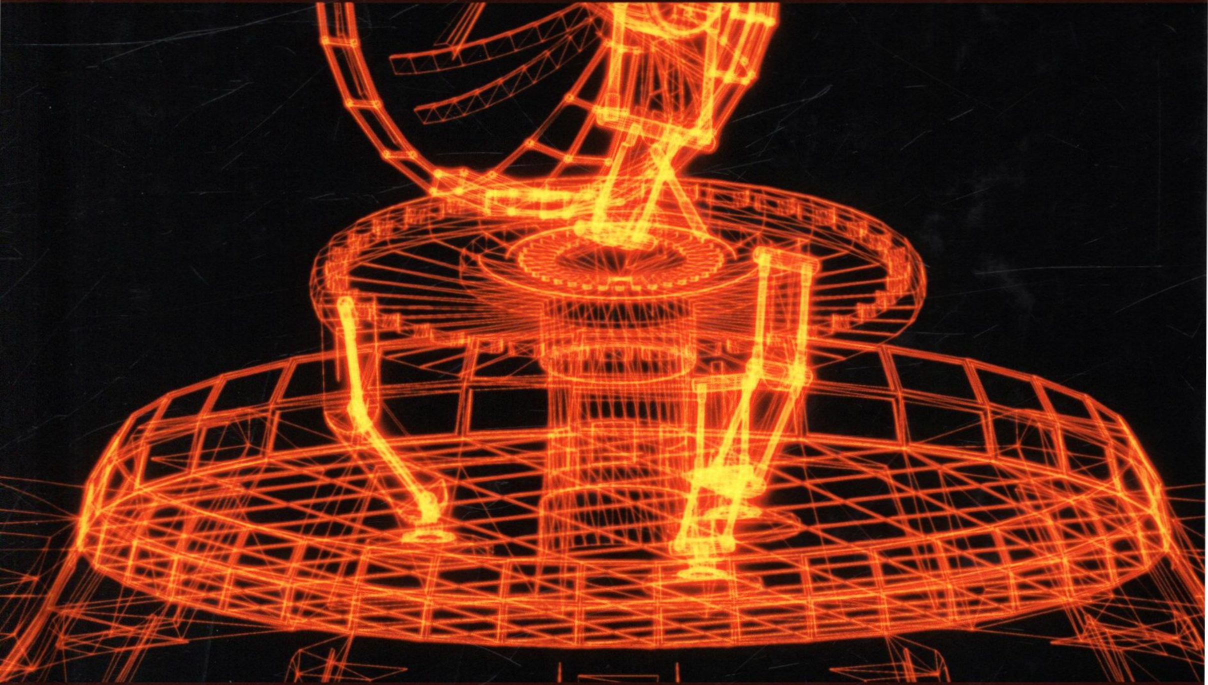
MECHANICAL ENGINEERING AND SOLID MECHANICS SERIES

# From Microstructure Investigations to Multiscale Modeling

*Bridging the Gap*


**Edited by**
**Delphine Brancherie**
**Pierre Feissel, Salima Bouvier**
**and Adnan Ibrahimbegović**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Mechanical behaviors of materials are highly influenced by their architectures and/or microstructures. Hence, progress in material science involves understanding and modeling the link between the microstructure and the material behavior at different scales.

This book gathers contributions from eminent researchers in the field of computational and experimental material modeling. It presents advanced experimental techniques to acquire the microstructure features together with dedicated numerical and analytical tools to take into account the randomness of the micro-structure.

Macro phenomenological models based on a fine modeling of the key phenomena at the micro-scale are presented and the influence of the parameters of the micro-scale models are analyzed in terms of their effects on the behavior at the upper scales.

Finally, this book illustrates how the increasing complexity of models brings challenging issues related to identification and simulation and presents on-the-edge numerical strategies to overcome those issues.

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From Microstructure Investigations to Multiscale Modeling

# Preface

Mechanical behaviors of materials are highly influenced by their microstructures. Therefore, progress in material science aims at understanding and modeling the link between the microstructure and the material behavior at different scales. This book comprises contributions from eminent researchers in the field of computational and experimental material modeling. The book focuses on experimental techniques, modeling approaches and computational strategies to understand and predict the behavior of materials in relation to its architecture and microstructure at different scales. Special attention is paid to the coupling of experimental techniques with advanced modeling tools, numerically or analytically.

The first four chapters are dedicated to the reconstruction of representative volume element (RVE) for different kinds of materials to study the mechanical behavior at the macro-scale. Advanced experimental techniques along with dedicated numerical and analytical tools are presented to efficiently analyze and represent the microstructural features. These tools are used to study synthetic materials, the key properties of RVEs, and to construct the behavior at the macro-scale through homogenization. The role of the randomness of the microstructure in the macro-scale behavior is also investigated, and stochastic dedicated tools are presented.

The following three chapters focus on complex mechanical behavior modeling at the macro-scale. Different modelization and simulation techniques are presented. These chapters discuss how the applications considered above enable the use and adaptation of numerical tools to analyze complex behaviors. The macro phenomenological models are based on a better understanding and modeling of key phenomena at the micro-scale, including multi-physics. The influence of the parameters of micro-scale models is analyzed in detail with respect to the macro-scale behavior.

The increasing complexity of models brings challenging issues related to identification and simulation. Due to these issues, models must be identified from complex experiments that are monitored richly, to imply the large amount of data. Dedicated identification strategies must be developed based on simulation, thereby requiring model reduction techniques. These reduction techniques will also be a key tool for large-scale (in terms of CPU time) predictive simulation, and new trends in data-driven simulations take advantage of the experimental data to propose a new modeling paradigm. The last two chapters focus on these issues.

This book is a collection of selected papers from the invited lectures presented at the 9th US–France symposium: "From microstructure observations to multi-scale modeling of deformation mechanisms and interfaces". This symposium was held in Compiègne in June 2016 under the auspices of the International Center for Applied Computational Mechanics, Compiègne, France, 1–3 June 2016.

We would like to thank all the ICACM participants for their lively exchanges, especially the authors of the chapters for their contributions.

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Pierre Feissel
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September 2017

# Contents

# 1

# Synchrotron Imaging and Diffraction for *In Situ* 3D Characterization of Polycrystalline Materials

## 1.1. Introduction

The last few years have seen material science progressing rapidly into three-dimensional (3D) characterization at different scales (e.g. atom probe tomography [PHI 09], transmission electron microscopy tomography [WEY 04], automated serial sectioning tomography [UCH 12, ECH 12] and X-ray tomography [MAI 14]). A wealth of 3D data sets can now be obtained with different modalities, allowing the 3D characterization of phases, crystallography, chemistry, defects or damage and in some cases strain fields.

In the last 10 years, one particular focus of the 3D imaging community (like 2D in its time with the advent of EBSD characterization) has been on obtaining reliable three-dimensional grain maps. As most structural materials are polycrystalline and the mechanical properties are determined by their internal microstructure, this is a critical issue. There has been considerable effort to develop characterization techniques at the mesoscale, which can image

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Chapter written by Henry PROUDHON.

typically 1 $mm^3$ of material with a spatial resolution in the order of micrometers.

Among 3D characterization, an important distinction exists between destructive and non-destructive techniques. Serial sectioning relies on repeated 2D imaging (which may include several modalities) of individual slices, where a thin layer of material is removed between each observation (see Figure 1.1(a,b)). The material removal can be achieved via mechanical polishing [ROW 10], ion [DUN 99, JIR 12] or femtosecond laser ablation [ECH 15] in a dedicated scanning electron microscope (SEM). Considerable progress has been made in this line in the last decade, bringing not only high-quality measurements in 3D of grain sizes and orientations but also detailed grain shapes and grain boundary characters. The most serious threat of serial sectioning is, however, the destruction of the sample.

In parallel, the advent of third-generation synchrotrons worldwide, with ESRF at the forefront, brought hard X-rays, with their high penetrating power, to the structural material science community. X-ray computed tomography (CT) rapidly developed as a key observation tool, allowing the non-destructive bulk evaluations of all types of materials [MAI 14]. This made the *in situ* study of damage possible using specifically designed stress rigs [BUF 10]. Unfortunately, CT imaging relies on absorption and phase contrasts and remains blind to crystal orientation. Accessing crystallographic information in the bulk of polycrystalline specimens (average orientation per grain) was subsequently achieved using the high penetrating power of hard X-rays and leveraging diffraction contrast. The pioneering work of Poulsen took advantage of high-brilliance synchrotron sources to study millimeter-sized specimens by tracking the diffraction of each individual crystal within the material volume while rotating the specimen over 360°. This led to the development of 3DXRD [POU 04] and its several grain mapping variants (DCT [LUD 08], HEDM [LIE 11], DAGT [TOD 13]). Among them, the near-field variant called diffraction contrast tomography (DCT, see Figure 1.1(c)) will be detailed in section 1.2.7.