微纳技术著作丛书（影印版）

纳米力学与材料：理论、多尺度方法和应用

Nano Mechanics and Materials

Liu Wing Kam
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内 容 简 介

合成与分析纳米物质特性的能力取得了革命性的进展，广泛应用于生物医学、机械、电子、精密材料以及军事工程等领域。纳米力学是研究和描述单个原子、系统和结构在各种载荷条件下响应的机械行为特性的学科，它的发展促进了该技术的进步。尤其是多尺度建模方法，它可以使此领域的工程师更好的理解微纳米材料。

本书由该领域内资深专家撰写，对纳米力学和材料的基本概念进行了介绍，侧重于多重尺度建模方法和技术的研究。本书内容包括：分子力学基础，微粒系统、晶格机械及现代多尺度建模理论等。

本书是一本相关领域电子工程师、材料科研工作者开发微纳米材料应用的全面的指南，同时也可作为微纳米力学和微纳米技术专业研究生的参考书。

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序

科学出版社准备出版一套《微纳技术著作丛书》，包括原创作品和引进作品（影印或翻译）两种形式，并聘请专家组成编委会。这是一件大事，希望能坚持把它办好。

微纳米技术作为21世纪重要的一项技术，已成为国际科学界和工程技术界研究的热点。近年来，微米纳米技术进展迅速，已经发展成为一个包含机械、材料、电子、光学、化学、生物、基因工程、医学等基础学科的综合领域，而不仅仅属于任何单一的科学和技术门类。就其产品而言，也早已超越了人们广为熟悉的微型加速度传感器和纳米碳管等，呈现出向各个科学和技术领域全面渗透的趋势。

由于微纳米技术使得人们除了可以在同一基片上实现包括机械、流体、化学、生物、光学等器件外，也可以将信号处理和传输系统集成在同一基片上用以处理信息，决定计划，控制周围环境，从而大大提高最终产品的综合性能，实现高度智能化。在未来的航空航天、生物医学、环境监控、无线通信、汽车和交通、石油化工、能源、工农业、国家安全、食品和消费的各个领域都将有广泛应用，对国民经济、科学技术、社会发展与国家安全具有重要意义。今后的几十年里，随着微米纳米技术的迅速发展和向现代科学和技术的各个门类渗透，其对我们现代生活的各个方面带来的影响将是长期和深远的。从某种意义上来说，微米纳米技术的发展，可能改变人类的工作和生活方式，乃至基本概念，其潜在的影响有可能和以计算机技术为代表的微电子工业对世界的影响相提并论。

正是由于其诱人的应用前景和巨大的潜在市场，微米纳米技术目前已成为世界各国大力投资进行研究和发展的热点领域，其研究范围包括了材料、器件和系统，涉及的技术包含机理研究、设计分析、计算仿真、制造工艺、系统集成或组装、测控技术和应用研究等。随着微纳米技术的迅猛发展，近年来国外有大量这方面的专业书籍出版。

《微纳技术著作丛书》涵盖材料开发、系统设计、检测技术、集成技术、通信网络、传感系统、微加工技术等方面，它们都是本领域的研究热点。这套丛书的出版对促进我国微米纳米技术的发展将有很大的推动作用。

这套丛书中，原创作品收录的都是国内从事微纳技术的一线研究人员在本领域的研究成果与心得，具有很强的独立性、创造性和系统性。引进作品都是与国际知名的出版集团合作，经国内专家的甄别，挑选出能反映国外最新研究成果、对国内读者又有借鉴价值的作品，具有权威性、前瞻性和可读性。因为微纳米技

术是一个交叉学科领域，我们有意识的选择了一些由多人合写的专著。通常这类著作都是由相关领域的知名专家，各自在每一章节涵盖一个专题，既有进行综合性的论述，也有个人的具体独创性研究。这样的书籍，通常能帮助读者既获得某一领域的研究概况，又能从一个具体的应用专题中获得收益。

2007 年初推出的第一批影印版图书，我和王万军教授进行了评读，此套丛书很实用，不少作者在该领域有很高的声望。我们建议致力于微米纳米技术的研究人员，包括研究生、技术人员，能够花些时间阅读。

总之，我们对科学出版社组织出版这套丛书的举措很赞赏，也希望他们能将这一工作认真、长期地做下去。同时，我们也希望国内的专家能够积极、踊跃地加盟，为我国微米纳米技术的推进做出贡献。

周兆英 王万军

2006 年 12 月 7 日

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1

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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efforts deal with the application of cell mechanics to neurobiology and cancer research. Currently, a key limitation is in understanding the behavior of the myriad of different cellular structures, interactions and adhesive forces. Once this is established, these mechanisms can be used to develop treatment strategies for cancer, for example, in the prevention of metastasis.

The design and production of materials from the atomic scale up is a goal that is becoming increasingly realizable by the application of DNA to nanotechnology and biotechnology. Owing to the predictable manner in which DNA strands interact, research is now being performed to design solid materials by manipulating individual DNA strands as the basic building blocks. Use of DNA will lead to new materials with novel mechanical, chemical and optical properties, controllable at the unit of the basic building block.

Nanotechnology also has the potential to greatly improve our resistance to terrorism and improve our national security by improving the technologies available to our armed forces. Nanoscale sensors are being developed for the purpose of detecting illegal and harmful airborne chemicals. Our soldiers will benefit from new, energy-absorbing polymer-based nanomaterials that will provide ballistic protection while being light enough to allow maximum mobility. Research along these crucial lines is being done, for example, at the MIT Institute for Soldier Nanotechnologies.

Protective coatings is another area that has greatly benefited from nanotechnology. These coatings have a wide range of applicability, examples being gears and bearings in the automotive industry, and naval vessels for the military. In all these applications, the goal has been to replace or augment previously known super hard materials such as diamond in designing tribological parts that use nanoceramic-type coatings to reduce friction and wear. Extending the lifetime of these parts is crucial, and will lead to a massive reduction in maintenance costs for these components.

Another key area in nanotechnology is in electronics, microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS). For example, the storage capacity of computer hard drives has been increased by orders of magnitude, thanks to magnetic materials whose thickness is on the order of nanometers. Medicine is another key area in which NEMS and MEMS devices have made, and will make, large contributions. Here, nanotechnology can be used to dynamically image living biological systems, such that the real-time study of bacteria and diseases can be performed.

1.2 Motivation for Multiple Scale Modeling

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

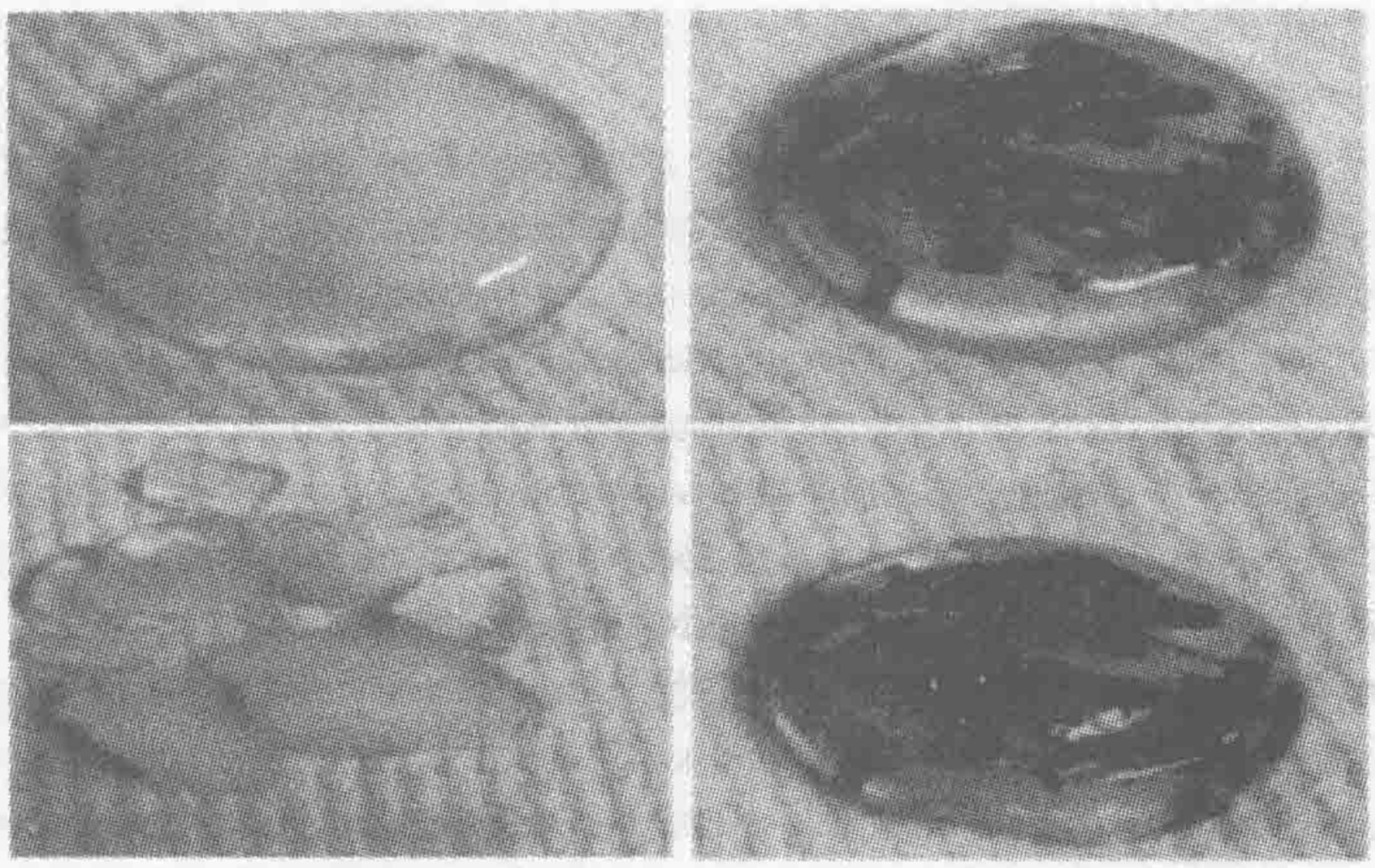

Figure 1.1 Left: brittle fracture of non-reinforced ice after drop test. Right: unbroken reinforced ice after drop test. Images are courtesy of Prof. Yip-Wah Chung, Northwestern University.

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

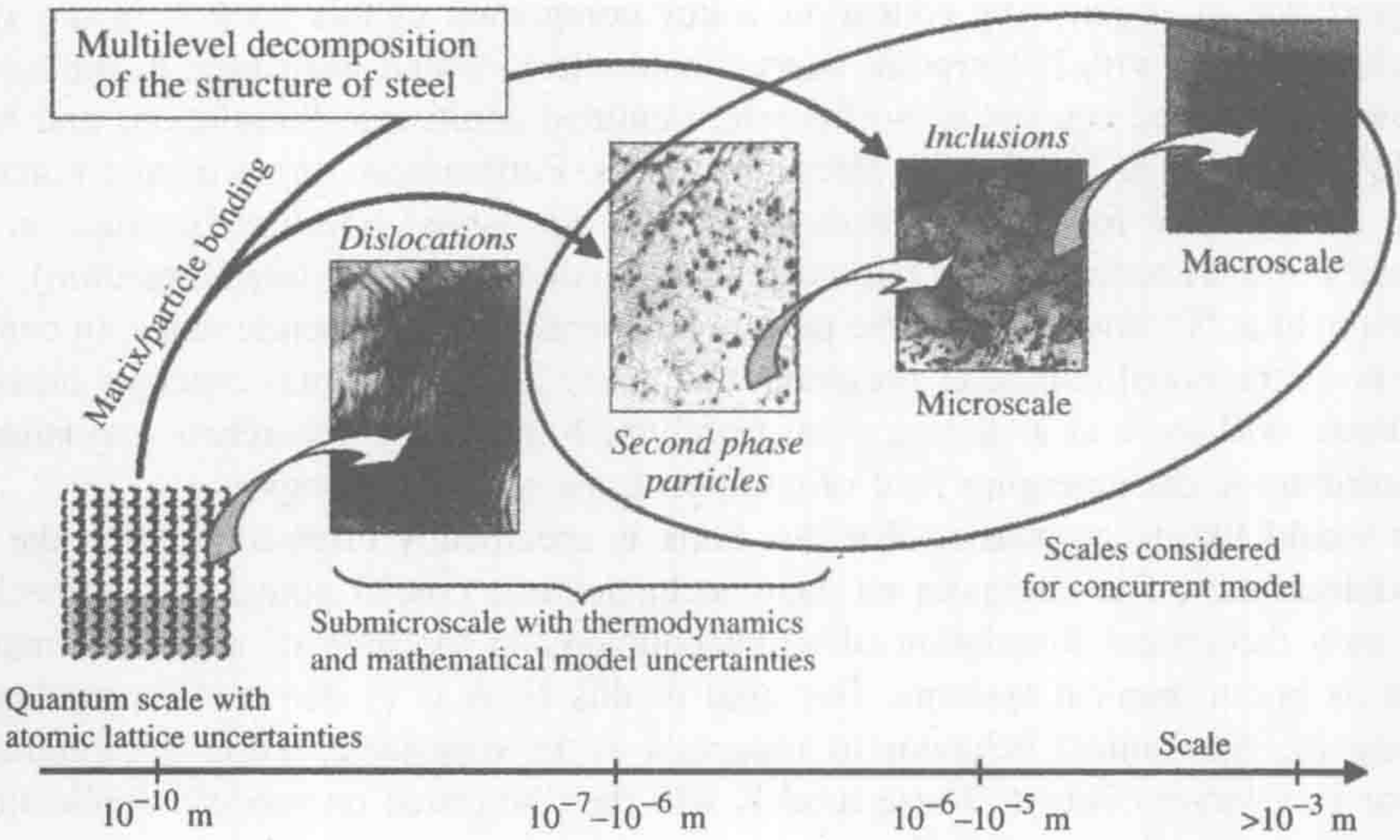

Figure 1.2 Multiple scale properties of steel.

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.

2

Classical Molecular Dynamics

This chapter is devoted to the methods of classical mechanics that allow the study of the motion of gas, liquid and solid particles as a system of interactive, dimensionless mass points. The classical dynamic equations of motion are valid for slow and heavy particles, with typical velocities $v \ll c$, c being the speed of light, and masses $m \gg m_e$, m_e being the electron mass. Therefore, only slow motion (slower than thermal vibrations) of atoms, ions and molecules can be considered, and the internal electronic structure is ignored. The atoms and molecules exert internal forces on each other that are determined by instantaneous values of the total potential energy of the system. The potential energy is typically considered only as a function of the system spatial configuration and is described by means of *interatomic potentials*. These potentials are considered as known input information; they are either found experimentally or are computed by averaging over the motion of the valence electrons in the ion's Coulomb field by means of quantum ab initio methods. During the course of the system's dynamics, the interatomic potentials are not perturbed by possible changes in the internal electronic states of the simulated particles.

Analytical solutions of the equations of particle dynamics are possible only for a limited set of interesting problems and only for systems with a small number of degrees of freedom. Numerical methods of solving the classical equations of motion for multiparticle systems with known interatomic potentials are collectively referred to as *molecular dynamics* (*MD*). MD is regarded as a major practical application of the classical particle dynamics. The subsequent computer postprocessing and visualization of the results accomplished in a dynamic manner are called the *molecular dynamics simulation*.

2.1 Mechanics of a System of Particles

Classical dynamics studies the motion of mass points (ideal dimensionless particles) due to known *forces* exerted on them. These forces serve as qualitative characteristics of the interaction of particles with each other (internal forces) and with exterior bodies (external forces). The general task of dynamics consists in solving for the positions (trajectories) of all particles in a given mechanical system over the course of time. In principle, such a solution

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