Preface

Within the past decade, the emphasis of scientific research worldwide has shifted to the study of the behavior of materials at the atomic scale of matter. The proliferation of scientists and engineers studying matter at this length scale has led to the coining of the phrase *nanotechnology*. This term can generally be taken to imply the investigation and technological utilization of the properties of matter at length scales of one thousand nanometers or smaller. Generally, a few thousand atoms will exist in the space of thousand nanometers.

As engineers typically study the mechanical properties of materials, the corresponding emphasis of research in the engineering community has been on *nano mechanics*. The term "nano mechanics" is typically associated with the study and characterization of the mechanical behavior of individual atoms, atomic-scale systems and structures in response to various types of forces and loading conditions. The specific nature of nano mechanics research generally varies depending on the discipline of the engineer; the topic of interest can involve the atomic-scale effect of fracture and wear on material performance, mechanical properties of nanocomposites, atomic-scale flow and locomotion of individual biological cells.

Regardless of the interest of the particular scientist or engineer, what is universally agreed upon is the overall potential that nanotechnology, and particularly nano mechanics, has for the betterment of our society, including the sectors of private industry, national defense and homeland security. An emphasis on nanoscale entities will make our manufacturing technologies and infrastructure more sustainable in terms of reduced energy usage and environmental pollution. Recent advances made by the research community in this topic have stimulated ever-broader research activities in science and engineering that are devoted to their development and applications.

Many areas of research are rapidly advancing owing to the combined efforts of science and engineering. In mechanics and materials, we are particularly excited with the progress in research and education that can be achieved by combining engineering and basic sciences through modeling and simulation together with experimentation. Owing to the combination of constantly increasing computational power and the increased knowledge and understanding of material behavior, *multiple scale modeling methods* have recently emerged as the tool of choice to link the mechanical behavior of materials from the smallest scale of atoms to the largest scale of structures. Multiple scale methods offer the best hope for bridging the traditional gap that exists between experimental approach, the theoretical approach and computational modeling for studying and understanding the behavior of materials.

Owing to the central role that multiple scale methodology appears poised to play in the computational mechanics and materials science in the foreseeable future, this book aims to summarize the past and the current developments in multiple scale modeling to

provide a coherent starting point from which interested scientists and engineers can begin their journey into this vast and rapidly expanding subject. We hope that this book is one of the first systematic works aimed at providing knowledge about fundamental concepts behind nanoscale mechanics and materials and the relevant applications. The book contains both published and previously unpublished material and is aimed at nanoscale engineers, designers, materials scientists and interested students and researchers.

A salient feature of this book is that it is also intended to be used as an educational tool. The major reason is to synthesize the state of the art in multiple scale modeling techniques into the classroom such that the crucial tools being made available today are passed onto the next generation of scientists and engineers. Thus, the materials in this book which were previously used for courses at Northwestern University and the National Science Foundation (NSF) Summer Institute on Nano Mechanics and Materials have been coherently combined with Powerpoint lecture notes and selected computer codes (available online at www.wiley.com/go/nanomechanics) to make the material presented readily accessible for those researchers who are interested in joining and contributing to the field of multiple scale modeling and analysis. Along with the review of basic theoretical concepts, they present the solutions and dynamic visualization of numerous practical problems, ranging from simple one-dimensional systems to state-of-the-art applications. The solutions of the simple illustrative problems are augmented by Matlab and Mathematica codes which serve to highlight the numerical implementation of the theoretical approaches presented in this book.

There are many other novel and unique aspects to this book. As mentioned above, the integration of teaching and research is one of the key features. The material contains detailed expositions on all the topics that are necessary to fully comprehend multiple scale analysis. As such, the book is logically divided into three parts. The first part consists of Chapters 2–4, which cover the theoretical basis needed to understand the behavior of multiparticle atomistic systems. The second part consists of Chapters 5–8, and introduces multiple scale methods. In particular, the bridging scale concurrent approach, which is based on the theoretical considerations provided in the first part of the book, is given special attention here. The third part comprising Chapters 9–10 is devoted to contemporary applications in the area of nanostructured and bioinspired materials, biofluidics and cell mechanics.

Chapter 1 contains an introduction, and emphasizes the need for multiple scale simulations by presenting case studies from different scientific disciplines, including materials design and biofluidics. Chapter 2 introduces the notion of Lagrangian dynamics description of systems of interacting particles, including nonconservative equations of motion, multibody interatomic potentials and arbitrary molecular shapes. Chapter 3 details the extension of the Lagrangian method to spatially periodic lattice structures; it reviews the relevant symmetry concepts, and derives the basic response solutions for a general three-dimensional lattice in semianalytical forms that are important in nanoscale engineering applications. Chapter 4 gives a systematic, though condensed, exposition on contemporary approaches that allow an averaged macroscopic characterization of multiparticle systems in thermodynamic equilibrium; these include the methods of thermodynamic potentials, statistical averaging, microcanonical and canonical ensemble theories.

Chapter 5 provides an overview of multiple scale modeling. As such, previously developed multiple scale methods are reviewed and analyzed, and capabilities that are needed in

multiple scale modeling are discussed and provided as a basis for the remaining chapters. Chapter 6 introduces the bridging scale concurrent method, which couples atomistic and continuum scale models; here, connections are made between the bridging scale, particle dynamics and lattice mechanics concepts introduced in Chapters 2–3.

Numerical validation of the bridging scale approach is given in Chapter 7. The numerical examples in one, two and three dimensions highlight the applicability of the bridging scale to highly nonlinear physical phenomena, including the fracture and subsequent failure of materials. The recent extension of the bridging scale to incorporate quantum mechanical information into the coupling of length scales framework is also described in this chapter. Chapter 8 provides an extension of the MD impedance force such that it can be utilized with long-ranged interatomic potentials; this extension is crucial as most realistic interatomic potentials incorporate non-nearest neighbor bonding. This chapter concludes the section on multiple scale modeling with comments on future research directions.

Chapter 9 highlights applications of multiple scale methods in crucial areas of physical interest. In the realm of solids, the topics covered are the hierarchical and concurrent design of realistic materials, including novel steel and metallic alloys, shape memory composites and self-healing materials. Lastly, Chapter 10 emphasizes new research in the area of computational biofluidics, electrohydrodynamics, bioengineering and nano-bio interfacial problems. The topics include electrophoresis multiscale and multiphysics modeling of red blood cell (RBC) aggregation and the effect on blood rheology, capillary flow, cell migration, nanomanipulation and assembly of macromolecules.

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