Integral Materials Modeling

Towards Physics-Based Through-Process Models

Edited by
Günter Gottstein

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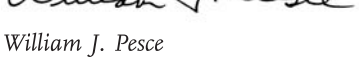

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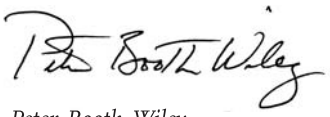

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1
Introduction

This book comprises the proceedings of the final symposium of the Collaborative Research Center (SFB 370) of the Deutsche Forschungsgemeinschaft on ''Integral Materials Modeling'' which took place in Aachen, Germany, on December 1–2, 2005. It is composed of the final reports of the projects and complementary manuscripts of renowned scientists in the field of materials modeling, covering a broad range of current simulation activities.

The projects are identified by their project numbers in their title. The manuscripts are organized such that after a list of persons involved in the SFB 370 the final through-process modeling exercises (group C) are introduced by the reports on supporting process and materials models (groups A and B) and complemented by the invited contributions. The first article on ''Integral Materials Modeling'' gives an introduction into the philosophy, history, and structure of the collaborative research center.

With the final symposium the SFB officially ended but its core topic was continued in a transfer program of the Deutsche Forschungsgemeinschaft (TFB 63) on ''Industrially Relevant Modeling Tools''.

As a chairman of the collaborative research center on ''Integral Materials Modeling'' (SFB 370) I would like to express my sincere gratitude to my colleagues for their continuous support and encouragement. As a university professor it was my great pleasure to see the interest and engagement of the young doctoral students in the research program, their fascination by the scientific challenge, and their natural openness to interdisciplinary cooperation, discussion, and information exchange. Last but not least my thanks go to the review panels for their valuable advice and the Deutsche Forschungsgemeinschaft which not only funded the collaborative research center for 12 years but also offered unbureaucratic support.

Günter Gottstein
Chairman, SFB 370
Aachen, December 2006

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2
Integral Materials Modeling

G. Gottstein

Abstract

This chapter reviews the historical background of computational materials science and introduces the scientific concept of ''integral materials modeling''. The objectives of the collaborative research center on this topic are formulated and an overview is given on the structure development and achievements of the research program.

2.1
Introduction

One of the ultimate dreams of materials science is the theoretical design of new materials. It would save tremendous costs that are currently invested in alloy development, e.g. for operating expensive pilot plants and conducting comprehensive materials testing, and in view of the fact that even today it takes more than 15 years before a new material eventually sees the market. That there is still need for research to develop new metallic materials although they have be successfully processed for more than 5000 years is not due to the large number of potential alloys that can be produced in multicomponent alloys out of 92 elements or even 70 elements with metallic character. On the contrary, if the properties of these alloys would only reflect the property mix of their components, it would be easy with current computer power to predict the properties of virtually any potential alloy system. However, the properties of a material do not reflect the properties of the constituent elements, rather the properties of a material are controlled by the spatial distribution of elements and crystal defects, which is also referred to as microstructure. The microstructure comprises phase distribution, elemental distribution, orientation distribution, as well as crystal defects like grain boundaries, dislocations, and point defects. What is more, the microstructure is seriously affected by materials processing. In essence, the properties of a material are not given by a superposition of elemental properties, but by a complex function of

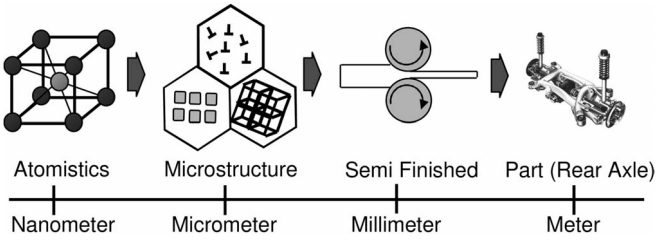

Fig. 2.1 The scale problem of materials modeling: the macroscopic properties are defined by the microstructure which develops by atomic mechanisms.

its chemical composition and its processing history, and there is a virtually infinite number of possible microstructures and, therefore, of material properties. This is good news for alloy development since material properties can be changed by processing at constant chemistry in a wide range but it is a nightmare for materials modeling that aims at predicting material properties from the knowledge of materials chemistry and processing, and it appears hopeless to design computational strategies for optimization of materials chemistry and processing for a given desired property spectrum.

As a result, it is practically impossible to establish relations between materials properties and both processing parameters and the overall chemistry. This is because of the fact that the processing conditions are not the state variables of materials properties even though that would be desirable for the materials engineer who is used to formulate the properties of a product in terms of the engineering control parameters. Processing–property relationship may be most desirable for engineering practice, but unfortunately this approach cannot be successful. It is common in materials engineering to establish correlations between material properties and processing conditions. These correlations, however, are not equations of state for the material, and thus liable to fail when the chemistry or processing parameters are changed.

The only correct way to formulate equations of state for the terminal properties of a processed material is in terms of microstructure development during processing because the microstructure constitutes the state variable of the material. In fact, the microstructure is a fingerprint of the processing history of a material and determines the current properties of a material. That is why geologists hope to derive the history of rocks from today's microstructure to understand the formation of the Earth's crust. Consequently, the very problem of property predictions is to adequately quantify a microstructure and, in particular, to establish microstructure–property relationships. This requires an understanding of the controlling microstructural elements and the microscopic processes that determine a specific property.

An adequate characterization of the microstructure requires knowledge of the atomistic arrangement in a material. Therefore, a deeper physical understanding

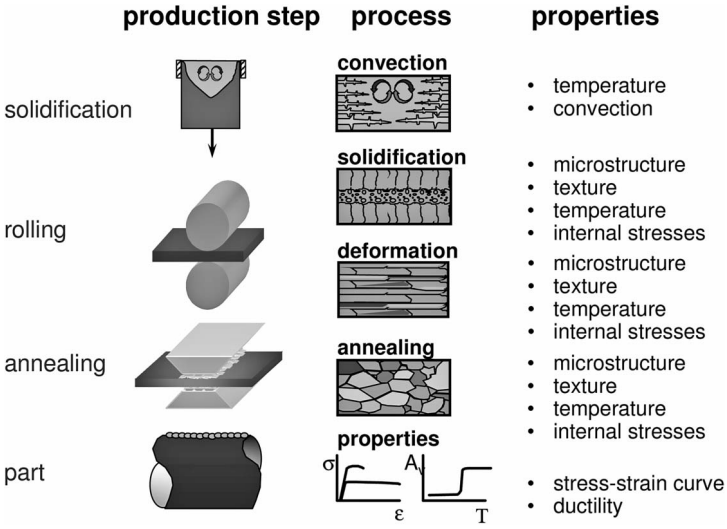

Fig. 2.2 During conventional processing of a metallic material to the final product (here a welded tube) the microstructure changes during each processing step.

of material properties and phenomena could only be developed after the discovery of X-rays and their application to crystallography in the beginning of the 20th century. This engendered an understanding of material behavior on the basis of its atomistic arrangements and atomistic transport processes. Application of X-ray diffraction and spectroscopy complemented much later by electron and neutron diffraction and spectroscopy revealed the importance of nanoscale configurations, notably the crystal structure, crystal defects, and nanoscale chemistry, in terms of solute distribution and dispersion of second phases, for an interpretation of material properties. In fact, materials science in the 20th century was essentially dedicated to an understanding of microstructure evolution and a formulation of microstructure–property relationships.

From this research it became clear, however, that there are only a few although complex physical processes that impact the microstructure of a bulk metallic material. The mechanisms of these processes have been the subject of investigations for many years, and the outcome of this research constitutes the foundations and concepts of modern materials science.

In essence, there are three major processes that affect the microstructure of a material, namely phase transformations, plastic deformation, and restoration processes like recovery, recrystallization, and grain growth. These processes and their impact on microstructure are complex in detail and interdependent in a highly nonlinear fashion. Their thermodynamics, kinetics, and atomic mechanisms have been subject of numerous investigations over the past 50 years, which have substantiated that microstructural evolution is strongly related to the properties

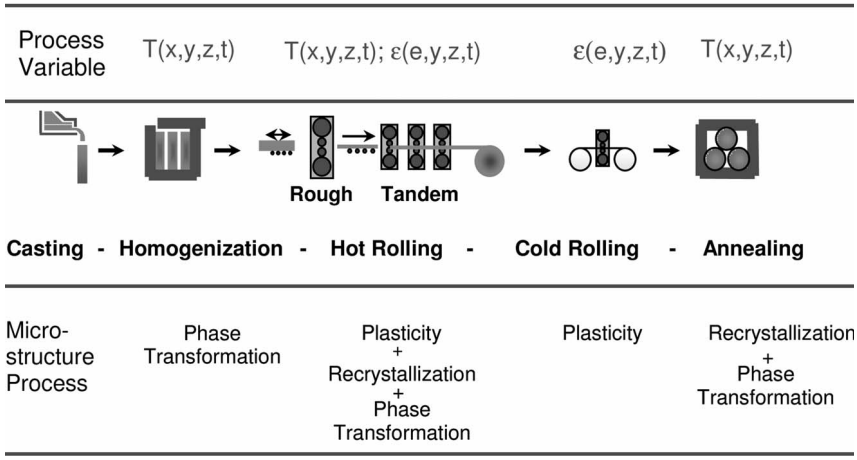

Fig. 2.3 For simulation of microstructure evolution the microstructure processes have to be interfaced to the process variables; here for sheet fabrication of an aluminum alloy.

and behavior of crystal defects: deformation of crystals proceeds by the generation, motion, interaction, and storage of dislocations; phase transformations are controlled by diffusion, the fundamental atomic transport mechanism; and recrystallization and grain growth involve the motion of grain boundaries.

These three microstructural processes affect each other, e.g. precipitation of a second phase hinders dislocation and grain boundary motion and, therefore, influences hardening during crystal plasticity and softening by recrystallization and grain growth. A major complication for the mathematical treatment of these processes is the local inhomogeneity that is introduced or even imposed by processing, e.g. fluctuation of composition, segregation of elements, deformation inhomogeneities, etc.

The theoretical foundations that govern the thermodynamics and kinetics of these processes have been developed during the past 50 years [1–4]. The respective equations of motion and equations of state for these processes are generally formulated in terms of partial differential equations. An analytical solution of these equations was in the vast majority of cases beyond reach, even impossible. Even 20 years ago such mathematical problems could be solved only by experts for very special cases. This situation changed dramatically with the advent of powerful computers, which could be utilized to solve numerically these difficult equations. With the increasingly powerful computers at hand to everybody nowadays, virtually every scientist can tackle these mathematical problems by utilizing sophisticated software. Moreover, the availability of high-performance computers has engendered novel computational techniques to address microstructural changes and thus the option to simulate microstructural evolution on the computer [5].

While the simulation of microstructure evolution constitutes a remarkable progress in computational materials science it does not yet solve the engineering problem to predict the properties of a material. Since the microstructure controls materials properties but is affected by each processing step, the prediction of terminal material properties or the behavior of a part under service conditions requires one to follow microstructural evolution along the entire processing chain, i.e. conventionally from the liquid state to the final product. To simulate this on the computer, it is necessary to connect the microstructural evolution to the processing parameters, which essentially means to subject each microstructural volume element to a temporal change of strain and temperature. In engineering applications this temperature and strain history of a material is typically computed by finite element (FE) approaches. On the other hand, the results of an FE simulation depend on the current properties of a material; hence microstructural evolution along the processing history and the local processing parameters, strain and temperature, are interdependent. In essence, both approaches, processing in terms of FE codes and microstructure in terms of physics-based microstructure evolution codes, have to be connected and interfaced in space and time. This means accounting for local and temporal changes of chemical composition, segregation, defect densities, etc., under changing boundary conditions. Therefore, it also requires advanced interface tools and sophisticated numerical techniques to solve the respective sets of mathematical equations and places a substantial demand on computing power.

2.2 The Collaborative Research Center on "Integral Materials Modeling"

In 1994 the collaborative research center on "Integral Materials Modeling" (SFB 370) of the Deutsche Forschungsgemeinschaft set out to tackle this problem and to develop strategies and techniques to predict terminal material properties from the knowledge of material chemistry and processing conditions. Since each processing step affects the microstructure, the microstructure evolution through the entire processing chain had to be traced to determine the final microstructure at the end of the processing chain in order to predict the properties associated with it. This though-process modeling approach on a physics-based microstructure definition was subject of research for a variety of materials and their processing. Two fundamental processing stages (A and B) were distinguished, which characterized virtually all materials fabrication procedures (Fig. 2.4):

(A) Generation of the solid state from the liquid phase (solidification) or gas phase (condensation).
(B) Processing of the solid by mechanical and thermal treatment.

They determined the properties of the product which constituted stage C:

(C) Determination of the specific properties of interest for a processed product.

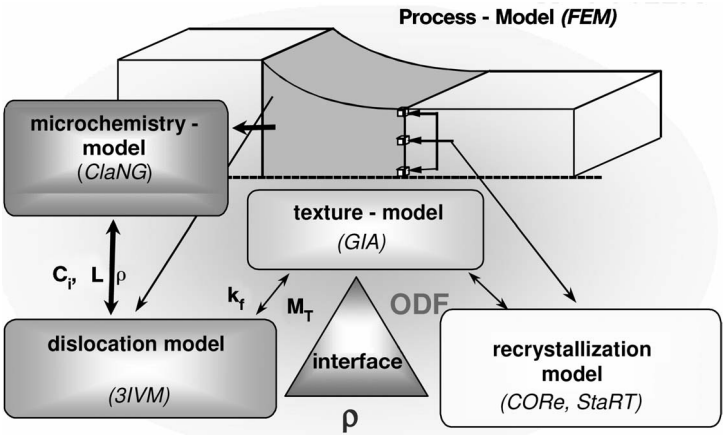

Fig. 2.4 Coupling of microstructure and processing by interfacing FEM and physics-based microstructure models. For each volume element the microstructural information has to be updated in every time step.

Depending on the specific product considered these processing stages can be connected in various ways (Fig. 2.5). For a net shape cast metallic part or an injection molded polymer, stage A directly connects to stage C. Stage A itself may be subdivided in to several steps, e.g. if a cast part is coated. A homogenization anneal

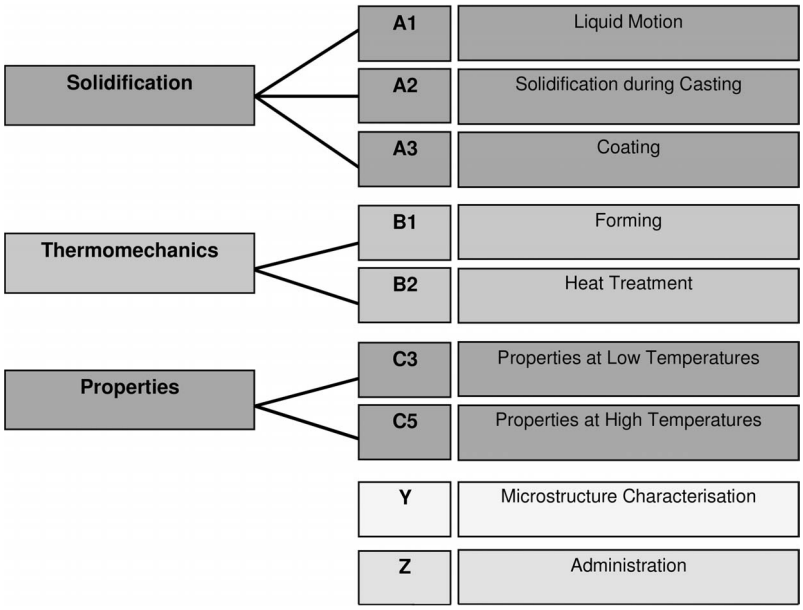

Fig. 2.5 Topical structure of the collaborative research center (SFB 370) ''Integral Materials Modeling'' of the Deutsche Forschungsgemeinschaft.