Part I
Concepts

Integrative Computational Materials Engineering: Concepts and Applications of a Modular Simulation Platform,
First Edition. Edited by Georg J. Schmitz and Ulrich Prahl.

1
Introduction

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1.1
Motivation

The production of increasingly complex and valuable goods requires highly advanced, knowledge-based, tailored materials and components. In general, production goes along with planning and design activities to elaborate suitable process chains, leading to the desired functionality of the component while simultaneously meeting reasonable cost targets. This leads to a dilemma where efforts spent in planning and design have to be related to the final value of the product and, accordingly, the price a customer is willing to pay for it. The quantity any producer is interested in is the profit to be made. In a very simple view, this profit may be defined as

$$\text{profit} = \text{value} - \text{costs}$$

Value here may be interpreted as the price a third party is willing to pay for the product, while costs comprise the costs of anything needed to produce the particular product. Especially, activities for designing and planning the product and its production process on the basis of experiments and simulations have to be considered here as well. Thus, any optimization of the planning process (Figure 1.1) will lead to either a reduced effort in terms of time and costs to be spent in planning or to more reliable predictions, reducing the necessity of experimental tests for verification or even enabling a production at ''first time right.'' In particular cases, even the value of the product may be increased, for example by including a virtual documentation of its production process and its properties, which may be used by the customer to elaborate better predictions for the maintenance and life cycle when using the product. A reduction in maintenance intervals or an extended service time represents an added value for this customer. Another benefit might be drawn from extending the service life of a product by entering it into service with properties being sufficient – but not yet optimal – while expecting their further optimization under operational conditions.

A fundamental requirement to meet the ambitious objective of life-cycle modeling of products is an integrative description of the history of the component, starting

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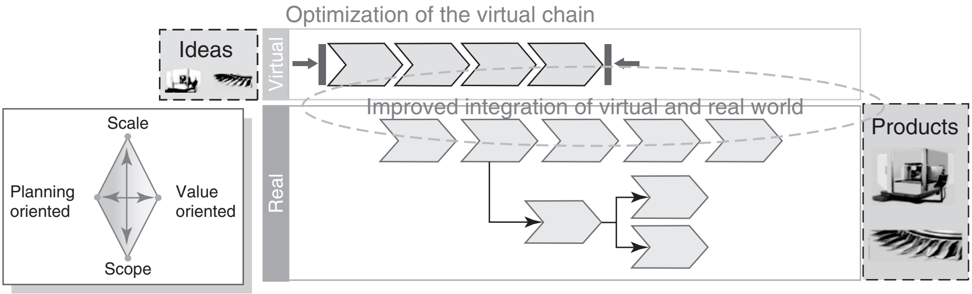

Figure 1.1 Efforts for planning production processes by simulations can be reduced by (i) optimization of individual modules and especially by (ii) improved communication between different modules. The real production process can be optimized, for example, by coupling the virtual world with on-line process control.

from the sound initial condition of a homogeneous, isotropic, and stress-free melt; continuing via subsequent processing steps; and eventually ending in the description of failure onset under operational load. The realization of such a modeling scenario is one of the key objectives of Integrated Computational Materials Engineering (ICME).

1.2 What Is ICME?

ICME or ''Integrative Computational Materials Engineering,'' as denoted in the title of this book, or ''Integrated Computational Materials Engineering,'' as used, for example, in Wikipedia – the slight differences in nomenclature already indicate that it is helpful to discuss the wording in all its aspects before entering the subject itself in more detail.

Looking at the four ingredients ''I,'' ''C,'' ''M,'' and ''E,'' materials scientists might discover an analogy with a quaternary phase diagram like for example the Fe–C–Mn–Si alloy system (Figure 1.2a–d). In order to construct a thermodynamic description of a quaternary alloy system one starts from the pure elements and continues via the binary systems. Those are then used to construct the ternary system and eventually ternary systems are used to construct the quaternary system. It is worthy to note that a ternary system might comprise information that cannot be obtained by a mere superposition of the binary subsystems.

Unveiling the complexity of the quaternary system, ICME will provide a common understanding of the wordings used in this book and best starts from exploiting the ''unaries'' I, C, M, and E first, before continuing via the ''binaries'' integrative computation (IC), integrative materials (IM), integrative engineering

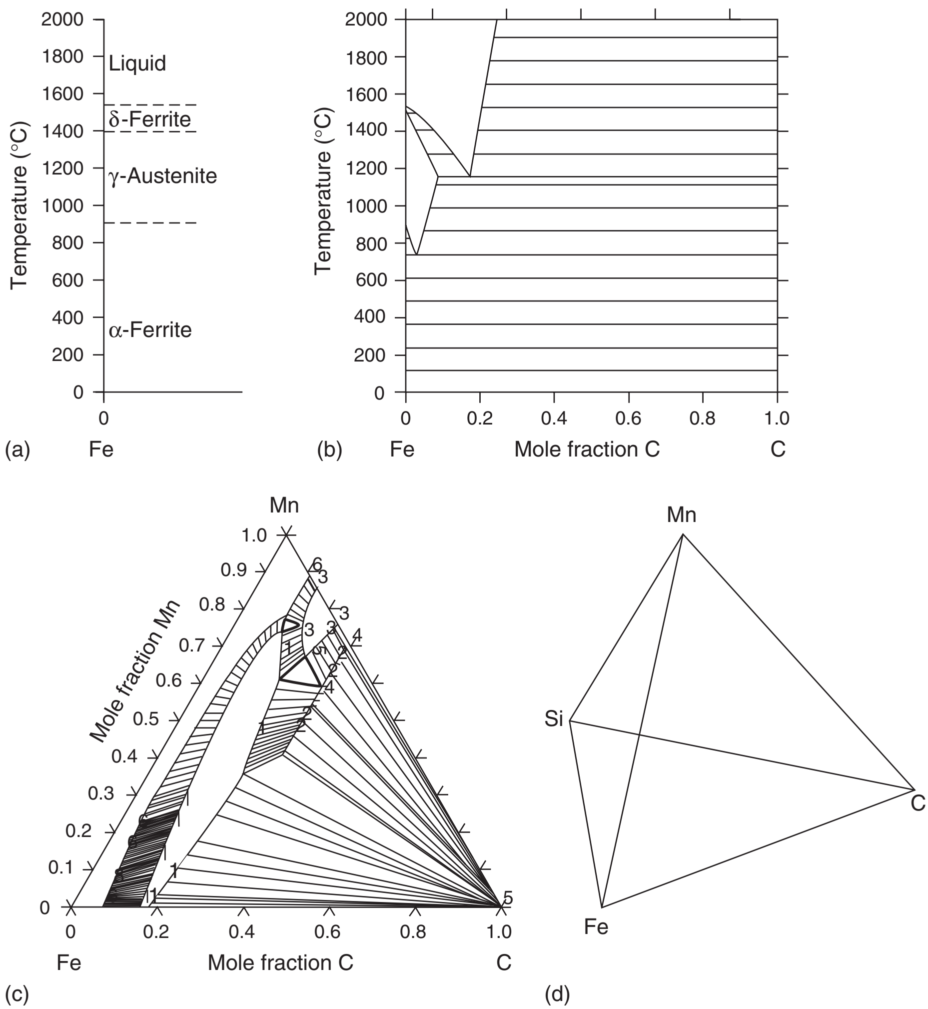

Figure 1.2 (a–d) Schematic thermodynamics of a quaternary alloy system (Fe–C–Mn–Si). (a) Unary phase diagram for pure Fe representing the left boundary for (b) the binary system Fe–C that itself for a given temperature ($T = 1200\ ^{\circ}C$) is a boundary of (c) an isothermal section of the ternary system Fe–C–Mn (calculated using Thermo-Calc). The quaternary diagram Fe–C–Mn–Si for a given temperature corresponds to a tetrahedron with four isothermal ternary sections (not shown in detail) forming the four faces of the tetrahedron (d).

(IE), computational materials (CM), computational engineering (CE), and materials engineering (ME) toward the ternaries integrated computational materials (ICM), integrative computational engineering (ICE), integrative materials engineering (IME), and computational materials engineering (CME).

1.2.1
The "Unaries": I, C, M, and E

- **"I" like integrative, integrated, integration, integr***: These expressions are found in a variety of contexts ranging from social life, mathematics, natural sciences, engineering, and others. Subjects of social integration are, for example, different cultures, and a key issue for a successful integration in social life is communication using a standard for information exchange – the common language. Integration in mathematics essentially means summing up different contributions to form a new entity – the integral. The difference between "integrated" and "integrative" may be seen in the fact that the first term implies the process of integration being already completed, while the second term considers it as still ongoing. With respect to integration in "time," the word history seems adequate, while integration of knowledge over time leads to experience. Usually, an integrative view generates additional information as compared to the mere superposition of the individual parts. Specific aspects of integration in engineering, materials, and computation are discussed in the "binaries" IE, IM, and IC.
- **"C" like computational, computers, computation, comput***: In short, anything that can be performed on a computer such as simulations, handling of large datasets, description of iterative processes, computer control and steering, storage of data and knowledge, mimicking of real processes in virtual reality, computer games, and e-learning. The computer hardware arrangements used for such purposes range from simple processors for simple control tasks to high-performance computing (HPC) for demanding simulation tasks and comprise methods such as parallel computing, grid/cloud computing, and many others. Nowadays, computer technology has reached a degree of maturity, being sufficient to handle large datasets and to tackle complex engineering tasks.
- **"M" like materials**: Classification of materials may be on the basis of different types such as plastics, rubbers, metallic alloys, ceramics, concrete, biomaterials, and wood. Other schemes hold for their individual shape such as bulk materials, thick films, thin films, coatings, or for specific functionalities such as conductors, isolators, structural materials, biocompatible materials, biodegradable materials, high-temperature materials, shape memory materials, self-healing materials, and many, many others.
- **"E" like engineering**: All activities related to design, construction, manufacture; production, assembly, operation and repair/recycling of materials, components, and systems, for example, for consumables, investment goods, public infrastructure, or exploitation of raw materials and resources. Engineering draws on fundamental understanding of phenomena in order to make them applicable for use.

1.2.2
The "Binaries" ME, IM, IE, IC, CE, and CM

The sequence of the description of the "binaries" has been selected according to the relevance for this book, meaning that those binaries without "C" are treated first because they historically have been present before the availability of computers and thus form an initial state especially for their later ternaries comprising a "C."

"ME" Like Materials Engineering or Engineering of Materials Any efforts aimed at influencing, controlling, and tailoring the properties of materials, especially for technical applications such as "engineering materials." These properties are largely determined by the microstructure of the material, which itself is the result of a subtle interplay of its chemical composition and the entire history of its manufacturing process. Typical ME parameters comprise grain size, grain boundaries, local and global crystallographic orientations ("texture,"), phase fractions, precipitates, dislocations and defects, and their arrangement in the microstructure. Other relevant quantities especially are the concentrations of the individual chemical elements at the scale of the microstructure – the so-called microsegregation – and their variation across the entire component, the macrosegregation. Segregations do contribute to the mechanical properties in terms of solid solution hardening. Their major impact, however, is in their role in determining the further evolution of the microstructure such as the formation or non-formation of precipitates during heat treatment.

Besides the alloy composition itself, a number of process parameters such as heating or cooling rates, dwell times in heat treatments, application of pressure and/or special atmospheric conditions, specific deformation and recrystallization procedures are especially used to control these ME parameters. External electric or magnetic fields, ultrasound agitation, and addition of numerous seeding particles for grain refinement or the use of only a single seed when aiming at a single crystal are some other methods to influence them. It should be noted that in special cases such as for amorphous materials with special properties, the design space for respective products is restricted, for example, to products being small in at least one dimension (powders, wires, foils), because reaching the amorphous state requires extremely high cooling rates, which can only be realized for thin products.

ME – even until the end of the twentieth century – has been based on skills, experience, special recipes, and traditions. Such traditions allowed the realization of exceptional properties by a well-defined sequence of dedicated process steps leading to special microstructures, for example, in ancient damascene swords. With the beginning of the twenty-first century, the availability of sufficient computer capacities and dedicated numerical models allowed for a deeper understanding of the underlying individual processes leading to a desired microstructure in the frame of "computational materials" and "integrative computational materials" (ICM) modeling, the latter being applied in the case of several processing steps. In this context, it is worthy to note that future efforts – in terms of time and resources – to elaborate a suitable process chain, including a well-suited set of parameters, can be drastically reduced as compared to the development of the above-mentioned damascene process, which took generations to evolve.

"IM" Like Integrative Materials Integrative Materials (IM) might be interpreted as materials combining the individual properties of several materials or integrating several functionalities in a material to form a new material with improved functionalities or properties. Thus, typical examples of IM would be metal-matrix composites such as fiber-reinforced or particle-reinforced metal-matrix composites; reinforced ceramics such as cermets, textile- or steel-reinforced concrete; and reinforced polymers such as CFC, and many others.

Besides arranging one material in the bulk matrix of another material, multilayers of different materials such as laminates or coatings can be considered as another type of IM, where, for example, a coating adds a "corrosion protection" (or an optical, a tribological, or an isolating) functionality to the "structural" (or electrical) functionality of the base material.

Whether such a composite material is considered as a product created by the combination of two different materials or whether it is interpreted as a new material with new effective properties is quite diffuse and frequently depends on its final application. It seems important to note that the properties of such a composite material cannot always be estimated as a weighted average of the individual properties. An important point is that the individual materials such as a technical metallic alloy may also be considered as "composites" being combined from several phases at the scale of their microstructure. Depending on the desired application, either detailed information about the different components/phases and their spatial distribution in the composite or an "effective property of the system" may represent the necessary resp. interesting and adequate description.

"IE" Like Integrative Engineering The term *integrative engineering* might be defined in different ways. It may be interpreted as a combination of different processes ("hybrid processes"), a combination of different technologies ("hybrid systems"), or combinations of a number of components ("system engineering"). Another aspect of IE aims at integrating an increasing number of functionalities in a decreasing system size, such as downsizing concepts in the automotive industry or integrated circuits in the electronics industry.

A modern aspect of IE is integrated production engineering, which is a holistic approach to production processes comprising the engineering of process and value chains from the basic level of understanding of materials and processes up to global production networks and all related logistics.

A success story of integrated production scenarios are platform concepts being essentially characterized by modularity and standardized interfaces. Such platforms, as, for example, platforms known from car manufacture, allow creation of individualized and customized products in spite of an underlying mass production process.

"IC" Like Integrative Computation In a similar sense, software integration in informatics is the combination of different software and/or hardware tools to form a new, more complex entity. Integration in this context may extend from full in-line integration, where the different tools directly interact at each time step, to handshake protocols, enabling an easy information transfer between different tools in a serial type of coupling. Although seemingly contradictory, "distributed" computation is a special form of integrated computation, as distributed resources are combined to form an integrated computational network. Special examples are cloud computing or ''Software as a Service'' approaches. Integrated computation also refers to special computer architectures such as shared memory architectures or special postprocessing procedures like immersed visualization.

Future developments – as already shown by present Internet browsers – increasingly will take directions of data accumulation, data integration, data retrieval, and knowledge management. Especially for ICME, such a data management is most important for both storage and retrieval of simulation parameters, particularly for a virtual documentation of the component life cycle.

''CE'' Like Computational Engineering All engineering tasks supported by computers form the area of ''CE.'' Engineering tasks, especially in the area of mechanical engineering such as design, construction, manufacture, production, assembly, and operation of components and systems, find their virtual counterparts in computational aided engineering (CAE) such as computer-aided design (CAD), computer-aided manufacture (CAM), virtual manufacturing systems (VMS), and finite element methods (FEMs).

Further aspects of production engineering such as factory planning and logistics are modeled on computers as well, for example, in the frame of condition-based factory planning (CBFP). CE of the materials-representing the basis for any production processes-and their properties proceeds in the areas of CM and CME.

''CM'' Like Computational Materials A number of keywords can be listed to describe the aspects of CM science such as *ab initio* calculations, density functional theory (DFT), molecular dynamics, CALPHAD approach, and computational thermodynamics. Most of these methods aim at descriptions of equilibrium situations or at models at the atomistic length scale. Nonequilibrium situations are tackled using cellular automata, phase-field and phase-field-crystal approaches, crystal plasticity FEM [37], and many more. Several books by now have summarized and reviewed the subject as ''computational thermodynamics'' [1] or ''computational materials'' [2]. CM science has been further extended to simulations of engineering materials [3], somehow directly bridging to the ternary CME. Note that the abbreviation ''CM'' is also used for continuum mechanics, which would match computational materials (when performed at the scale of the microstructure) or computational engineering (when performed at the process/component and system scales).

1.2.3
The ''Ternary Systems'': CME, ICM, IME, ICE

''CME'' Like Computational Materials Engineering It is worthy to note that ''engineering'' in the CME context is rather understood as engineering the properties of a material than engineering the properties of a component, product, or system. A number of books by now have been published on CME such as [3] or [4].

"ICM" Like Integrative Computational Materials Modeling The classical scope of ICM approaches (e.g., [5]) is the description of materials *evolution* in two directions of integration. The horizontal integration along the processing chain aims at through process modeling and eventually shall describe materials starting from the homogeneous liquid up to the final failure. The vertical integration is well known as the multiscale approach and aims at the description of the properties of the materials starting from the *ab initio* level of the Schrödinger equation and ending at the scale of the material and/or component. This scale bridging is based on the same approaches as CM and CME. Modern ICM developments accept that in many cases a full integration over all scales is neither possible nor mandatory. A scale-hopping approach is thus introduced, focusing on only those effects being relevant for the final process and material property design.[1)]

"IME" Like Integrative Materials Engineering The abbreviation IME may be interpreted as either engineering of integrative materials or integrative engineering of materials. It does not contain a "C" and thus does not relate to "computational" approaches. Thus, either experimental or analytical methods (i) to engineer integrative materials such as composites or (ii) to engineer materials in an integrative approach may be understood here. Examples might be analytical approaches to calculate the properties of a composite by a mixture rule and empirical materials laws being derived from experimental information or experience-based tailoring of alloy compositions or process parameters. Respective models are extremely useful in the context of ICME in view of bridging gaps in the virtual chain, for speeding up individual simulation tools, for validation of simulation results, and many other aspects.

"ICE" Like Integrative Computational Engineering ICE might be understood as any combination of CE activities such as, for example, a virtual description of a production process comprising product design, machining of components, assembly and logistics, and even considering global markets providing the economic and ecologic boundary conditions for the respective component/product.

1.2.4
The "Quaternary" System: "ICME"

Summarizing the above interpretations, there is a discrepancy in the term *Engineering*, which is applied to a product/component on the one hand and to a specific material on the other hand. The adequate interpretation of "E" in ICME is focused on engineering of an entire component and its manufacture in the

1) Special Research Area "steel *ab initio*" at the RWTH Aachen University.

sense of "ICE," with the engineering of the material eventually constituting the component in the sense of Materials Engineering ("ME" or "CME") being only a very important part of the entire effort.

The focus of ICME is thus on engineering the properties of the component as a function of the *local properties of the material* inside the component [6]. These properties themselves have experienced an evolution and depend on the entire process history as well as on the shape of the component and the alloy composition. An instructive benchmark example for a successful ICME could be the prediction of the distortions of a transmission component, which are based on the eigenstrains within the component being influenced by almost each of the process steps during its manufacture and still reveal a dependence on the segregation pattern resulting from the continuous casting process at the very beginning of the component's life-cycle.

1.3
Historical Development of ICME

As computers and computation represent the key ingredient of ICME, the development of this discipline follows the development of computers and their use in society (Figure 1.3).Increasing computational capabilities increasingly allowed for mimicking of real processes in a virtual world. For this purpose models had to be developed, allowing describing physical processes on a computer at all. The most prominent method is the description of phenomena occurring in the continuum of the real world on a numerical grid using the finite difference methods (FDMs) and FEMs and their further derivatives. In the meantime, these methods have

Figure 1.3 Development of computers and computational power goes along with significant changes in their applications. In the 1960s, computers filled entire rooms, still had limited capabilities, and essentially were operated by experts only. Computers of the twenty-first century find a place on a table with their performance largely exceeding the one of a 1960s computer. Their "operators" changed into "users" and in general are normal people without special computational skills. Nowadays, research and development could not proceed as rapidly without computers.

reached a degree of maturity, making them even applicable to the qualification and certification of products.

FEMs, extended FEMs "X-FEMs," computational fluid dynamics "CFD," and computational damage mechanics "CDM" have been extremely successful and a number of relevant software packages are frequently used to describe and optimize individual processes in the frame of "CE." Most progress in terms of "ICE" by now has been made in the area of structural materials and their mechanical properties. Computer simulations of macroscopic processes nowadays range from CAD-data to the finished product and in the past decade have been intensively used in many fields of application such as virtual crash tests.

Material data entering such simulations, however, by now in many cases have to be taken from experiments, from literature, or from other sources of information. Owing to a lack of more detailed information or high costs for their determination, such data are frequently assumed as constant, isotropic, homogeneous, and/or are based on other simplifications. Values for a dedicated material often are not available and are then approximated by drawing on similar materials. The variation in these values across the component, their dependence on temperature, and anisotropy are by now, in general, even entirely neglected.

The necessity for such approximations is due to the fact that computational models for materials, allowing for the prediction of materials properties, did not keep pace with the rapid developments of the macroscopic FEM models.

The historic development of CM aiming at the prediction of material properties has at least two different roots, one originating from the atomistic scale in a bottom-up approach and one starting from a thermodynamic, statistical perspective. The latter has proved the potential to tackle technical alloy systems. On the basis of the description of the Gibbs energy of the individual phases and the development of respective models, the CALPHAD method was established in the 1970s to assess a variety of data and combine them into suitable databases [1, 7]. Software and databases such as Thermo-Calc [8], JMatPro [9], FactSage [10], or Pandat [11] have meanwhile become key tools for modern alloy development.

The thermodynamic nature of these programs and databases, however, in general only allows the prediction of equilibrium conditions such as the fractions of individual phases being in equilibrium at a given temperature, the onset temperatures for the formation of specific phases, and many other most interesting thermodynamic data. Information can, however, be neither drawn on the evolution of these phase fractions in time (being mandatory to describe the kinetics of phase evolution) nor about their distribution in space (essentially corresponding to the microstructure, which eventually defines the properties of the material).

In the late 1990s, theoretical developments in the area of microstructure modeling such as the phase-field theory [12] and multiphase-field models [13, 14] have been combined with the above thermodynamic models [15–17]. Such combined models nowadays provide the key to describe and to control the microstructure evolution and eventually to tailor effective properties of technical materials and products [18]. The required data and parameter sets for such models can be obtained from even more fundamental models such as the DFT, atomistic modeling, and molecular dynamic simulations e.g. by multi-scale modeling schemes [35].

Currently, all these approaches have reached a level allowing for valuable contributions to modern engineering tasks within the knowledge-driven production models. The capabilities of the software tools and the present availability of computational power make efforts toward the integration of all these approaches possible, meaningful, and timely. Such integration offers a relevant step forward in the direction of knowledge-based optimal design of tailored materials, components, and products with regard to their specific applications. Future ''ICME as an emerging discipline aiming to integrate CM science tools into a holistic system will accelerate materials development, transform the engineering design optimization process, and unify design and manufacturing'' [19].

1.4 Current Activities Toward ICME

Describing or even predicting the properties of a component is a key objective of ICME. These properties are essentially determined by the microstructure of the component. Tracking the local microstructure evolution – besides a number of other data – requires boundary conditions for all processes affecting the microstructure during the life cycle of the component. These boundary conditions can be provided by a variety of different FEM simulations on the component scale being daisy-chained to cover the entire production sequence and subsequent operational conditions.

Efforts to standardize and generalize data formats for the exchange of simulation results thus represent a major step toward successful future applications of ICME. Such a standard facilitates information exchange between the different software tools for numerous processes and also across the different length and time scales, affecting both the properties and the life-cycle of an engineering component. A suitable data standard easily links the successful FEM models used in mechanical engineering and CFD, amongst each other and especially with microstructure models such as the phase-field method, which actually seems to become the ''FEM for metallurgists''. This eventually will allow for tracking of the microstructure – and thus the properties of the component – starting from the sound initial condition of a homogeneous, isotropic, and stress-free melt and eventually ending in the prediction of failure under operational conditions. Furthermore, the effects of transformations in the microstructure on the properties of the component can be tackled by extracting local effective properties from the microstructure information and feeding them back into the simulation tools on the component level.

A structural framework for ICME, comprising a variety of academic and/or commercial simulation tools operating on different scales and being modular interconnected by a standardized data exchange, will allow integrating different disciplines along the production chain, which by now have only scarcely interacted.

This will substantially improve the understanding of individual processes by integrating the component history originating from the preceding steps as the initial condition for the actual process. Eventually, this will lead to optimized process and production scenarios and will allow effective tailoring of specific materials and component properties.

Recently, the high importance of an ''ICME'' [20] for the future economic development and competitiveness has been strongly emphasized in a study by the National Research Council of the United States [19]. A number of industrial companies and joint ventures already make use of an ICME' approach and obviously draw significant benefits from doing so (Tables 2.1–2.3 in [19]). The materials being addressed by now comprise Al-alloys, Mg-alloys, superalloys, titanium alloys, solders, and advanced high-strength steels. The benefits being specified by these companies are related to (i) the development, (ii) manufacture, and (iii) the application of products.

The *benefits for planning/development* are identified as

- reductions in materials development *time*,
- *improved materials properties* such as brittleness and strength,
- shorter material certification *times*,
- reductions in product development *time* (15–25% in some cases up to 50%),
- substantial reduction in experimental testing *efforts* in terms of *time* and *costs*,
- weight *savings* for specific components while maintaining the desired *functionality*,
- *improved capabilities* of the components,

The *benefits for manufacture/production*, among others, are exemplarily:

- reduction in manufacturing *costs*,
- *optimized* forging *processes*,
- *fast* and *cost-effective* optimized rolling *processes*,
- *optimized* microstructure *control* in investment castings,

For *operation/maintenance*, the following benefits are exemplarily stated:

- *savings* in operation and, especially, maintenance,
- *prediction of life cycles* of solder joints, (no alternative to ICME),

Looking at the expressions emphasized by *italics*, all these benefits are a result of pursuing the strategy of decreasing the dilemma between planning efforts taken and the eventual product value. During the materials/product design and development stage, ICME significantly reduces these planning efforts in terms of both the time and cost, while simultaneously increasing the product value by improved material properties and/or improved capabilities of the component.

In the United States, a number of universities and academic institutions started working on ICME [38], especially in large consortia, with industry, such as the ''Virtual Aluminum Castings'' [21]. Organizations such as the TMS, ASM, and

MRS aim at structuring all ICME activities in the United States and even in the world by a joint committee on ICME, by organizing a first world congress on ICME (TMS) or by composing the most valuable information about materials simulation in a recent handbook [22].

Although some companies already promote ICME on their web site, for example [23], details about the individual approaches to ICME being taken by industry and the results by now, however, are published only in a few cases such as ''Virtual Aluminum Castings'' [21], structural magnesium parts in automotive applications [24], and the development of superalloys for aerospace and power applications [25, 26]. These approaches, in general, draw back on proprietary developments of the individual companies for interfacing with available commercial tools and complementing them toward the desired ICME functionality.

In Europe, materials modeling on the basis of an integrative simulation approach has been investigated within the project ''Integrated Materials Simulation'' in the period 1993–2005 [5]. The conceptual approach of this project being characterized by modular, integrated multilevel models in the meantime has been adapted by the European industry within the framework of ''Through Process Modeling'' programs for commercial materials within the ''VIR.*''-projects [27, 28]. Several other European groups follow the objectives of integrated modeling such as the IMMPETUS group in Sheffield [29], the Hero-M activity at the KTH Stockholm [30], a through process modeling including in-service operations at the Imperial College [31] and the Interdisciplinary Centre for Advanced Materials Simulation in Germany [32]. Eventually, the AixViPMaP® platform for ICME [36] described in this book is also based on an academic, nonprofit activity. Some preliminary simulations of industrial steel components have been performed on the basis of this platform [33].

The efforts of commercial providers of simulation software aim at a steadily increasing integration of more and more functionalities into their own specific codes. This frequently leads to large general purpose tools instead of modular structures. Examples are the ESI Virtual Try-Out Space (VTOS) or the ANSYS Workbench Platform. These commercial software structures can be considered as strong in modeling a number of coupled processes (e.g., forging and heat treatments) at the component scale using FEM methods in the sense of an ICE. The underlying materials models most relevant for a successful ICME, however, are in most cases empirical and, in general, do not account for the preceding history of the material with respect to the component.

1.5 Toward a Modular Standardized Platform for ICME

In view of the common perception of the significant benefits being related to a successful implementation and application of ICME scenarios, the question arises about how to realize such scenarios successfully while at the same time taking care of the interests of academia, the producing industry and the providers of simulation software.

Industrial approaches to ICME, as exemplarily detailed for Mg and Al castings above, by now often are stand-alone island solutions being designed to tackle dedicated problems. Such solutions in general draw back on commercial software codes being complemented by proprietary software to allow for an integrative description of specific, commercially relevant phenomena. Economic competition will prevent or at least substantially hinder the exchange of codes or interface routines and data.

Commercial providers of simulation software are highly interested and active in developing their own standards linking their proprietary codes toward their own ICME platforms, making their product portfolio more competitive. Although many of them already provide interfaces to their tools, their interest in creating and developing a generalized, open standard that also allows information exchange, for example, with software tools of their competitors or with tools originating from academia, is less pronounced. It does not seem probable that a general standard will be proposed or realized by one of the commercial simulation software providers in the near future.

To circumvent such limitations arising from competition issues, establishing a generalized, open standard in the frame of an academic setting seems meaningful. The expertise of an individual academic institute alone, however, is not sufficient to meet this ambitious objective. In contrast, the task requires the combined effort of a number of institutions contributing a broad range of expertise for various materials, for all processes along the value chain of a product, for the relevant phenomena and their modeling, for efficient computation and algorithms and much more.

Hierarchical structures with few experts aiming at coordinating such an activity thus will be less effective as compared to a self-organization of teams of experts with a broad spectrum of expertise heading for generalized solutions.

A German initiative aiming at fostering the excellence of German universities provided funding to a number of institutes at the RWTH Aachen University to investigate ''Integrative production technologies for high-wage countries'' in the frame of a cluster of excellence at the end of 2006 [34]. One of the larger projects in this cluster combined the profound expertise of nine university institutes renowned in materials and process development and simulation along the entire value chain. Already in the very early work-group meetings, the urgent need for a ''common language'' for the exchange of simulation results was identified. In the further course of this project, such a standard has been elaborated and implemented in a number of dedicated simulation tools. Simulation chains for dedicated test scenarios were then created and validated. In a second step, several of the simulation tools were implemented in a web-based grid infrastructure, allowing for setting up simulation chains and automatically running them remotely.

1.6 Scope of This Book

The scope of the book is to demonstrate a promising strategy toward a successful ICME being based on the standardization of information exchange. This pathway and its benefits are highlighted using the example of the AixViPMaP® platform and some test cases that have been used for its verification. The special scope of the AixViPMaP® platform is the definition and provision of an open, generalized standard allowing for information exchange between a variety of simulation tools. The major scope of this book is the communication of this standard and of the first experiences made in using it. Several further reasons extended the basis for writing this book:

- **First**: A major reason for publishing this book was to comprehensively summarize all work being performed during the period 2006–2011 within the project ''Virtual Process Chains for Processing of Materials'' of the Cluster of Excellence ''Integrative Production Technologies for High-Wage Countries.'' This work comprises the efforts of a consortium of nine institutes of the RWTH Aachen, all being renowned in the area of materials science and processing (casting, forming, annealing, joining, and coating) of metallic alloys (especially steels), polymers, and composites and two further institutes being well known in the areas of scientific computing and information management.
- **Second**: Only a publication in the form of a book allows to describe all structural ideas, underlying concepts, defined standards, results obtained for verification using the different test cases, and eventually even a description of how to use the platform as a user and how to join the platform as a provider. Many aspects being necessary for the successful operation of such a platform – especially the definition of standards – are hard to publish as stand-alone articles in journals.
- **Third**: The book might serve as a first handbook for future users of the simulation platform (especially small and midsize enterprises (SMEs) and academia) as well as for providers of simulation software, which would like to make their software/services available via such a platform.
- **Fourth**: The book will provide an integrative view on production processes and the resulting properties of materials and components for students of materials science and engineering, for students of mechanical engineering, and eventually also for people responsible for the design and layout of production processes.
- **Fifth**: A book on ICME seems timely in view of a particular community actually establishing itself with a First International World Congress on ICME, which took place in Pennsylvania in July 2011.

In fact, this book is not a book on ICME in general, as the area is huge and still not sufficiently mature for a sound review. The scope of the book is to summarize the general ideas of ICME, but especially to demonstrate a promising strategy toward a successful ICME being based on standardization of information exchange. This pathway and its benefits are then highlighted using the example of the AixViPMaP® platform and the test cases used for its verification. In this context, the AixViPMaP® platform should not be identified as a dedicated software requiring an ''own manual'' and ''regular releases.'' The special scope (and content) of the AixViPMaP® platform is the definition and provision of an open standard allowing for information exchange between a variety of commercial and academic research tools. A second scope of the AixViPMaP® is the realization of simulation chains in an Internet-based environment – a GRID – drawing back on this particular standard.

To the best of our knowledge, such an open, modular standardization approach toward ICME involving both commercial and academic software tools has not been made till now. Communication of this first version of a standard for exchange of simulation results along a process chain and across different length scales (and of the benefits resulting from using it) thus is the major objective for writing this book. Such standards must be communicated in order to be spread, to find acceptance, and eventually to become a worldwide standard. As for standards in general, the authors are well aware that such a standard will surely further evolve in future.

This book is structured in two parts. In the first part (Chapters 2–7), the platform concept and its background are detailed. The second part (Chapters 8–12) describes several test cases being used to verify the platform functionality and to demonstrate the benefits of an ICME approach. Eventually, future perspectives for the further development of ICME using the approaches being detailed in this book are outlined in the final chapter.

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