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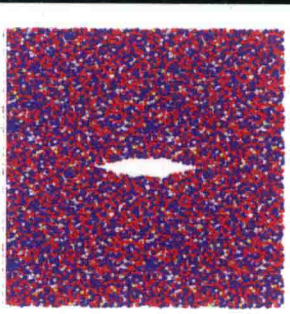
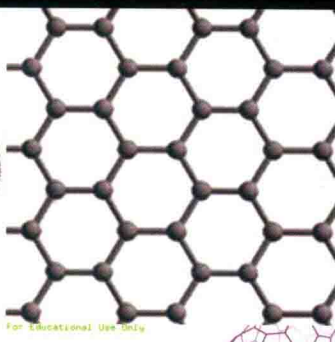
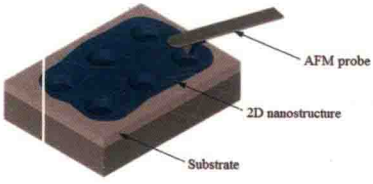
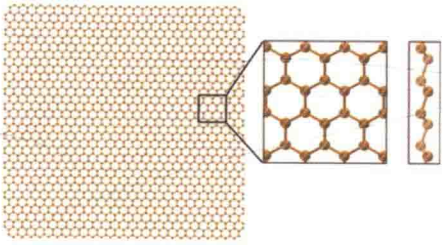
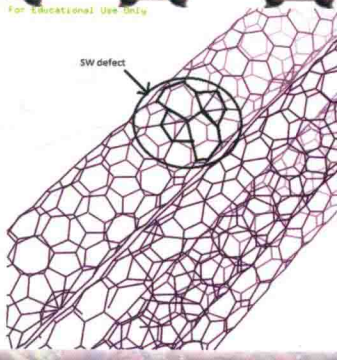






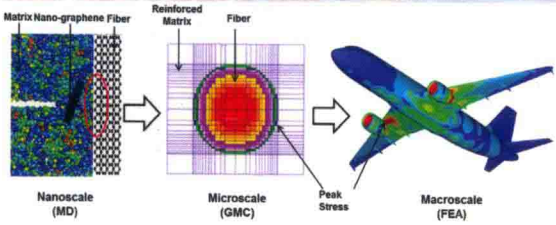




Advanced Computational Nanomechanics

Editor

NUNO SILVESTRE



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ADVANCED COMPUTATIONAL NANOMECHANICS

Edited by

Nuno Silvestre

University of Lisbon
Portugal

WILEY

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Advanced Computational Nanomechanics

Silvestre, February 2016

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Morgan and Green, January 2003

Microfluidic Technology and Applications

Koch et al., November 2000

List of Contributors

Avinash Akepati, Graduate Research Assistant, Department of Aerospace Engineering and Mechanics, University of Alabama, Tuscaloosa, AL, USA

Ganesh Balasubramanian, Assistant Professor, Department of Mechanical Engineering, Iowa State University, Ames, IA, USA

Irene J. Beyerlein, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA

Khoa Bui, School of Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, OK, USA

Steven W. Cranford, Assistant Professor, Department of Civil and Environmental Engineering, Northeastern University, Boston, MA, USA

Ghasem Ghadyani, Faculty of Mechanical Engineering, University Malaya, Kuala Lumpur, Malaysia

Ali Ghavamian, Research Assistant, School of Engineering, Griffith University, Gold Coast Campus, Southport, Queensland, Australia

Yuantong Gu, Professor, School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD, Australia

Mesut Kirca, Assistant Professor, Department of Mechanical Engineering, Istanbul Technical University, Istanbul, Turkey

Huong Nguyen, School of Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, OK, USA

Andreas Öchsner, Prof. Dr.-Ing., School of Engineering, Griffith University, Gold Coast Campus, Southport, Queensland, Australia

Dimitrios V. Papavassiliou, Professor, School of Chemical, Biological and Materials Engineering, The University of Oklahoma, Norman, OK, USA; Division for Chemical, Bioengineering and Environmental Transport Systems, National Science Foundation, Arlington, VA, USA

Nicola M. Pugno, Professor, Department of Civil, Environmental and Mechanical Engineering, University of Trento, Trento, Italy; Centre of Materials and Microsystems, Bruno Kessler Foundation, Trento, Italy; School of Engineering and Materials Science, Queen Mary University, London, UK

Moones Rahmandoust, Dr., Protein Research Center, Shahid Beheshti University, G.C., Velenjak, Tehran, Iran; School of Engineering, Griffith University, Gold Coast Campus, Southport, Queensland, Australia; Deputy Vice Chancellor Office of Research and Innovation, Universiti Teknologi Malaysia, Johor Bahru, Johor, Malaysia

Ruth E. Roman, Graduate Research Assistant, Department of Civil and Environmental Engineering, Northeastern University, Boston, MA, USA

Samit Roy, William D Jordan Professor, Department of Aerospace Engineering and Mechanics, University of Alabama, Tuscaloosa, AL, USA

Hiroyuki Shima, Associate Professor, Department of Environmental Sciences, University of Yamanashi, Kofu, Yamanashi, Japan

Yoshiyuki Suda, Associate Professor, Department of Electrical and Electronic Information Engineering, Toyohashi University of Technology, Toyohashi, Aichi, Japan

Keka Talukdar, HOD, Department of Physics, Nadiha High School, Durgapur, West Bengal, India

Albert C. To, Associate Professor, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, PA, USA

Chien Ming Wang, Professor, Engineering Science Programme, Faculty of Engineering, National University of Singapore, Singapore, Singapore

Yu Wang, PhD Student, School of Computing, Engineering and Mathematics, University of Western Sydney, Sydney, NSW, Australia

Xi F. Xu, Professor, School of Civil Engineering, Beijing Jiaotong University, Beijing, China

Yingyan Zhang, Senior Lecturer, School of Computing, Engineering and Mathematics, University of Western Sydney, Sydney, NSW, Australia

Series Preface

Books in the Wiley's Microsystem and Nanotechnology Series are intended, through scholarly works of the highest quality, to serve researchers and scientists wishing to keep abreast of advances in this expanding and increasingly important field of technology. Each book in the series is also intended to be a rich interdisciplinary resource for not only researchers but also teachers and students of specialized undergraduate and postgraduate courses.

Past books in the series include the university textbook *Introduction to Microsystem Technology* by Gerlach and Dötzel, covering the design, production and application of miniaturized technical systems from the viewpoint that for engineers to be able to solve problems in this field, they need to have interdisciplinary knowledge over several areas as well as the capability of thinking at the system level. In their book *Fluid Properties at Nano/Meso Scale*, Dyson *et al.* take us step by step through the fluidic world bridging the nanoscale, where molecular physics is required as our guide, and the microscale where macro continuum laws operate. Jinghong Fan in *Multiscale Analysis of Deformation and Failure of Materials* provides a comprehensive coverage of a wide range of multiscale modelling methods and simulations of the solid state at the atomistic/nano/submicron scales and up through those covering the micro/meso/macroscopic scale. Most recently, *Nano and Cell Mechanics: Fundamentals and Frontiers*, edited by Espinosa and Bao, assembled through their own inputs and those of 47 other experts of their chosen fields of endeavour, 17 timely and exciting chapters that represent the most comprehensive coverage yet presented of all aspects of the mechanics of cells and biomolecules.

In this book edited by Professor Nuno Silvestre, who is well known for his own work in the modelling and simulation of carbon nanotube structures, he has assembled 11 chapters written by international experts that comprehensively cover the experimental, modelling and theoretical studies of the mechanical and thermal properties of carbon nanotubes, polymer nanocomposites and other nanostructures. The research literature on *Computational Nanomechanics* is spread among many journals specialising in mechanics, computer science, materials science and nanotechnology. The latest advances in this rapidly moving field of nanotechnologies have been collected together in a single book!

Although the chapters are primarily intended for established scientists, research engineers and PhD students who have knowledge in materials science and numerical simulation methods, the clarity of writing and pedagogical style of the various chapters make much of this book's content suitable for inclusion in undergraduate and postgraduate courses.

Ronald Pethig
School of Engineering
The University of Edinburgh

Preface

During the last decade, nanomechanics emerged on the crossroads of classical mechanics, solid-state physics, statistical mechanics, materials science, and quantum chemistry. As an area of nanoscience, nanomechanics provides a scientific foundation of nanotechnology, that is, an applied area with a focus on the mechanical properties of engineered nanostructures and nanosystems. Owing to smallness of the studied objects (atomic and molecular systems), nanomechanics also accounts for discreteness of the object, whose size is comparable with the interatomic distances, plurality, but finiteness, of degrees of freedom in the object, thermal fluctuations, entropic effects, and quantum effects. These quantum effects determine forces of interaction between individual atoms in physical objects, which are introduced in nanomechanics by means of some averaged mathematical models called interatomic potentials. Subsequent utilization of the interatomic potentials within the classical multibody dynamics provides deterministic mechanical models of nanostructures and systems at the atomic scale/resolution. This book focuses on a variety of numerical and computational methods to analyze the mechanical behavior of materials and devices, including molecular dynamics, molecular mechanics, and continuum approaches (finite element simulations). In resume, several computational methods exist to model and simulate the behavior of nanostructures. All of them present advantages and drawbacks. This book presents a survey on the computational modeling of the mechanical behavior of nanostructures, with particular emphasis on CNTs, graphene, and composites. It includes 11 chapters and each chapter is an independent contribution by scientists with worldwide expertise and international reputation in the technological area.

In Chapter 1, Y.Y. Zhang, Y. Wang, C.M. Wang, and Y.T. Gu present a state-of-the art review on the thermal conductivity of graphene and its polymer nanocomposites. It is known that some progress has been achieved in producing graphene–polymer nanocomposites with good thermal conductivity, but interfacial thermal resistance at the graphene/polymer interfaces still hinders this improvement. This chapter reports recent research studies, which have shown that covalent and noncovalent functionalization techniques are promising in reducing the interfacial thermal resistance. The authors argue that further in-depth research studies are needed to explore the mechanisms of thermal transport across the graphene/polymer interfaces and achieve graphene–polymer nanocomposites with superior thermal conductivity.

In Chapter 2, M. Kirca and A.C. To describe the mechanics of CNT network materials. Recently, the application of CNTs has been extended to CNT networks in which the CNTs are joined together in two- or three-dimensional space and CNT networks. In this chapter,

a thorough literature review including the most recent theoretical and experimental studies are presented, with a focus on the mechanical characteristics of CNT network materials. As a supporting material, some recent studies of authors are also introduced to provide deeper understanding in mechanical behavior of CNT network materials.

In Chapter 3, H. Shima and Y. Suda present the "Helical carbon nanomaterial," which refers to exotic nanocarbons having a long, thin, and helical morphology. Their spiral shape can be exploited for the development of novel mechanical devices such as highly sensitive tactile nanosensors, nanomechanical resonators, and reinforced nanofibers in high-strain composites. Because the quantitative determination of their mechanical properties and performance in actual applications remains largely unexamined, advanced computational techniques will play an important role, especially for the nanomaterials that hold the promise for use in next-generation nanodevices that have been unfeasible by the current fabrication techniques. This chapter gives a bird's eye view on the mechanical properties of helical carbon nanomaterials, paying particular attention to the latest findings obtained by both theoretical and experimental efforts.

In Chapter 4, G. Ghadyani and M. Rahmandoust present a review of the fundamental concepts of the Newtonian mechanics including Lagrangian and Hamiltonian functions, and then the developed equations of motion of a system with interacting material points are introduced. After that, based on the physics of nanosystems, which can be applicable in any material phases, basic concepts of molecular dynamic simulations are introduced. The link between molecular dynamics and quantum mechanics is explained using a simple classical example of two interacting hydrogen atoms and the major limitations of the simulation method are discussed. Length and timescale limitation of molecular dynamic simulation techniques are the major reasons behind opting multiscale simulations rather than molecular dynamics, which are explained briefly at the final sections of this chapter.

In Chapter 5, a probabilistic strength theory is presented by X. Frank Xu to formulate and model probability distribution for strength of CNTs and CNT fibers. A generalized Weibull distribution is formulated to explain statistical features of CNT strength, and a multiscale method is described to show how to upscale strength distribution from nanoscale CNTs to microscale CNT fibers. The probabilistic theory is considered applicable to fracture strength of all brittle materials, and with certain modifications, to failure of non-brittle materials as well. The benchmark model on strength upscaling from CNTs to fibers indicates that the full potential of CNT fibers for exploitation is expected to be in the range between 10 and 20 GPa with respect to mean strength, due to universal thermodynamic effects and inherent geometric constraints.

In Chapter 6, A. Ghavamian, M. Rahmandoust, and A. Öchsner review and present the latest developments on nanomechanics of perfect and defective heterojunction CNTs. Homogeneous and heterojunction CNTs are of a great importance because of their exceptional properties. In this chapter, the studies on considerable number of different types of perfect and atomically defective heterojunction CNTs with all possible connection types as well as their constructive homogeneous CNTs of different chiralities and configurations are presented and their elastic, torsional, and buckling properties are numerically investigated based on the finite element method with the assumption of linear elastic behavior. They conclude that the atomic defects in the structure of heterojunction CNTs lead to an almost linear decrease in the mechanical stability and strength of heterojunction CNTs, which appeared to be considerably more in the models with carbon vacancy rather than Si-doped models.

In Chapter 7, S. Roy and A. Akepati present a methodology for the prediction of fracture properties in polymer nanocomposites. These authors propose a new methodology to compute J-integral using atomistic data obtained from LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator). As a case study, the feasibility of computing the dynamic atomistic J-integral over the MD domain is evaluated for a graphene nano-platelet with a central crack using OPLS (Optimized Potentials for Liquid Simulations) potential. For model verification, the values of atomistic J-integral are compared with results from linear elastic fracture mechanics (LEFM) for isothermal crack initiation at 300 K. Computational results related to the path-independence of the atomistic J-Integral are also presented. Further, a novel approach that circumvents the complexities of direct computation of entropic contributions in polymers is also discussed.

In Chapter 8, R.E. Roman, N.M. Pugno, and S.W. Cranford characterize the mechanical behavior of 2D nanomaterials and composites. They relate the recent isolation of graphene from graphite with the discovery and synthesis of a multitude of similar two-dimensional crystalline. These single-atom thick materials (2D materials) have shown great promise for emerging nanotechnology applications, and a full understanding of their mechanistic behavior, properties, and failure modes is essential for the successful implementation of 2D materials in design. R.E. Roman, N.M. Pugno, and S.W. Cranford focus on the fundamental nanomechanics of 2D materials, describing how to characterize basic properties such as strength, stiffness, bending rigidity, and adhesion using computational methods such as molecular dynamics (MD). Failure is discussed in terms of the local, atomistic interpretation of quantized fracture mechanics (QFM) and extended to bulk systems via Nanoscale Weibull Statistics (NWS).

In Chapter 9, K. Talukdar studied the effect of chirality on the mechanical properties of defective CNTs. In spite of many existing studies, the experimental values of the mechanical properties of the CNTs vary in magnitude up to one order as the actual internal structure of the CNTs is still not completely known and the properties vary largely with their chirality and size. For better understanding of the internal molecular details, computer modeling and simulation may serve as an important tool, and MD simulations provide the internal dynamical change that the system is running through in course of time under various external forces. In this chapter, a comprehensive investigation is presented to find out the influence of chirality on the defective CNTs.

In Chapter 10, G. Balasubramanian describes the mechanics of thermal transport in mass disordered nanostructures. Its scope is to provide a flavor of a set of computational approaches that are employed to investigate heat transfer mechanisms in mass disordered nanostructures, and in particular those containing isotope impurities. Carbon nanomaterials have been attractive case studies for their remarkable properties. Although the examples below demonstrate effects of isotopes mostly in carbon nanotubes and graphene, the approaches are generic and applicable to a wide array of nanomaterials. This chapter begins from the fundamentals of thermal transport in nanomaterials, moves to engineering material properties and their computation, and finally concludes with data-driven methods for designing defect-engineered nanostructures.

In Chapter 11, D.V. Papavassiliou, K. Bui, and H. Nguyen present a study on the thermal boundary resistance (TBR) effects in CNT composites. In this work, the authors review briefly predictive models for the thermal behavior of CNTs in composites, and simulation efforts to investigate improvements in Keff with an increase in CNT volume fraction. Emphasis is placed in the investigation of the TBR in CNTs coated with silica in order to reduce the overall TBR

of the composites. The authors propose the use of multiwalled CNTs (instead of single-walled CNTs), because heat can be transferred mainly through the outer wall offering the advantage of a larger area of heat transfer. A better approach proposed by the authors might be to design composites where the CNT orientation, when it leads to anisotropic thermal properties, or thermal rectification could be explored.

Finally, the editor would like to thank all authors for having accepted the challenge of writing these chapters and also for they support to achieve this high-quality book. The editor also acknowledges Wiley professionals (Clive Lawson and Anne Hunt) and SPi Global (Durgadevi Shanmughasundaram) for their enthusiastic and professional support.

Nuno Silvestre
Lisbon, May 2015

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