovery process through which waste products are processed to products, materials or substances either for their original purpose or for other uses. It includes the processing of organic materials, but not energetic recovery or the processing of materials purposed as fuel or back filling" [4].

This chapter covers all processes along the entire life cycle of a typical product in individual subchapters starting from primary shaping (2.2), via forming (2.3),

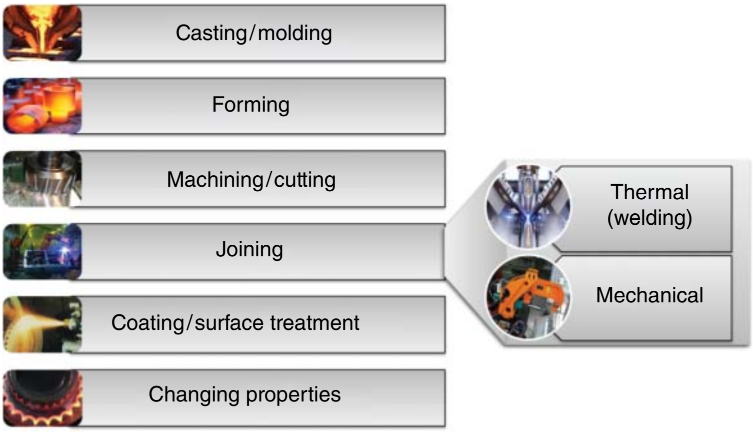
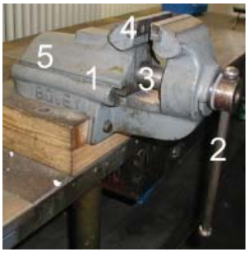


Figure 2.1.2 Main methods of manufacturing processes according to German Norm DIN standard 8580.



1. Base body: primary shaping: melting (formless substance) → casting (primary shaping) → work piece (vise body) and semi-finished parts for other components
2. Crank handle: Forming: raw part (billets) → rolling on a roll stand (forming) → component (Round material for the lever)
3. Vise spindle: Cutting (by machining): semi-finished product (round material) → turning, threading → component (Spindle)
4. Hardened vise jaws: Changing material properties: raw material (steel) → Hardening of the jaws (changing material properties) → component material (hardened steel)
5. Painting: coating: raw component → varnish application (coating) → painted component
6. Final assembly: Joining: individual parts → assembly (joining) → finished part (vise)

Figure 2.1.3 Manufacturing steps for components of a product for the example of a vise after [9]. (Benutzer https://commons.wikimedia.org/wiki/File:Schraubstock-800.jpg#. Used under CC BY 3.0 license https://creativecommons.org/licenses/by-sa/3.0/deed.en.)

heat treatment (2.4), joining (2.5), coating with thick (2.6) and thin (2.7) films, machining (2.8), fatigue (2.9), corrosion (2.10), and eventually recycling (2.11).

2.1.4
Processes and Process Chains

A technical *process* in the sense of manufacturing a product after DIN 66201 can be summarized as the entirety of processes in a system in which the state of the product is specifically altered. This change in state can entail an alteration of the geometric form and/or of the properties of the product. DIN 66201 also states: "A technical process is a process, the physical quantities of which can be determined and influenced with technical means."

A correlation between the process, the microstructure of the finished product, and accordingly its properties exists in all manufacturing processes:

> Process influences microstructure and microstructure determines properties.

The interpretation of this statement means that any processing of a material by any of the manufacturing processes automatically results in a change of its microstructure and therefore in the (local) properties. These changes may be small and even almost nondetectable or may be dramatic in some cases, for example, phase transitions in the materials are evoked by the process.

One of the oldest and globally well-known *process chains* in the field of metal forming was already applied to the manufacturing of Damascus steel in order to achieve a targeted geometric form and a specific combination of properties [11]. The origins of Damascus steel date back to the year 600 B.C. and took place in modern-day India and Sri Lanka. Essentially, after an initial primary shaping process (melting and casting), a multistage hot forming process (forging) is

Figure 2.1.4 "Disassembly of a car." (Paul Hudson https://commons.wikimedia.org/wiki/File:Disassembly_of_a_car_(3).jpg. Used under CC BY 2.0 license https://creativecommons.org/licenses/by/2.0/deed.en.)

linked with a joining process (forge welding) with intermediary heat treatments (quenching and tempering) and cutting operations. The basic idea is to join two single bars of materials of varying hardness, heat them, and create a form by forging. The early craftsmen already understood that the joining of two different materials results in a product that is not only very hard and durable (hard steel) but also possesses sufficient toughness (soft steel). Furthermore it was perceived that if the process is repeated very often, the continuous combination of forming, folding, and heating results in a very fine microstructure in terms of the number of "folded layers."

Recently it was discovered that "the forge masters of the time used trial and error of different methods to create nanostructures, which constituted the key to the particular hardness. Periodic heating and forming of the steel fostered the creation of carbon nanotubes, which in turn contribute to the formation of microscopically thin fibers of iron carbide" [12]

The necessity of linking different individual processes and repeatedly applying them in a process chain therefore are an evident prerequisite to reach the superior properties of the Damascus steel.

It is obvious that the combination of processes results in an arbitrary number of different process chains with an arbitrary number of complex combinations. Even each of the individual processes in such a chain reveals an almost infinite option to adjust its parameter set such as temperature–time profiles. Different process chains can further be combined to form a final sequence, which typically happens when individual components are assembled into a system. These components are joined and assembled in a specific assembly sequence to form a system – each component representing the process chain in itself, which has been run to manufacture it (Figure 2.1.4)

2.1.5
Benefits of Modeling Process Chains

"Customers neither buy products nor features, but benefits" – this statement can be ubiquitously found in standard literature about marketing and communications. "But benefits are determined through properties" – only this clarification explains the necessity for the current shift in the manufacturing industry from product-oriented to property-oriented development and manufacturing.

As already discussed in Chapter 1, “properties” in this context are now increasingly replaced by the demand for “functionality” (e.g., determined by a number of properties) and even further by the demand for “performance,” meaning the provision of a functionality for a given life cycle.

Manufacturers are increasingly facing the challenge of reliably manufacturing new products with high-dimensional accuracy and only revealing small tolerances for the local properties. They further need to operate their processes and process chains not only economically but also ecologically in terms of energy and resource efficiency [13]. Possible solutions are customized and tailored materials, specified for the component requirements, and adjusted processes for their manufacturing and processing. The focus is on the *entire* process chain, which is generally heterogeneous in terms of the process owners in the supply chain and also in terms of the variety of process types.

To meet the demands for individually adjustable product properties at the end of the process chain, the complex relationship between material design (e.g., the alloy composition for metallic materials) and the desired local creation of different microstructures and phase components (e.g., fiber form and orientation in fiber composites) and the specific process parameters have to be analyzed along the entire process chain and across the different scales of relevance. In the end, locally occurring effects in microstructure of different length scales determine the distribution of properties at the component level. Properties in this context are not limited to strength requirements. The terms “life cycle” and “performance characteristics” also include, fatigue, abrasion, and corrosion – here the focus is on the machining and heat treatment processes as well as the methods of surface treatment and joining.

All the aforementioned statements have a common and central denominator: the importance of the materials used and their (local) properties in compliance with their operational performance. For a targeted design and robust adjustment of the required component properties, the early knowledge and design of the following parameters are indispensable:

- Type, proportion, distribution (segregation), and mode of action respectively purpose of alloy elements
- Phase fractions and their local distribution and properties of the phases
- Grain size and their (statistical) distribution and derivable properties
- Type, proportion, size, shape, and distribution of precipitates
- Existence of preferred property orientations (anisotropy effects)
- Consideration of micro-/macrodefects/damage (porosity, inclusions, blowholes)
- Undesired inclusions (e.g., oxides in casting processes)

In order to control these parameters, appropriate process designs have to be developed in advance, and robust process situations must be found for every single process step. Taking into account the history of the previous manufacturing steps is the only way to reach this objective. The biggest challenge is that the aforementioned factors are often controlled by effects in the micro- and nanoscale and are in most cases not homogeneously but stochastically distributed over the component.

Using the example of a safety-critical automotive component, the outstanding importance of a virtual design approach can be clearly demonstrated: Redesign of such a component first requires selection of a suitable alloy, which has to be ordered from suppliers of semifinished products in an amount of typically 5 tons in business practice. Samples being produced by the desired production process are then subjected to durability tests and – according to the client's specification – to static and/or cyclic torsion or bending tests. Structural analyses, the creation of entire tool sets, and a prototype production under near-series conditions drive the costs for one loop to the six-digit euro range. A similar reasoning also holds for the approval of new aerospace components [14].

2.1.6
Available Modeling Tools at Component Scale

There is a large variety of available software codes and modeling tools at component scale. Subchapters 2.2–2.11 provide a list with respective tools in the different fields. Independent of the dedicated application field and methods being used, three types of software can be distinguished:

- General-purpose (GP) codes
- Commercial codes
- Proprietary codes

GP codes – as the name implies – are not limited (or only to a certain extent) in terms of applicable problems. They enable users to define a wide range of problems with respect to manufacturing processes at the component scale. Their biggest advantage is the unbeatable flexibility. On the other hand, they demand for very experienced users. Handling of simulations may become very complex and time consuming. In some cases such codes would be able to model manufacturing processes, but modeling and computational efforts to spend make it unattractive to use the software.

Commercial codes mostly make use of the same or similar solver solutions like GP codes, but they are specialized for a single main application – in the manufacturing areas this can be commercial codes for primary shaping or plastic forming or welding or heat treatment or surface treatment or machining applications. Specialization in this context means the best fit to the specific areas of application.

Proprietary codes are most of the time highly specialized solutions to cover one given process type or process chain of a company. They have nearly no flexibility to solve other problems but may provide excellent output for the very specific application. Such codes are not available on the market.

All types of software packages shall predict – for the selected manufacturing processes – integral quantities like forces, moments, work, and energy.

Furthermore they shall predict the viability of the process design approach, the existence of potential failure sources, and the evolution and distribution of typical scalar field variables like temperatures, strains, strain rates, and others.

The microstructure of a material has a huge impact on the properties of the component after each process stage and is itself influenced by the process. Modeling tools being designed to compute manufacturing processes at the component level mostly provide averaged output for microstructure features like phase transformation rates and phase fractions, grain growth, and grain size along with some information on recrystallized fraction and in few cases information about diffusion-driven processes. Methods and models to describe the microstructures and their evolution in more detail are discussed in Chapter 3.

When combining different codes, one has to differentiate carefully between the so-called incremental (fully coupled) and offline calculations (decoupled, postvariables). Fully coupled approaches considering the dynamic change of the material conditions (e.g., workability) are expensive with respect to computational efforts. Aspects of numerically coupling different modeling tools are discussed in Chapters 7 and 8.

Within the existing variety of software codes, no single software vendor can provide all the necessary answers. In order to virtually describe the entire manufacturing process of a component, thus several solutions are needed to cover the different process types by suitable modeling approaches. In the existing heterogeneous world of software solutions, it is, however, still hardly possible to consider the manufacturing history of the previous process steps and hence their impact on initial and boundary conditions with respect to the material state and the component properties. This will be one of the major challenges of introducing ICME approaches to a broader industrial community [15].

The following subchapters provide an introduction to the different individual processes in the process chain according to the categorization depicted in Figure 2.1.2 and provide lists of software tools currently available in the individual fields: casting – forming – joining – heat treatment – machining – coating – operations – corrosion – recycling.

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