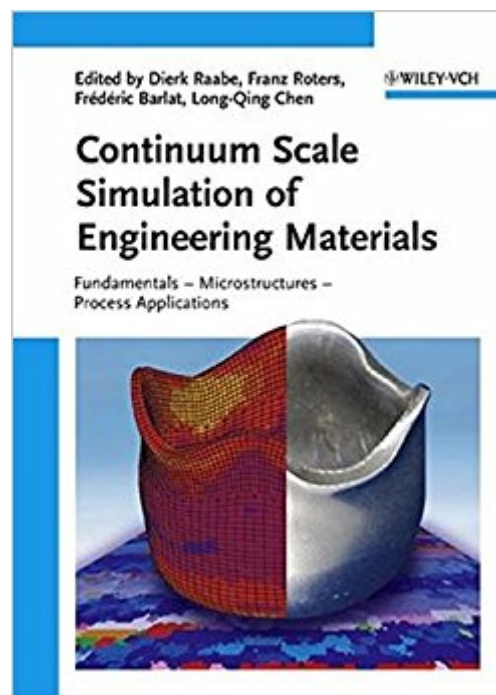




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# Continuum Scale Simulation Of Engineering Materials: Fundamentals - Microstructures - Process Applications



## Synopsis

This book fills a gap by presenting 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. The volume provides an excellent overview on the different methods, comparing the different methods in terms of their respective particular weaknesses and advantages. This trains readers to identify appropriate approaches to the new challenges that emerge every day in this exciting domain. Divided into three main parts, the first is a basic overview covering fundamental key methods in the field of continuum scale materials simulation. The second one then goes on to look at applications of these methods to the prediction of microstructures, dealing with explicit simulation examples, while the third part discusses example applications in the field of process simulation. By presenting a spectrum of different computational approaches to materials, the book aims to initiate the development of corresponding virtual laboratories in the industry in which these methods are exploited. As such, it addresses graduates and undergraduates, lecturers, materials scientists and engineers, physicists, biologists, chemists, mathematicians, and mechanical engineers.

## Book Information

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"The recently published book on Continuum Scale Simulation of Engineering Materials ... provides an updated excellent overview on the computational modeling above the atomic scale of a wide

variety of problems related to advanced engineering materials. ... It should be considered as one of the important reference books in the area of computational material science." *Advanced Engineering Materials* "This collection of chapters would be useful for graduate students, scientists, and engineers working in this field." *Materials and Manufacturing Processes* "It is likely to be of most use to final year undergraduates, postgraduate students, postdoctoral researchers and other established researchers." *Materials World*

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 some excellent overviews no such collection was presented for the field of continuum scale materials simulation concepts. This book tries to fill that gap. By presenting in this volume a spectrum of different computational approaches to materials we also hope to initiate the development of corresponding virtual laboratories in the industry in which these methods are exploited. Another field which might substantially profit from the field of computational continuum materials science is the domain of computational bio-materials science which increasingly makes use of modeling approaches which have been developed by the materials community. We feel 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 critical evaluation is important since continuum models do as a rule not emerge directly from ab-initio calculations. In other words, continuum simulations of materials rely on approximate constitutive models which are usually not derived by the help of 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 train the reader in its ability 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, phase field simulations of solid-state phase transformations and strain/stress-dominated microstructure evolution, statistical theory of grain growth, curvature-driven grain growth and coarsening including the motion of multiple interfaces, deformation and recrystallization of particle-containing aluminum alloys, cellular automaton simulation with variable cell size of grain growth, vertex grain boundary modeling, fluid mechanics of suspensions, thermal activation in discrete dislocation dynamics, statistical dislocation modeling, discrete dislocation simulations of thin film plasticity and brittle to ductile transition in fracture mechanics, coarse graining of dislocation dynamics, constitutive modeling of polymer deformation, Taylor-type homogenization methods for texture and anisotropy, continuum thermodynamic modeling, self consistent homogenization methods for texture and anisotropy , crystal plasticity finite element simulations, texture component crystal plasticity finite element methods, coupling of continuum fields to materials properties through microstructure (the OOF project), micromechanical simulations of composites, as well as computational fracture mechanics.

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