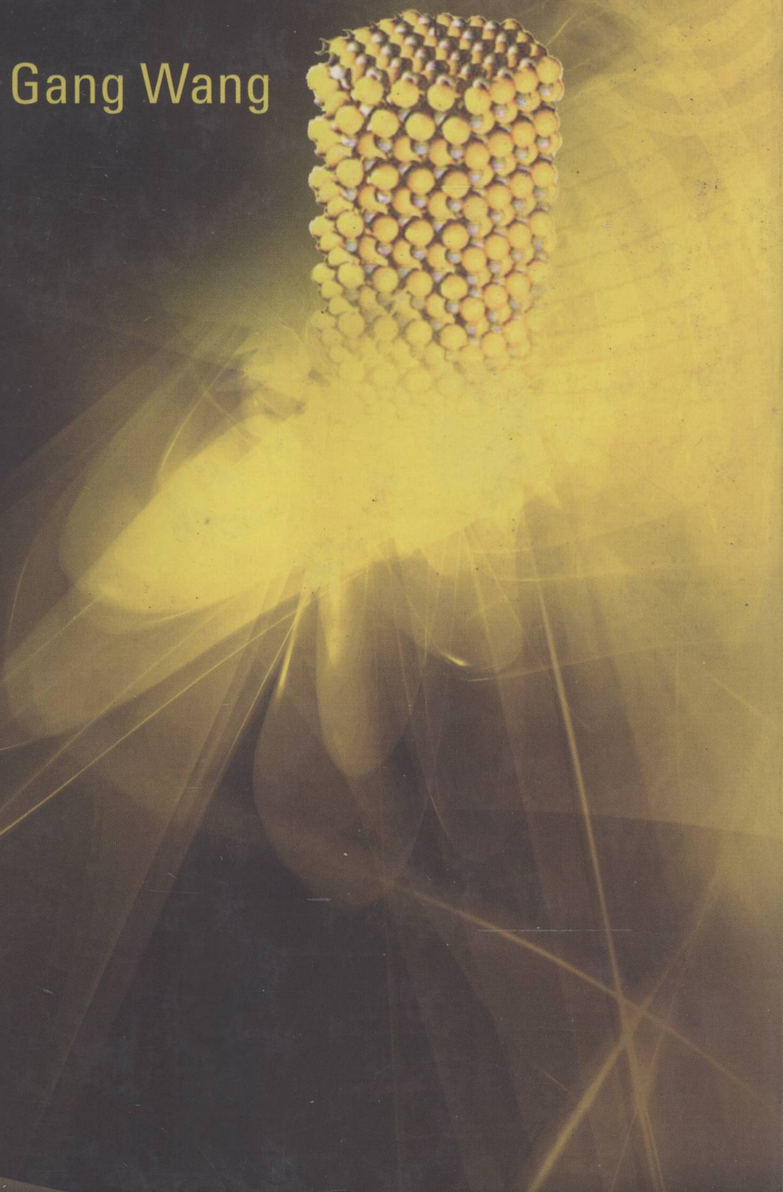
Introduction to Micromechanics and Nanomechanics

Shaofan Li • Gang Wang



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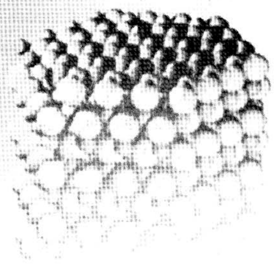

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In memory of my mother,
Yu-zheng Zhang,
for her love and perpetual inspirations.

S. Li

To my mother,
Pei-xue Gong,
for her love and sacrifice.

G. Wang

Preface

My early interests in Micromechanics was largely inspired by Professor Toshio Mura. I had been studied under Professor Mura from 1994-1998, during which I had taken his graduate class *Micromechanics* I and II, and I had worked with him in the same office for almost four years. In specific, Professor Mura taught me equivalent eigenstrain theory (which should be labeled as the Eshelby-Mura theory), dislocation theory, and lattice statics/dynamics. As I can remember, one favorite line of Professor Mura's is: *the eigenstrain method is panacea.* My current interests in Nanomechanics and Computational Nanomechanics researches are mainly motivated by my Ph.D. dissertation advisor, Professor Wing Kam Liu, who is one of the leading experts in Computational Nanomechanics today. Readers may find that this book is greatly influenced by Professor Mura's book, *Micromechanics of Defects in Solids* (Kluwer Academic Publisher, 1987) and Professor Liu's book, *Nano Mechanics and Materials: Theory, Multiscale Methods and Applications* (John Wiley & Sons, Ltd., 2005).

Since spring 2001, I have been regularly teaching a graduate course on *Micromechanics* (CE236) in the University of California at Berkeley. This book is the outcome of the lecture notes as well as research projects of that course. In recent years, more focus of the course has been placed on the presentation of nanomechanics — an emerging field that is still very much under development. Therefore, aside from traditional Micromechanics, a unique feature of this book is its in-depth discussions of the latest topics on Nanomechanics and its applications. This includes: lattice Green's function method (LGFM), embedded atom method (EAM), quasi-continuum method, discrete dislocation dynamics (DDD), the Peierls-Nabarro model, the Gurtin-Murdoch surface elasticity model, and the concept of the virial stress, etc.

Many students who had taken the class have participated in the related class research projects. Most of those researches have been published in peer-reviewed journals, and constitute a significant part of materials presented in this book. My co-author, Dr. Gang Wang, is among the first group of students participating in the class research project. Since then, we have been working together for several years, and he has contributed significantly on many subjects discussed in this book.

I would also like to thank those who have made unique contributions to this book. They are: Dr. Roger Sauer, Dr. Christian Linder, Dr. Chin-long Lee, Dr. Xiaohu Liu, Dr. James Foulk III, Dr. Daniel Simkins, Jr., Dr. Elif Ertekin, Dr. Albert To, Dr. Elisa Morgan, Dr. Anurag Gupta, Dr. Ni Sheng, Ms. Veronique Le Corvec, Mr. Morteza Mahyari, Mr. Noang-Nam Nguyen among others.

During the writing of this book, many colleagues have given us encouragements and suggestions. In particular, Professor Dong Qian of University of Cincinnati, Professor L. Z. Sun of the University of California at Irvine, Professor H. Wang of the Texas A & M University, Professor P. Sharma of University of Houston, Professor X. Markenscoff of the University of California at San Diego, and Dr. L. P. Liu of California Institute of Technology, who have generously provided their own research results or materials helping us writing the book. I would also like to acknowledge the financial support from National Science Foundation through the Career Award (Grant No. CMS-0239130), which makes this book and related researches possible.

The objective of the book is twofold: it can serve as a graduate textbook on Micromechanics and Nanomechanics for the first-year graduate students, and also a research guide book for researchers who want to master the fundamental theories of Micromechanics and Nanomechanics through self-study. One of the main features of this book is to give as many detailed derivations as necessary to assist the readers in understanding the theoretical assumptions, mathematical techniques, and possible limitations. To make the self-learning an enjoyable journey for our readers, our motto is to *spell out all the details even if they may be trivial.* By doing so, we hope to fill the gap between the literature and the actual research notes.

Due to our limitations, the book may contain mistakes, misrepresentations, and errors; Moreover, we are aware the fact that some of the presentations in the book may be biased or limited by our own technical capacities and inadequacies. Readers can send their comments and suggestions to the following email address:

`micro.and.nanomechanics@gmail.com`

which, we hope, can be used to correct and improve the quality of the book in the future.

Finally, we would also like to thank our wives, Yan Zhang (SL) and Furong Wang (GW), and our families. Without their supports and encouragements, this book will never be finished.

Shaofan Li

Spring 2007, Berkeley, California

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Chapter 1

INTRODUCTION

1.1 What are micromechanics and nanomechanics?

Generally speaking, MICROMECHANICS is a scientific discipline that studies mechanical, electrical, and thermodynamical behaviors of materials with microstructure; NANOMECHANICS is a research field that studies material behaviors at nanoscale level.

In recent years, micromechanics has become an indispensable part of theoretical foundation for many engineering fields and emerging technologies such as nanotechnology as well as biomedical and bioenvironmental technologies. Because of its multidisciplinary characteristics, the term *micromechanics* has 'multidisciplinary interpretations', and it has been used with different meanings in different contexts. In the area of applied mechanics, micromechanics is often referred to as a hierarchical mechanics and mathematics paradigm that is mainly used to study the effective material properties of composite materials. A major objective of this kind of study is to find the statistical average material properties of the heterogeneous material through various homogenization methods. In condensed solid state physics and statistical mechanics, this process is called the *Coarse Graining*. One of the fundamental challenge of the contemporary statistical physics is how to construct accurate coarse grain models.

Traditionally, the standard micromechanics methodology in engineering applications treats a composite material as a generic continuum model with a two-level paradigm: microscopic structure and macroscopic structure. The material properties at microscale are usually given as a priori, and the task is to find the material behaviors at macroscale, which are also called as the effective or overall material properties. From this perspective, a material point at the macro-level may be viewed as a microscopic material ensemble. In principle, the constitutive relations at macro level should be able to be derived from the ensemble average of micro-objects that are governed by the microscale physical laws, which can be quantum mechanics, lattice dynamics, microscale plasticity, or elasticity, etc. Two subtle points worth further clarification: (1) the constitutive relations or material behaviors at macroscale may be very much different from their counterparts at microscale, so the task of micromechanics is to find the unknown macroscale constitutive laws. One of such examples is the well-known Gurson's model, in which the microscale constitutive law is the rigid perfectly plasticity whereas the macroscale constitutive law obtained by homogenization is a pressure sensitive damage plasticity; (2) in many other cases, the microscale and macroscale constitutive laws are the same type, e.g. elastic behaviors, however, the detailed elastic stiffness tensors at the different scales are different. The effective material properties at a macroscale point are average material properties of a microscale ensemble or a unit cell.

The conventional two-level paradigm of micromechanics is a special mathematical homogenization model that is usually not associated with any fixed length scale. When studying material properties of a metal, 1 mm may be viewed as macroscale, and the length scale at microlevel may range from nm to μm ; whereas studying the deformation of a dam, the macroscale may be up to $10^3 m$, and the length scale of micro-structure may be around $10^{-2} m$.

In the conventional micromechanics, the classical ergodic assumption is usually adopted: *if a mesoscale is large enough, the underline micro-structure is assumed to statistically homogeneous and stable in both space and in time.* Therefore, one simply uses spatial average to replace the temporal average of a random stochastic process. In this sense, traditional micromechanics is essentially a particular ensemble averaging theory that takes into account the overall effects of microstructure.

In engineering applications, the conventional micromechanics deals with practical engineering problems of a broad spectrum: effective material properties of composite/synthetic materials, such as cementitious materials, geotechnical materials, etc.; constitutive modeling of bio-materials, such as bone, muscle, blood flow, etc.; phase transformations; defects in solids, such as dislocation motion and crack growth; and environmental problems, such as air pollution, ground water flow and chemical transport, etc.

Contemporary condensed matter physics and applied mechanics in general agree that the physics at molecular or atomic level (Å) can be described by the quantum mechanics or related approximation theories, e.g. density functional theory; the physics between the nm scale to sub-μm scale is governed by nanomechanics though presently we are mainly relying on the molecular dynamics simulation; from μm scale to or sub-mm length scale, micromechanics and related mesoscale mechanics are playing more important roles; and the macroscopic phenomenological theory is generally valid at the length scale mm level or up.

In this book, we shall focus on several areas of nanomechanics and micromechanics. Different from traditional micromechanics, a salient feature of nanomechanics is its multiscale and multiphysics characteristics. It has some features presented in quantum mechanics, or quantum statistical mechanics, manifesting the statistical effects at atomic or sub-atomic level; on the other hand, it also shares many features of continuum mechanics, because a nanostructure could contain millions of atoms.

The impetus for contemporary micromechanics and nanomechanics is primarily due to the emergence of nanoscience and biomedical technology. It appears that traditional physics alone is not sufficient to deal with many engineering problems that are emerging from nanotechnologies and nanoengineering. There is a call for nanomechanics and nanocomputational mechanics to serve as the infrastructure of these developing engineering fields. For instance, much attention has been focused recently on material properties of thin films; manufacturing devices and components of a microelectromechanical system (MEMS), such as sub-micro sized sensors, motors; mechanics of nanotubes and nanowires; and micro-biophysics/biochemistry systems, e.g. protein/DNA interaction in biomolecular simulation, etc.

From the perspective of higher learning and intellectual advancement, micromechanics has been developed into a rigorous and beautiful mathematical framework, philosophical methodology, and powerful computational realization. Forty years ago, micro-elasticity started with simple definitions of eigenstrain and inclusion, came along with Eshelby's equivalent homogenization theory [Eshelby (1957, 1959, 1961)]) and Hashin & Shtrikman's variational principle [Hashin and Shtrikman (1962a,b)], it is now the foundation of composite material research. Even though the conventional micromechanics deals with the objects with the length scale around μm, it has been extensively used to estimate or to analyze the behaviors of nanocomposites and nanoscale structures, such as the composite made by nanowires and quantum dots.

Besides homogenization, another main aspect of mciromechanics is the study of defect mechanics at small scale. This includes: crack growth, dislocation motion, and evolution of vacancies and interstitial, etc. In parallel to the development of micro-mechanics, another major paradigm of defect mechanics is the Configurational Force Mechanics. It seems to us that future trend of micro-mechanics is to develop multiscale configurational mechanics that can describe defect motions in a multiscale thermodynamic environment.

The main task of nanomechanics is to establish *coarse-graining models* at small scales or to bridge the gap between the atomic scale and continuum scale. For example, an efficient coarse-graining technique is the so-called Cauchy-Born rule. The Cauchy-Born rule may be viewed as a simple "homogenization approximation" in lattice statics and it serves as a passage or linkage between molecular mechanics and continuum mechanics. The Cauchy-Born rule assumes that under certain kinematic conditions, for instance, uniformity of local deformation gradient, the continuum energy density can be computed directly by using the atomistic potential, which links the continuum elastic potential energy with the atomistic potential. By using the Cauchy-Born rule, one may be able to derive the expressions for stress tensors and elastic stiffness tensors directly from the interatomic potential, which allows the use of the standard nonlinear finite element method in nanoscale computations.

Another useful nanomechanics approach is the Lattice Green's Function (LGF) method. It provides an important limit case for continuum mechanics, which allows us examine the differences between the molecular mechanics and the continuum mechanics.

Presently, nanomechanics is only at its infancy. There are many approaches to be explored and many new phenomena to be studied. In this book, we are attempting to synthesize some recent research results at the forefront of nanomechanics research while presenting traditional micromechanics in a coherent fashion. By doing so, we hope that it may serve as a stepping stone for nanomechanics research in the quest for a multiscale mechanics of our time.

Many research monographs on Micromechanics and Composite Materials have been published over the years, notably the classical treatises by Professor Mura [Mura (1987)], Christensen [Christensen (1979)], Nemat-Nasser and Hori [Nemat-Nasser and Hori (1999)], Teodosiu [Teodosiu (1982)], Hahn and Tsai [Hahn and Tsai (1980)], Kim and Karrila [Kim and Karrila (1991)], and Krajcinovic [Krajcinovic (1996)]. In recent years, quite a number of books have been published focusing on various different aspects of micromechanics and defect mechanics, such as statistical micro-mechanics [Torquato (1997)], translation method and variational bounds for composite materials [Milton (2002)], general introductions to micromechanics and composite materials [Cristescu *et al.* (2004)] and [Qu and Cherkaoui (2006)], micro-poromechanics [Dormieux *et al.* (2006)], and comprehensive treatise and handbook on micromechanics as well [Buryachenko (2007)], among others.

The current literature on Micromechanics and Nanomechanics is either too specialized, too esoteric, to be understood, or too elementary to be applied. The objective of the present book is to fill the gap between the graduate study or self-study and the independent or creative research. To do so, firstly, we would like to provide a self-study guide or a readable graduate textbook on Micromechanics and Nanomechanics that is easy to read without much prerequisites and experiences on applied mathematics, continuum mechanics or elasticity theories; Secondly, we would like to merge the theory of micromechanics into the theory of nanomechanics by find internal links and coherence between the two subjects and making the subject more contemporary and more interesting to readers.

1.2 Vectors and tensors

For self-containedness and easy reference, the presentation starts with an outline of some basic prerequisites: mathematics preliminaries, the element of elasticity theory, and lattice and molecular statics and dynamics.

1.2.1 *Vector algebra*

Consider a Cartesian coordinate in a three dimensional space, $\mathbb{R}^3$ with unit vector basis, $\{\mathbf{e}_i\}, i = 1, 2, 3$. An arbitrary position vector, $\mathbf{x}$, may be expressed as

$$\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3 = x_i\mathbf{e}_i = (\mathbf{x}\cdot\mathbf{e}_i)\mathbf{e}_i \tag{1.1}$$