Multiscale Modeling In Solid Mechanics Computational Approaches Computational And Experimental Methods In Structures

Nanotechnology is a progressive research and development topic with large amounts of venture capital and government funding being invested worldwide. Nano mechanics, in particular, is the study and characterization of the mechanical behaviour of individual atoms, systems and structures in response to various types of forces and loading conditions. This text, written by respected researchers in the field, informs researchers and practitioners about the fundamental concepts in nano mechanics and materials, focusing on their modelling via multiple scale methods and techniques. The book systematically covers the theory behind multi-particle and nanoscale systems, introduces multiple scale methods, and finally looks at contemporary applications in nano-structured and bio-inspired materials.

State-of-the-technology tools for designing, optimizing, and manufacturing new materials Integrated computational materials engineering (ICME) uses computational materials science tools within a holistic system in order to accelerate materials development, improve design optimization, and unify design and manufacturing. Increasingly, ICME is the preferred paradigm for design, development, and manufacturing of structural products. Written by one of the world's leading ICME experts, this text delivers a comprehensive, practical introduction to the field, guiding readers through multiscale materials processing modeling and simulation with easy-to-follow explanations and examples. Following an introductory chapter exploring the

core concepts and the various disciplines that have contributed to the development of ICME, the text covers the following important topics with their associated length scale bridging methodologies: Macroscale continuum internal state variable plasticity and damage theory and multistage fatigue Mesoscale analysis: continuum theory methods with discrete features and methods Discrete dislocation dynamics simulations Atomistic modeling methods Electronics structures calculations Next, the author provides three chapters dedicated to detailed case studies, including "From Atoms to Autos: A Redesign of a Cadillac Control Arm," that show how the principles and methods of ICME work in practice. The final chapter examines the future of ICME, forecasting the development of new materials and engineering structures with the help of a cyberinfrastructure that has been recently established. Integrated Computational Materials Engineering (ICME) for Metals is recommended for both students and professionals in engineering and materials science, providing them with new state-of-the-technology tools for selecting, designing, optimizing, and manufacturing new materials. Instructors who adopt this text for coursework can take advantage of PowerPoint lecture notes, a questions and solutions manual, and tutorials to guide students through the models and codes discussed in the text. Multiscale Simulations and Mechanics of BiologicalMaterials A compilation of recent developments in multiscalesimulation and computational biomaterials written by leadingspecialists in the field Presenting the latest developments in multiscale mechanics andmultiscale simulations, and offering a unique viewpoint onmultiscale modelling of biological materials, this book outlinesthe latest developments in computational biological materials fromatomistic and molecular scale simulation on DNA, proteins, andnano-particles, to meoscale soft matter modelling of cells, and tomacroscale soft tissue and blood vessel, and

bone simulations.Traditionally, computational biomaterials researchers come frombiological chemistry and biomedical engineering, so this isprobably the first edited book to present work from these talentedcomputational mechanics researchers. The book has been written to honor Professor Wing Liu ofNorthwestern University, USA, who has made pioneering contributionsin multiscale simulation and computational biomaterial in specificsimulation of drag delivery at atomistic and molecular scale andcomputational cardiovascular fluid mechanics via immersed finiteelement method. Key features: Offers a unique interdisciplinary approach to multiscalebiomaterial modelling aimed at both accessible introductory andadvanced levels Presents a breadth of computational approaches for modellingbiological materials across multiple length scales (molecular towhole-tissue scale), including solid and fluid basedapproaches A companion website for supplementary materials plus links tocontributors' websites (www.wiley.com/go/li/multiscale)

Solid State Physics, Volume 50 continues the series' tradition of excellence by focusing on the optical and electronic properties and applications of semiconductors. All of the topics in this volume are at thecutting-edge of research in the semiconductor field and will be of great interest to the scientific community.

The book presents a series of concise papers by researchers specialized in various fields of continuum and computational mechanics and of material science. The focus is on principles and strategies for multiscale modeling and simulation of complex heterogeneous materials, with periodic or random microstructure, subjected to various types of mechanical, thermal, chemical loadings and environmental effects. A wide overview of complex behavior of materials (plasticity, damage, fracture, growth, etc.) is provided. Among various approaches,

attention is given to advanced non-classical continua modeling which, provided by constitutive characterization for the internal and external actions (in particular boundary conditions), is a very powerful frame for the gross mechanical description of complex material behaviors, able to circumvent the restrictions of classical coarse–graining multiscale approaches.

This unique volume presents the state of the art in the field of multiscale modeling in solid mechanics, with particular emphasis on computational approaches. For the first time, contributions from both leading experts in the field and younger promising researchers are combined to give a comprehensive description of the recently proposed techniques and the engineering problems tackled using these techniques. The book begins with a detailed introduction to the theories on which different multiscale approaches are based, with regards to linear homogenization as well as various nonlinear approaches. It then presents advanced applications of multiscale approaches applied to nonlinear mechanical problems. Finally, the novel topic of materials with self-similar structure is discussed.

The idea of the book is to provide a comprehensive overview of computational physics methods and techniques, that are used for materials modeling on different length and time scales. Each chapter first provides an overview of the physical basic principles which are the basis for the numerical and mathematical modeling on the respective length-scale. The book includes the micro-scale, the meso-scale and the macro-scale. The chapters follow this classification. The book will explain in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution. Case studies are occasionally included to further illustrate some methods or theoretical considerations. Example applications for all techniques

are provided, some of which are from the author's own contributions to some of the research areas. Methods are explained, if possible, on the basis of the original publications but also references to standard text books established in the various fields are mentioned.

This book presents a unique combination of chapters that together provide a practical introduction to multiscale modeling applied to nanoscale materials mechanics. The goal of this book is to present a balanced treatment of both the theory of the methodology, as well as some practical aspects of conducting the simulations and models. The first half of the book covers some fundamental modeling and simulation techniques ranging from ab-inito methods to the continuum scale. Included in this set of methods are several different concurrent multiscale methods for bridging time and length scales applicable to mechanics at the nanoscale regime. The second half of the book presents a range of case studies from a varied selection of research groups focusing either on a the application of multiscale modeling to a specific nanomaterial, or novel analysis techniques aimed at exploring nanomechanics. Readers are also directed to helpful sites and other resources throughout the book where the simulation codes and methodologies discussed herein can be accessed. Emphasis on the practicality of the detailed techniques is especially felt in the latter half of the book, which is dedicated to specific examples to study nanomechanics and multiscale materials behavior. An instructive avenue for learning how to effectively apply these simulation tools to solve nanomechanics problems is to study previous endeavors. Therefore, each chapter is written by a unique team of experts who have used multiscale materials modeling to solve a practical nanomechanics problem. These chapters provide an extensive picture of the multiscale materials landscape from problem statement through the final results and outlook, providing

readers with a roadmap for incorporating these techniques into their own research.

The experience of people working with different perspectives in different fields of masonry modeling, from mathematics to applied engineering and practice, is brought together in this book. It presents both the theoretical background and an overview of the state-of-the-art in static and dynamic masonry modeling.

The papers in this proceeding are a collection of the works presented at the IUTAM symposium-Marrakech 2002 (October 20-25) which brought together scientists from various countries. These papers cover contemporary topics in multiscale modeling and characterization of materials behavior of engineering materials. They were selected to focus on topics related to deformation and failure in metals, alloys, intermetallics and polymers including: experimental techniques, deformation and failure mechanisms, dislocation-based modelling, microscopic-macroscopic averaging schemes, application to forming processes and to phase transformation, localization and failure phenomena, and computational advances. Key areas that are covered by some of the papers include modeling of material deformation at various scales. At the atomistic scale, results from MD simulations pertaining to deformation mechanisms in nano-crystalline materials as well as dislocation-defect interactions are presented. Advances in modeling of deformation in metals using discrete dislocation

analyses are also presented, providing an insight into this emerging scientific technique that can be used to model deformation at the microscale. These papers address current engineering problems, including deformation of thin fIlms, dislocation behavior and strength during nanoindentation, strength in metal matrix composites, dislocation-crack interaction, development of textures in polycrystals, and problems involving twining and shape memory behavior. On Behalf of the organizing committee, I would like to thank Professor P.

Bringing together the world's leading researchers and practitioners of computational mechanics, these new volumes meet and build on the eight key challenges for research and development in computational mechanics.

Researchers have recently identified eight critical research tasks facing the field of computational mechanics. These tasks have come about because it appears possible to reach a new level of mathematical modelling and numerical solution that will lead to a much deeper understanding of nature and to great improvements in engineering design. The eight tasks are: The automatic solution of mathematical models Effective numerical schemes for fluid flows The development of an effective mesh-free numerical solution method The development of numerical procedures for multiphysics problems The development of numerical procedures for multiscale problems The modelling of

uncertainties The analysis of complete life cycles of systems Education - teaching sound engineering and scientific judgement Readers of Computational Fluid and Solid Mechanics 2003 will be able to apply the combined experience of many of the world's leading researchers to their own research needs. Those in academic environments will gain a better insight into the needs and constraints of the industries they are involved with; those in industry will gain a competitive advantage by gaining insight into the cutting edge research being carried out by colleagues in academia. Features Bridges the gap between academic researchers and practitioners in industry Outlines the eight main challenges facing Research and Design in Computational mechanics and offers new insights into the shifting the research agenda Provides a vision of how strong, basic and exciting education at university can be harmonized with life-long learning to obtain maximum value from the new powerful tools of analysis

This book provides an overview of the current of the state of the art in the multiscale mechanics of solids and structures. It comprehensively discusses new materials, including theoretical and experimental investigations their durability and strength, as well as fractures and damage

Presenting a state-of-the-art overview of theoretical and computational models that link characteristic biomechanical phenomena, this book provides guidelines

and examples for creating multiscale models in representative systems and organisms. It develops the reader's understanding of and intuition for multiscale phenomena in biomechanics and mechanobiology, and introduces a mathematical framework and computational techniques paramount to creating predictive multiscale models. Biomechanics involves the study of the interactions of physical forces with biological systems at all scales – including molecular, cellular, tissue and organ scales. The emerging field of mechanobiology focuses on the way that cells produce and respond to mechanical forces – bridging the science of mechanics with the disciplines of genetics and molecular biology. Linking disparate spatial and temporal scales using computational techniques is emerging as a key concept in investigating some of the complex problems underlying these disciplines. Providing an invaluable field manual for graduate students and researchers of theoretical and computational modelling in biology, this book is also intended for readers interested in biomedical engineering, applied mechanics and mathematical biology.

The latest state of simulation techniques to model plasticity and fracture in crystalline materials on the nano- and microscale is presented. Discrete dislocation mechanics and the neighbouring fields molecular dynamics and crystal plasticity are central parts. The physical phenomena, the theoretical

basics, their mathematical description and the simulation techniques are introduced and important problems from the formation of dislocation structures to fatigue and fracture from the nano- to microscale as well as it's impact on the macro behaviour are considered.

A systematic discussion of the fundamental principles, written by a leading contributor to the field.

Multiscale Modeling in Solid MechanicsComputational ApproachesImperial College Press

The combination of readily available computing power and progress in numerical techniques has made nonlinear systems - the kind that only a few years ago were ignored as too complex - open to analysis for the first time. Now realistic models of living systems incorporating the nonlinear variation and anisotropic nature of physical properties can be solved numerically on modern computers to give realistically usable results. This has opened up new and exciting possibilities for the fusing of ideas from physiology and engineering in the burgeoning new field that is biomechanics. Computational Biomechanics presents pioneering work focusing on the areas of orthopedic and circulatory mechanics, using experimental results to confirm or improve the relevant mathematical models and parameters. Together with two companion volumes, Biomechanics: Functional Adaptation and Remodeling and the Data Book on

Mechanical Properties of Living Cells, Tissues, and Organs, this monograph will prove invaluable to those working in fields ranging from medical science and clinical medicine to biomedical engineering and applied mechanics.

Temam and Miranville present core topics within the general themes of fluid and solid mechanics. The brisk style allows the text to cover a wide range of topics including viscous flow, magnetohydrodynamics, atmospheric flows, shock equations, turbulence, nonlinear solid mechanics, solitons, and the nonlinear Schrödinger equation. This second edition will be a unique resource for those studying continuum mechanics at the advanced undergraduate and beginning graduate level whether in engineering, mathematics, physics or the applied sciences. Exercises and hints for solutions have been added to the majority of chapters, and the final part on solid mechanics has been substantially expanded. These additions have now made it appropriate for use as a textbook, but it also remains an ideal reference book for students and anyone interested in continuum mechanics.

Summary: A Generalized Multiscale Analysis Approach brings together comprehensive background information on the multiscale nature of the composite, constituent material behaviour, damage models and key techniques for multiscale modelling, as well as presenting the findings and methods, developed over a lifetime's research, of three leading experts in the field. The unified approach presented in the book for conducting multiscale analysis and design of conventional and smart composite materials is also

applicable for structures with complete linear and nonlinear material behavior, with numerous applications provided to illustrate use. Modeling composite behaviour is a key challenge in research and industry; when done efficiently and reliably it can save money, decrease time to market with new innovations and prevent component failure. Uncertainty Quantification in Multiscale Materials Modeling provides a complete overview of uncertainty quantification (UQ) in computational materials science. It provides practical tools and methods along with examples of their application to problems in materials modeling. UQ methods are applied to various multiscale models ranging from the nanoscale to macroscale. This book presents a thorough synthesis of the state-of-the-art in UQ methods for materials modeling, including Bayesian inference, surrogate modeling, random fields, interval analysis, and sensitivity analysis, providing insight into the unique characteristics of models framed at each scale, as well as common issues in modeling across scales.

The idea of the book is to provide a comprehensive overview of computational physics methods and techniques, that are used for materials modeling on different length and time scales. Each chapter first provides an overview of the basic physical principles which are the basis for the numerical and mathematical modeling on the respective length-scale. The book includes the micro-scale, the meso-scale and the macro-scale, and the chapters follow this classification. The book explains in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate

materials on the perspective levels of spatial and temporal resolution. Case studies are included to further illustrate some methods or theoretical considerations. Example applications for all techniques are provided, some of which are from the author's own contributions to some of the research areas. The second edition has been expanded by new sections in computational models on meso/macroscopic scales for ocean and atmosphere dynamics. Numerous applications in environmental physics and geophysics had been added.

In August 2003, ETHZ Computational Laboratory (CoLab), together with the Swiss Center for Scientific Computing in Manno and the Universit della Svizzera Italiana (USI), organized the Summer School in "Multiscale Modelling and Simulation" in Lugano, Switzerland. This summer school brought together experts in different disciplines to exchange ideas on how to link methodologies on different scales. Relevant examples of practical interest include: structural analysis of materials, flow through porous media, turbulent transport in high Reynolds number flows, large-scale molecular dynamic simulations, ab-initio physics and chemistry, and a multitude of others. Though multiple scale models are not new, the topic has recently taken on a new sense of urgency. A number of hybrid approaches are now created in which ideas coming from distinct disciplines or modelling approaches are unified to produce new and computationally efficient techniques

This work gives a modern, up-to-date account of recent developments in computational

multiscale mechanics. Both upscaling and concurrent computing methodologies will be addressed for a range of application areas in computational solid and fluid mechanics: Scale transitions in materials, turbulence in fluid-structure interaction problems, multiscale/multilevel optimization, multiscale poromechanics. A Dutch-German research group that consists of qualified and well-known researchers in the field has worked for six years on the topic of computational multiscale mechanics. This text provides a unique opportunity to consolidate and disseminate the knowledge gained in this project. The addition of chapters written by experts outside this working group provides a broad and multifaceted view of this rapidly evolving field.

Deformation Based Processing of Materials: Behavior, Performance, Modeling and Control focuses on deformation based process behaviors and process performance in terms of the quality of the needed shape, geometries, and the requested properties of the deformed products. In addition, modelling and simulation is covered to create an in-depth and epistemological understanding of the process. Other topics discussed include ways to efficiently reduce or avoid defects and effectively improve the quality of deformed parts. The book is ideal as a technical document, but also serves as scientific literature for engineers, scientists, academics, research students and management professionals involved in deformation based materials processing. Covers process behaviors, such as non-uniform deformation, unstable deformation, material flow phenomena, and process performance Includes modelling and simulation of the entire

deformation process Looks at control of the preferred deformation, undesirable material flow, avoidance and reduction of defects, and improving the dimensional accuracy, surface quality and microstructure construction of the produced products

This volume consists of a collection of chapters by recognized experts to provide a comprehensive fundamental theoretical continuum treatment of constitutive laws used for modelling the mechanical and coupled-field properties of various types of solid materials. It covers the main types of solid material behaviour, including isotropic and anisotropic nonlinear elasticity, implicit theories, viscoelasticity, plasticity, electro- and magneto-mechanical interactions, growth, damage, thermomechanics, poroelasticity, composites and homogenization. The volume provides a general framework for research in a wide range of applications involving the deformation of solid materials. It will be of considerable benefit to both established and early career researchers concerned with fundamental theory in solid mechanics and its applications by collecting diverse material in a single volume. The readership ranges from beginning graduate students to senior researchers in academia and industry.

An updated account of the state of the art in the subject, presenting recent progress in two active and related areas of continuum mechanics: fracture mechanics and structured deformations.

The minisymposium “Parametric and Non-Parametric Methods of Data Analysis at Multiscale Modeling” provided an opportunity to exchange ideas and experiences at the crossroads of three disciplines: materials science, image analysis and statistical data analysis, where new research possibilities have appeared with the rapid development of computer hardware: an increase in the processing speed and the size of the memory available – there has been a rapid development of data analysis methods that were previously not possible to use in practice due to the required computing power. The minisymposium was organized as part of the WCCM 2014, 11th World Congress on Computational Mechanics, which was held in Barcelona, Spain on 20-25 July, 2014.
Multiscale Biomechanics provides new insights on multiscale static and dynamic behavior of both soft and hard biological tissues, including bone, the intervertebral disk, biological membranes and tendons. The physiological aspects of bones and biological membranes are introduced, along with micromechanical models used to compute mechanical response. A modern account of continuum mechanics of growth and remodeling, generalized continuum models to capture internal lengths scales, and dedicated homogenization methods are provided to help the reader with the necessary theoretical foundations. Topics discussed include multiscale methods for fibrous media based on discrete homogenization,

generalized continua constitutive models for bone, and a presentation of recent theoretical and numerical advances. In addition, a refresher on continuum mechanics and more advanced background related to differential geometry, configurational mechanics, mechanics of growth, thermodynamics of open systems and homogenization methods is given in separate chapters. Numerical aspects are treated in detail, and simulations are presented to illustrate models. This book is intended for graduate students and researchers in biomechanics interested in the latest research developments, as well as those who wish to gain insight into the field of biomechanics. Provides a clear exposition of multiscale methods for fibrous media based on discrete homogenization and the consideration of generalized continua constitutive models for bone Presents recent theoretical and numerical advances for bone remodeling and growth Includes the necessary theoretical background that is exposed in a clear and self-contained manner Covers continuum mechanics and more advanced background related to differential geometry, configurational mechanics, mechanics of growth, thermodynamics of open systems and homogenization methods

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.

This book presents the state-of-the-art in multiscale modeling and simulation techniques for composite materials and structures. It focuses on the structural and functional properties of engineering composites and the sustainable high performance of components and structures. The multiscale techniques can be also applied to nanocomposites which are important application areas in nanotechnology. There are few books available on this topic.

Gradient-Enhanced Continuum Plasticity provides an expansive review of gradient-enhanced continuum plasticity from the initial stage to current research trends in experimental, theoretical, computational and numerical investigations. Starting with an overview of continuum mechanics and classical plasticity, the book then delves into concise lessons covering basic principles and applications, such as outlining the use of the finite element method to solve problems with size effects, mesh sensitivity and high velocity impact loading. All major theories are explored, providing readers with a guide to understanding the various concepts of

and differences between an array of gradient-enhanced continuum plasticity models. Outlines the concepts of, and differences between, various gradient-enhanced continuum plasticity models Provides guidance on problem-solving for size effects, mesh-sensitivity tests and thermo-mechanical coupling Reviews experimental, numerical and theoretical issues in gradient-enhanced continuum plasticity Describes micromechanical aspects from experimental observations This unique volume presents the state of the art in the field of multiscale modeling in solid mechanics, with particular emphasis on computational approaches. For the first time, contributions from both leading experts in the field and younger promising researchers are combined to give a comprehensive description of the recently proposed techniques and the engineering problems tackled using these techniques. The book begins with a detailed introduction to the theories on which different multiscale approaches are based, with regards to linear Homogenisation as well as various nonlinear approaches. It then presents advanced applications of multiscale approaches applied to nonlinear mechanical problems. Finally, the novel topic of materials with self-similar structure is discussed. Sample Chapter(s). Chapter 1: Computational Homogenisation for Non-Linear Heterogeneous Solids (808 KB). Contents: Computational Homogenisation for Non-Linear Heterogeneous Solids (V G Kouznetsova et al.);

Two-Scale Asymptotic Homogenisation-Based Finite Element Analysis of Composite Materials (Q-Z Xiao & B L Karihaloo); Multi-Scale Boundary Element Modelling of Material Degradation and Fracture (G K Sfantos & M H Aliabadi); Non-Uniform Transformation Field Analysis: A Reduced Model for Multiscale Non-Linear Problems in Solid Mechanics (J-C Michel & P Suquet); Multiscale Approach for the Thermomechanical Analysis of Hierarchical Structures (M J Lefik et al.); Recent Advances in Masonry Modelling: Micro-Modelling and Homogenisation (P B Louren o); Mechanics of Materials with Self-Similar Hierarchical Microstructure (R C Picu & M A Soare). Readership: Researchers and academics in the field of heterogeneous materials and mechanical engineering; professionals in aeronautical engineering and materials science.

The EURO-C conference series (Split 1984, Zell am See 1990, Innsbruck 1994, Badgastein 1998, St. Johann im Pongau 2003, Mayrhofen 2006, Schladming 2010, St. Anton am Arlberg 2014, and Bad Hofgastein 2018) brings together researchers and practising engineers concerned with theoretical, algorithmic and validation aspects associated with computational simulations of concrete and concrete structures. Computational Modelling of Concrete Structures reviews and discusses research advancements and the applicability and robustness of methods and models for reliable analysis of complex concrete, reinforced concrete and pre-stressed concrete structures in engineering practice. The contributions cover both computational mechanics and computational modelling aspects of the analysis and design of

concrete and concrete structures: Multi-scale cement and concrete research: experiments and modelling Aging concrete: from very early ages to decades-long durability Advances in material modelling of plain concrete Analysis of reinforced concrete structures Steel-concrete interaction, fibre-reinforced concrete, and masonry Dynamic behaviour: from seismic retrofit to impact simulation Computational Modelling of Concrete Structures is of special interest to academics and researchers in computational concrete mechanics, as well as industry experts in complex nonlinear simulations of concrete structures.

"Practical Aspects of Computational Chemistry" presents contributions on a range of aspects of Computational Chemistry applied to a variety of research fields. The chapters focus on recent theoretical developments which have been used to investigate structures and properties of large systems with minimal computational resources. Studies include those in the gas phase, various solvents, various aspects of computational multiscale modeling, Monte Carlo simulations, chirality, the multiple minima problem for protein folding, the nature of binding in different species and dihydrogen bonds, carbon nanotubes and hydrogen storage, adsorption and decomposition of organophosphorus compounds, X-ray crystallography, proton transfer, structure-activity relationships, a description of the REACH programs of the European Union for chemical regulatory purposes, reactions of nucleic acid bases with endogenous and exogenous reactive oxygen species and different aspects of nucleic acid bases, base pairs and base tetrads.

This book provides an overview of multiscale approaches and homogenization procedures as well as damage evaluation and crack initiation, and addresses recent advances in the analysis and discretization of heterogeneous materials. It also highlights the state of the art in this

research area with respect to different computational methods, software development and applications to engineering structures. The first part focuses on defects in composite materials including their numerical and experimental investigations; elastic as well as elastoplastic constitutive models are considered, where the modeling has been performed at macro- and micro levels. The second part is devoted to novel computational schemes applied on different scales and discusses the validation of numerical results. The third part discusses gradient enhanced modeling, in particular quasi-brittle and ductile damage, using the gradient enhanced approach. The final part addresses thermoplasticity, solid-liquid mixtures and ferroelectric models. The contents are based on the international workshop “Multiscale Modeling of Heterogeneous Structures” (MUMO 2016), held in Dubrovnik, Croatia in September 2016.

Material properties emerge from phenomena on scales ranging from Angstroms to millimeters, and only a multiscale treatment can provide a complete understanding. Materials researchers must therefore understand fundamental concepts and techniques from different fields, and these are presented in a comprehensive and integrated fashion for the first time in this book. Incorporating continuum mechanics, quantum mechanics, statistical mechanics, atomistic simulations and multiscale techniques, the book explains many of the key theoretical ideas behind multiscale modeling. Classical topics are blended with new techniques to demonstrate the connections between different fields and highlight current research trends. Example applications drawn from modern research on the thermo-mechanical properties of crystalline solids are used as a unifying focus throughout the text. Together with its companion book, Continuum Mechanics and Thermodynamics (Cambridge University Press, 2011), this work

presents the complete fundamentals of materials modeling for graduate students and researchers in physics, materials science, chemistry and engineering.

This book presents a multiscale modeling framework combining computational chemistry and computational mechanics to study the stiffness, damage initiation and failure process of polymer-clay nanocomposites (PCNs). It demonstrates the feasibility of a virtual material characterization tool for PCNs, which could accelerate their development and application. It is useful for researchers in fields of solid mechanics and material science.

With its discussion of strategies for modeling complex materials using new numerical techniques, mainly those based on the finite element method, this monograph covers a range of topics including computational plasticity, multi-scale formulations, optimization and parameter identification, damage mechanics and nonlinear finite elements.

Most problems in science involve many scales in time and space. An example is turbulent ?ow where the important large scale quantities of lift and drag of a wing depend on the behavior of the small vortices in the boundarylayer. Another example is chemical reactions with concentrations of the species varying over seconds and hours while the time scale of the oscillations of the chemical bonds is of the order of femtoseconds. A third example from structural mechanics is the stress and strain in a solid beam which is well described by macroscopic equations but at the tip of a crack modeling details on a microscale are needed. A common dif?culty with the simulation of these problems and many others in physics, chemistry and biology is that an attempt to represent all scales will lead to an enormous computational problem with unacceptably long computation times and large memory requirements. On the other hand, if the discretization at a coarse level ignoresthe?nescale

informationthenthesolutionwillnotbephysicallymeaningful. The in?uence of the ?ne scales must be incorporated into the model. This volume is the result of a Summer School on Multiscale Modeling and S- ulation in Science held at Boso ¤n, Lidingo ¤ outside Stockholm, Sweden, in June 2007. Sixty PhD students from applied mathematics, the sciences and engineering parti- pated in the summer school.