Continuum Scale Simulation of Engineering Materials

Fundamentals – Microstructures – Process Applications

Edited by
Dierk Raabe, Franz Roters, Frédéric Barlat, Long-Qing Chen

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Cover Picture

The cover picture shows an experimental result and a corresponding simulation of an aluminium cup drawing process. The background figure shows a Potts Monte Carlo modeling result of a subgrain coarsening process during a simulation annealing treatment of a cold rolled automotive sheet steel.

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Contents

Preface

This book presents our current knowledge and understanding of continuum-based concepts behind computational methods used for microstructure and process simulation of engineering materials above the atomic scale. While the area of ground-state and molecular dynamics simulation techniques has recently been reviewed in various books, no such collection exists for continuum scale materials simulation concepts. This book tries to fill that gap.

By presenting for the first time a wide spectrum of different continuum-based computational approaches to materials microstructure simulations within a single volume, we also hope to initiate the development of corresponding scientific centers in academic research institutions as well as virtual laboratories in the industry in which these methods are exploited. Moreover, we feel that other fields such as computational bio–materials science, where modeling approaches developed in the materials community have been used increasingly, might substantially benefit from the methods presented in this book.

We think that students and scientists who increasingly work in the field of continuum–based materials simulations should have a chance to compare the different methods in terms of their respective particular weaknesses and advantages. Such a critical evaluation is important since continuum models, as a rule, do not emerge directly from ab-initio calculations. In other words, continuum simulations of materials rely on approximate constitutive models which are usually not derived through quantum mechanics. This means that one should carefully check the underlying model assumptions of such approaches with respect to their applicability to a given problem. We hope that this volume provides a good overview on the different methods and allows the reader to identify appropriate approaches to the new challenges emerging every day in this exciting domain.

Continuum-based simulation approaches cover a wide class of activities in the materials research community ranging from basic thermodynamics and kinetics to large scale structural materials mechanics and microstructure-oriented process simulations. This spectrum of tasks is matched by a variety of simulation methods. The volume, therefore, consists of three main parts. The first one presents basic overview chapters which cover fundamental key methods in the field of continuum scale materials simulation. Prominent examples are the phase field model, cellular automata, crystal elasticity-plasticity finite element methods, Potts models, lattice gas approaches, discrete dislocation dynamics, yield surface plasticity, as well as artificial neural networks.

The second one presents applications of these methods to the prediction of microstructures. This part deals with explicit simulation examples such as phase field simulations of solidification, modeling of dendritic structures by means of cellular automata, statistical theory of grain growth, curvature-driven grain growth, deformation and recrystallization of particlecontaining aluminum alloys, cellular automaton simulations of grain growth, thermal activation in discrete dislocation dynamics, coarse graining of dislocation dynamics, and texture component crystal plasticity finite element methods to name but a few.

The third part presents applications in the field of process simulation. Examples are the integration of physically based materials concepts into process simulations, modeling of casting and solidification, integrated simulations of rolling, sheet forming and hydroforming simulations, springback simulation, and automotive crash simulation.

This book is intended for students at the undergraduate and graduate levels, lecturers, materials and mechanical scientists and engineers, physicists, biologists, chemists, and mathematicians. The editors would greatly appreciate any suggestions, criticisms, advice, or examples that might improve the content of this volume.

The editors and authors are very grateful to Mr. Uwe Krieg and to Dr. Jörn Ritterbusch from Wiley-VCH for the excellent cooperation.

Dierk Raabe, Franz Roters, Frédéric Barlat, Long-Qing Chen

May 2004

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