THE HANDBOOK OF NANOTECHNOLOGY

# NANOMETER STRUCTURES

## Theory, Modeling, and Simulation

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*About the cover:* The images shown are part of a simulation studying the formation of complex junction structures in metals undergoing work-hardening induced by tensile strain. The work was produced by Farid Abraham of IBM Almaden Research in collaboration with Lawrence Livermore National Laboratory (LLNL) personnel Mark Duchaineau and Tomas Diaz De La Rubia. The images are screenshots from a movie depicting a billion-atom dislocation simulation in copper. Further information on this simulation can be found at www.llnl.gov/largevis/atoms/ductile-failure/ and in Reference 56 in Chapter 7 of this book. Special thanks are due to the University of California, LLNL, and the U.S. Department of Energy, under whose auspices the work was performed.

Dedicated to all who strive for peace

# Order of Chapters

# Foreword

It is both a rare privilege and a distinct challenge to prepare a short foreword to this volume of the *Handbook of Nanotechnology*. So, why me and why did I agree? The answer to that is certainly not the usual answer. Traditionally, someone pre-eminent in the field of nanometer structures would be asked to provide a short overview of this subfield, its importance, and its trajectory. Obviously, I am not an expert in this particular branch of science and technology; the fact is that I am intellectually challenged by the material in its totality even though I feel comfortable and at home with a significant fraction of that totality as stand-alone components.

The answer to "why me?" is perhaps because I have always championed the integrated approach to science and engineering, specifically optical science and engineering. This approach involves the integration of theory, modeling, setting up and evaluating specific examples, testing those examples, and applying the results to specific experimental and engineering studies. The resultant knowledge is then used to devise new technology, implement that technology, and apply it to problem solving and to the development of new components and systems. The final step is to design and create new instruments and products to serve the local world in which we live.

Having now taken the time to accept the challenge of working through this volume, I can certainly report that it was well worth the effort. Those readers who follow my example will find that it will provide a significant stimulation to those already working in the field and encourage others to make an intellectual investment in moving nanotechnology forward.

This handbook is not presenting a fully developed theoretical model, but is presenting significant theory based on sound physical laws augmented by other approaches to provide a framework to test ideas and make progress. We have all learned over the years that there are a number of valuable ways to approach the mathematical description of physical observations: modeling, simulation, algorithms, interactive processes, transformations to other spaces and coordinates, curve fitting, and statistical methods, to name a few. The reader will find many of these techniques used in the text.

There is no doubt that nanotechnology will play a very important role in the coming years in a variety of areas that are listed in Professor Lakhtakia's preface and in the table of contents. These areas will certainly be interdisciplinary between science and engineering, but also interdisciplinary in the traditional sense between optical science, optical engineering mechanics, electronics, material science, etc.

It is not without significance that this volume is published as a joint venture between SPIE—The International Society for Optical Engineering and ASME, The American Society of Mechanical Engineering.

My expectation (and hence my prediction) is that this volume may well become a milestone volume for some time to come with perhaps new editions in the future as the field progresses. I hope the editor will ask someone more qualified than I am to prepare the foreword to future editions!

**Brian J. Thompson**
*University of Rochester*
*May 2004*

# Preface

The *Handbook of Nanotechnology* series is intended to provide a reference to researchers in nanotechnology, offering readers a combination of tutorial material and review of the state of the art. This volume focuses on modeling and simulation at the nanoscale. Being sponsored by both SPIE—The International Society for Optical Engineering and the American Society of Mechanical Engineering, its coverage is confined to optical and mechanical topics.

The eight substantive chapters of this volume—entitled *Nanometer Structures: Theory, Modeling, and Simulation*—cover nanostructured thin films, photonic bandgap structures, quantum dots, carbon nanotubes, atomistic techniques, nanomechanics, nanofluidics, and quantum information processing. Modeling and simulation research on these topics has acquired a sufficient degree of maturity as to merit inclusion. While the intent is to serve as a reference source for expert researchers, there is sufficient content for novice researchers as well. The level of presentation in each chapter assumes a fundamental background at the level of an engineering or science graduate.

I am appreciative of both SPIE and ASME for undertaking this project at a pivotal point in the evolution of nanotechnology, just when actual devices and applications seem poised to spring forth. My employer, Pennsylvania State University, kindly provided me a sabbatical leave-of-absence during the Spring 2003 semester, when the major part of my editorial duties were performed.

All contributing authors cooperated graciously during the various phases of the production of this volume and its contents, and they deserve the applause of all colleagues for putting their normal research and teaching activities aside while writing their chapters for the common good. Tim Lamkins of SPIE Press coordinated the production of this volume promptly and efficiently. I consider myself specially privileged to have worked with all of these fine people.

**Akhlesh Lakhtakia**
*University Park, PA*
*May 2004*

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