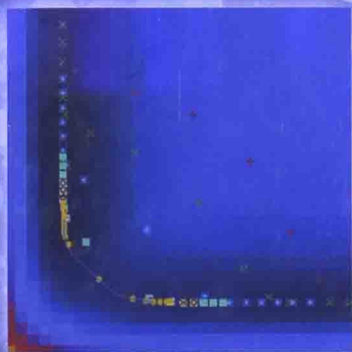

Multiscale Analysis of Deformation and Failure of Materials

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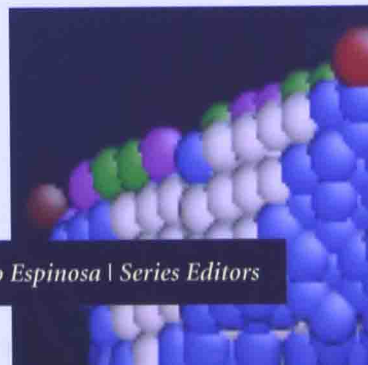

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MULTISCALE ANALYSIS OF DEFORMATION AND FAILURE OF MATERIALS

Jinghong Fan

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WILEY

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To my wife, Zheng Ying
Daughter Ying Fan and Son Qiang Fan
for
inspiration and loving support

About the Author

Dr. Jinghong Fan is a Professor at the Kazuo Inamori School of Engineering at Alfred University, New York, USA. Dr. Fan graduated from the Department of Naval Architecture, Shanghai Jiao Tong University, China and received MS and Ph.D. degrees from the Department of Aerospace Engineering and Engineering Mechanics at the University of Cincinnati, USA. Dr. Fan serves as the Chairman of the Scientific Committee of the Research Center on Materials Mechanics at Chongqing University. He is Co-Chair of the International Conference on Heterogeneous Materials Mechanics (ICHMM) 2004, 2008, and 2011.

Dr. Fan has developed the generalized particle dynamics method by which classical molecular dynamics can be extended to a large material domain. His pioneering work includes showing experimentally the quantitative size effects of layer thickness of microstructure of pearlitic steel on ratcheting (cyclic creep) and then developed a hierarchical multiscale method to describe the discovered size effects by linking variables at micro/meso/macroscopic scales of continuum and the scale of dislocation. Publications include *Foundation of Nonlinear Continuum Mechanics* and the Chinese version of *Multiscale Analysis of Deformation and Failure of Materials* as well as more than 140 papers. His research interests include multiscale modeling and simulation for deformation, defect initiation and evolution under mechanical loading and processing conditions of thin-layer ceramics coating as well as multiscale analysis for interactions between medical implants and bio-cells. His traditional research fields include constitutive laws, plasticity, composite materials, damage, fracture, and fatigue.

Series Preface

In the past decade, micro- and nano-technology have received unprecedented attention from governments around the world, industry, the press, and the public in the hope to witness revolutionary discoveries, which when translated to products could impact and transform our everyday lives. Following the success of the semiconducting industry, and more recently the information technology industry, the expectation for major nanotechnology breakthroughs, in the early part of the 21st century, is very high. However, micro and nano technologies are less mature and rely on scientific advances to fulfil their promise. In this regard, the development of model capabilities with *predictive power* is essential. Taking advantage of modern supercomputers, *in-silico* modelling of bottom up fabrication of complex 3-D molecular systems, prediction of mechanical, electrical, optical and thermal performance of new nanomaterials (e.g., metallic and semiconducting nanowires and carbon nanotubes), and protein-protein interactions, just to mention a few examples, is now possible. Such advances are poised to impact and accelerate developments in materials, manufacturing, electronics, medicine and healthcare, energy, the environment and world security. Books in this series focus in promoting the dissemination of such advances through scholarly work of the highest quality. The Series is intended to serve researchers and scientists who wish to keep abreast of advances in the expanding field of nano- and micro-technology, and as a resource for teachers and students of specialized undergraduate and post-graduate courses.

The earlier book *Fluid Properties at Nano/Meso Scale*, by Peter Dyson, Rajesh Ransing, Paul Williams and Rhodri Williams, provides a comprehensive numerical treatment of fluidics bridging the nanoscale, where molecular physics is required as a guiding principle, and the microscale where macro continuum laws operate. In this book Jinghong Fan takes us step by step through a wide range of multiscale modeling methods and simulations of the solid state at the atomistic/nano/submicron scales and up through those covering the micro/meso/macroscopic scale. The book is a timely and very useful presentation of modelling approaches and algorithms with a reach to a broad set of problems in nano and biotechnologies. We are introduced to the concept of material-cells that act as links to provide seamless, bottom-up and top-down, transitions between neighbouring sub-scales. This can be used for a progressive understanding of crystal lattice defects at the atomic scale, through to the dynamics of lattice dislocations, and then to macroscopic properties such as plasticity and electrical resistivity. Other examples include a description of how an atom-based continuum theory can be developed to understand hydrogen storage in carbon nanotubes, and how a multiscale analysis of biological cell-surface interactions can aid the development of medical implants.

The pedagogic treatment given by Professor Fan to his book makes it suitable for inclusion in the final year of undergraduate materials science courses in engineering and physical sciences, as well as in computational graduate courses. The book as a whole should be considered as recommended reading for researchers across a wide range of disciplines including materials science, mechanical engineering, applied chemistry and applied physics.

Ronald Pethig Horacio D. Espinosa

Preface

Experience shows that in-depth understanding of material properties can result in great improvement to products and promote the development of novel ones through synergies with other disciplines, for example design. Therefore it is essential to recognize that materials are inherently of a hierarchical, multiscale character. Properties should not be considered as monolithic quantities only at macroscopic levels, as historically taught. Rather, important material properties can arise at a myriad of length scales ranging from atomic to microscopic to mesoscopic to macroscopic. Computational simulation is also recognized now as an essential element between theory and experimentation. These concepts comprise the foundations of a new interdisciplinary field of study at the interface of engineering and material science, which is referred to in the current literature as multiscale, multi-physics modeling and simulation.

Study of this field necessarily draws from foundations in electronic structure and atomistic-scale phenomena, which are the basic building blocks of materials. Engineers and scientists are increasingly drawn together by this unifying theme to develop multiscale methods to bridge the gaps between lower-scale and macroscopic theory. This amalgam of fields demands a departure from classical solid mechanics curricula in engineering colleges, as well as condensed matter curricula in the fields of physics and chemistry. The need for curricula changes has been accelerated by recent advances in bio- and nanotechnologies.

This book describes the author's research experience in developing multiscale modeling methods across atomistic/nano/submicron scales and micro/meso/macroscopic continuum analysis. Researchers may be interested in how the concept of material neighbor-link cells can seamlessly transform information bottom-up and top-down, how meso-cells link micro- and macroscopic scales, and how their connection to dislocation theory can help investigate, for example, the size effects of cyclic plasticity and failure.

Wide applications of multiscale analysis are introduced in the book, including how atomistic-based continuum theory can be developed for hydrogen storage of carbon nanotubes, how rate effects on dislocation nucleation can be identified by atomistic analysis so its results can be compared with laboratory testing, how new states can be predicted by using the nudged elastic band method to find minimum energy path and saddle point to distinguish the large-scale separation of activation volume which is the physical basis for the distinction between yield and creep and to find the mechanism for the high strength and high ductility of nanostructured metals (e.g., nano-twinned copper), and how multiscale problems can be extracted from biology, such as the multiscale analysis of cell/surface interactions for medical implants.

Students and practitioners interested in these emerging ideas and approaches must develop an appropriate background. This textbook is written with the intention of providing students with the necessary background and advanced knowledge for multiscale modeling and simulation. The enthusiastic feedback provided by undergraduate and graduate students at Alfred University, USA and Shanghai University, China while using this book in a multiscale analysis course has been rewarding and encouraging.

This book not only describes the background, principles, methods, and applications of various atomistic and multiscale analyses, but also emphasizes new concepts and algorithmic developments through various homeworks. Emphasis is placed on the development of simulation skills and use of software for computer atomistic simulations. Associated with Chapter 10 is a Computational Simulation Laboratory Infrastructure (CSLI). CSLI contains computer UNITS with one-to-one correspondence to the sections of Chapter 10, which can be downloaded from the book's website http://multiscale.alfred.edu and used for computational lab practice through courses or self-learning.

My great thanks are due to Prof. D. McDowell of Georgia Institute of Technology, Dr. V. Yamakov of National Institute of Aerospace, Prof. A. Clare of New York State College of Ceramics and Prof. R. Loucks of the Physical Department of Alfred University for constructive suggestions. Thanks are also due to Dr. M. Chinappi, Dr. A. Cao, Dr. Y. Chen, Mr. B. Wang, Mr. D. Parker, Mr. R. Stewert, Mr. H. Lu, and Ms. L. He who have made contributions to various sections of the book. I would also like to express my gratitude to my colleagues, Professors X. Peng, J. Zhang, X. Zeng, and B. Chen in China for their extensive collaboration.

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Alfred Village, New York

Abbreviations

1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
ADP	Angular dependent potential
BCC	Body-centered cubic
CADD	Couple atomistic analysis with discrete dislocation
CNT	Carbon nanotube
CSLI	Computational simulation laboratory infrastructure
DC	Direct coupling
DFT	Density function theory
DT	Deformation twinning
EAM	Embedded atom method
ESCM	Embedded statistical coupling method
FCC	Face-centered cubic
FE	Finite element
FEA	Finite element analysis
FEAt	Finite element and atomistic model
FEM	Finite element method
GP	Generalized particle dynamics
GULP	General Utility Lattice Program
kMC	Kinetic Monte Carlo
k_B	Boltzmann constant
HCP	Hexagonal close-packed cell
HF	Hartree-Fock
LAMMPS	Large-scale atomic/molecular massively parallel simulation
LCAO	Linear combination of atomic orbitals
LDA	Local density approximation
LF	leap-frog
LJ	Lennard-Jones
MAAD	Macroscopic atomistic *ab initio* dynamics
MC	Monte Carlo
MD	Molecular dynamics
MEAM	Modified embedded atom method
MEP	Minimum energy path
MEMS	Micro electro-mechanical systems
MO	Molecular orbital
MS	Molecular statics
NAMD	Nanoscale molecular dynamics
NEB	Nudged elastic band
NEMS	Nano electro-mechanical systems
NLC	Neighbor-link cell
PBC	Periodic boundary condition(s)
PDB	Protein data bank
PES	Potential energy surface
PSF	Protein structure file
PN	Peierls-Nabarro
QC	Quasicontinuum method
QM	Quantum mechanics
R_{cut}	Cutoff radius for interatomic potential
RT	Rice-Thomson *or* Room temperature
RVE	Representative volume element (= Representative unit cell)
SCS	Self-consistent scheme
SOFC	Solid oxide fuel cells
TB	Tight binding
TST	Transition state theory
U^{tot}	Total system energy
VMD	Visual molecular dynamics
VV	Velocity Verlet
XRD	X-ray diffraction
YAG	$Y_3Al_5O_{12}$ synthetic garnet
YSZ	Yttria stabilized zirconia

Contents