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Introduction

Over the past three decades, we have acquired new tools and techniques to synthesize nanoscale objects and learn their many incredible properties. The high-resolution electron microscopes that are available today enable the visualization of single atoms; furthermore, the manipulation of these individual atoms is possible using scanning probe techniques. Synthesis of advanced materials provides the technology to tailor-design systems from as small as molecules to as large as the fuselage of a plane. We now have the technology to detect single molecules, bacteria or virus particles. We can make protective coatings more wear-resistant than diamond and fabricate alloys and composites such that they are stronger than ever before. Advances in the synthesis of nanoscale materials have stimulated ever-broader research activities in science and engineering devoted entirely to these materials and their applications. This is due in large part to the combination of their expected structural perfection, small size, low density, high stiffness, high strength and excellent electronic properties. As a result, nanoscale materials may find use in a wide range of applications in material reinforcement, field emission panel display, chemical sensing, drug delivery, nanoelectronics and tailor-designed materials. Nanoscale devices have a great potential as sensors and medical diagnostic and delivery systems.

With the confluence of interest in nanotechnology, the availability of experimental tools to synthesize and characterize systems at the nanometer scale, and computational tools widely accessible to model microscale systems by coupled continuum/molecular/quantum mechanics, we are poised to unravel the traditional gap between the atomic and the macroscopic world of mechanics and materials. This in turn opens up new opportunities in education and research.

1.1 Potential of Nanoscale Engineering

Nanotechnology is making, and will continue to make, an impact in key areas for societal improvement. In particular, it has been found that basic mechanics principles have found many applications in nanoscience and nanoengineering. For example, current research
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Current research in engineering is just beginning to impact molecular scale mechanics and materials and would benefit from interaction with the basic sciences. For solids, research in the area of plasticity and damage has experienced some success in advancing microscale component design. The development of carbon nanotubes is also an area in which nanoscale research has clearly played a major role. For fluids, coupling physics phenomena at the nanoscale is crucial in designing components at the microscale. Electrophoresis and electroosmotic flows coupled with particulate motion in a liquid have been important research areas that have had great impact in the homeland security area. Microfluidic devices often comprise components that couple chemistry, and even electrochemistry, with fluid motion. Once the physics-based models are determined for the solids and fluids,
computational approaches will need to be employed or developed to capture the coupled physics phenomena.

While microscale and nanoscale systems and processes are becoming more viable for engineering applications, our knowledge of their behavior and our ability to model their performance remains limited. Continuum-based computational capabilities are obviously not applicable over the full range of operational conditions of these devices. Noncontinuum behavior is observed in large deformation behavior of nanotubes, ion deposition processes, gas dynamic transport, and material mechanics as characteristic scales drop toward the micron scale. At the scales of nanodevices, interactions between thermal effects and mechanical response can become increasingly important.

Furthermore, nanoscale components will be used in conjunction with components that are larger and respond at different timescales. In such hybrid systems, the interaction of different time and length scales may play a crucial role in the performance of the complete system. Single scale methods such as ab initio methods or molecular dynamics (MD) would have difficulty in analyzing such hybrid structures owing to the large range of timescales and length scales. For the design and study of nanoscale materials and devices in microscale systems, models must span length scales from nanometers to hundreds of microns.

Computational power has doubled approximately every 18 months, in accordance with Moore’s law. Despite this fact and the fact that desktop computers can now routinely simulate million atom systems, simulations of realistic atomic system require at least tens of billions of atoms. In short, such systems cannot be modeled by continuum methods, because they are too small, nor can they be modeled by molecular methods because they are too large. Hence, coupled multiscale methods are urgently needed for this class of problems.

Multiple scale methods generally imply the utilization of information at one length scale to subsequently model the response of the material at larger length scales. These methods can be divided into two categories: hierarchical and concurrent. Hierarchical multiple scale methods directly utilize the information at a small length scale as an input into a larger model via some type of averaging process. The Young’s modulus is a good example of this; the structural material stiffness is found as a single quantity, through homogenization of all defects and microstructure at the micro- and nanoscales. Concurrent multiple scale methods are those that run simultaneously; in these methods, the information at the smaller length scale is calculated and inputted into the larger scale model on the fly. In this book, we shall concentrate on the development of concurrent multiple scale methods, much of which has occurred within the past decade. We note in particular the work of Li and Liu (2004), as well as two excellent review papers that comprehensively cover the field, namely, those of Liu et al. (2004c) and Curtin and Miller (2003).

Multiscale simulation methods will be a valuable tool in design; just as computer-aided engineering (CAE) on the microscale was facilitated by finite element methods. We envision that the availability of tools for multiscale analysis will provide a powerful impetus to the development of new nanodevices. More specifically, we believe that the next generation of CAE software will integrate nano and microstructures into the fundamental CAE capabilities for design and manufacturing. To move toward this goal, the development and validation of predictive multiscale simulation models that integrate materials design into virtual manufacturing processes is imperative. These multiscale models must incorporate
the statistical nature of defects and uncertainty analysis in processing and modeling in order to be considered complete.

A simple example of the necessity to account for microstructure in material modeling is shown in Figure 1.1. In the first case, a simple block of ice is dropped from a certain height onto the ground; as can be seen, the ice fractures into multiple pieces, reflecting its brittle nature. In the second case, the ice has been reinforced by strips of newspaper. Upon being dropped from the same height, the block of ice stays intact, and does not break. Clearly, the added microstructural effects in the form of the newspaper dramatically enhanced the strength of the ice.

A real-life example of the strengthening properties of material microstructure is given in Figure 1.2. There, the various complicated deformation mechanisms that exist at different material length scales in a typical high-strength steel is illustrated in a schematic. As can be seen, the overall structural response of the ship is governed by the interactions between the inclusions, second phase particles and defects that occur in the steel at different length scales. The TiN primary inclusions are typically micron sized, and govern fracture toughness due to decohesion and debonding. The secondary TiC inclusions are typically nanometer sized, and provide strengthening after yield by controlling the interfacial separation. Thus, the resultant mechanical properties of the steel are a competition between strength and toughness, with the inclusions at different scales dominating at each end of the spectrum.

We emphasize that while the mechanical response of the steel can be modeled hierarchically, that is, by using average properties from smaller length scales to control the macroscopic response, it is currently impossible to concurrently model all the way from atomistics to continuum without leaving out the crucial intermediate, mesoscopic length scales. Modeling from atoms to continuum represents a grand challenge in material design.
and solid mechanics; a focus of this book is on the development of efficient computational techniques and algorithms to assist in the modeling process.

In nano-bio systems, the multiple scale mechanics of the human heart is seen in Plate 1. The heart and its associated arteries, veins, valves and blood represent the smallest scale at which continuum solid and fluids mechanics can be utilized to model the heart as an elastic body. The second scale is the vessel scale, where the properties of the vessel wall and thrombus deposition on the wall are the interactions of interest. The third scale is the cellular scale, where blood components such as red blood cells, white cells, platelets, as well as their interactions are considered. At these small scales, the blood needs to be simulated using a non-Newtonian model. The smallest scale under consideration is the subcellular scale, where the biofibers, focal adhesion complexes, and other macromolecules and substructures are studied utilizing MD or some hybrid method. The goal of the multiple scale modeling is to better understand the nature of cellular forces and adhesion; as the blood flows in the vessel, cells and proteins in the blood may deposit onto the vessel wall and may finally block the blood flow, leading to heart attacks. The understanding of cellular interactions will result in the development of computational models that can assist in the accuracy of treatments to retard metastasis.

1.3 Educational Approach

The material presented in this book provides information to researchers and educators about specific fundamental concepts and tools in nanomechanics and materials, including solids and fluids, and their modeling via multiple scale methods and techniques. In recognition of
the importance of engineering education, a key component of this book is in the synthesis of the literature with Powerpoint instructional slides, which were used as the basis for two newly developed courses at Northwestern entitled Multiscale Simulations and Molecular Modeling and the Interface to Micromechanics. Furthermore, these lecture notes were utilized as the basis for the interdisciplinary NSF-sponsored Summer Institute on Nano Mechanics and Materials (www.tam.northwestern.edu/summerinstitute/Home.htm), which has been held at Northwestern for the past three summers. These lecture notes, in combination with instructional computer programs that cover all fundamental concepts introduced in the book, will serve as a starting point from which interested researchers may jump into and contribute to the emerging field of computational nanotechnology.

We would like to emphasize that this book is specifically oriented towards the study of nanomechanics. The emphasis on nanomechanics is a crucial point, as nanomechanics serves as a theoretical foundation of nanotechnology in the area of nanoscale materials as well as biomechanical systems. Our goal in this book is to demonstrate methods for modeling the mechanical behavior of materials at the nanoscale, while interpreting that behavior in a larger context. These models will then be tested on modern applications to validate the approaches presented.

Traditional educators and researchers in mechanics and materials are well versed in continuum mechanics including topics such as elasticity, plasticity, dislocations and fracture. As we evolve toward smaller and smaller components and systems, there is no doubt that we must move beyond continuum treatments into characterizations of mechanics and materials at the nanoscale. Therefore, the material presented in this book is invaluable for introducing engineers to the fundamental methods of modeling and characterization of nano and multiscale systems, that is, molecular dynamics, statistical physics and quantum mechanics. These tools, when combined with continuum mechanics and multiple scale modeling, will allow engineers to continue the fruitful collaborations with scientists who have been responsible for the surge in interest in nanoscale engineering.

One important impact of engineering education is the multiplying effect. Participants may launch their own initiatives in nanotechnology, such as curriculum development or enhancement, initiation of new research ideas or products, and so on. Since engineers are not trained in the fields that bridge the nanosciences with engineering, their training is of great importance in providing society useful applications of these technologies. Training for those in the basic sciences is also needed to bring products of practical use from these technologies to the marketplace. This book will serve these needs by providing education and resource for both engineers and scientists in the technologies that bridge the nanosciences with engineering.