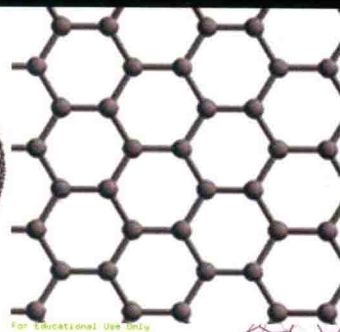
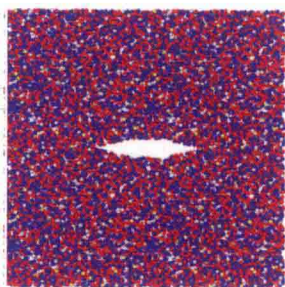
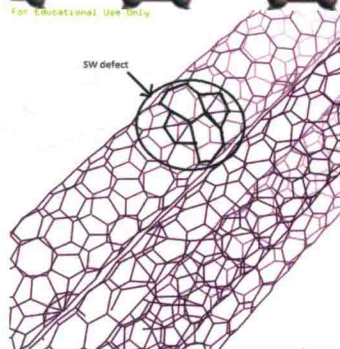
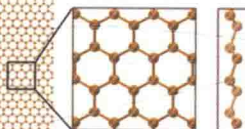
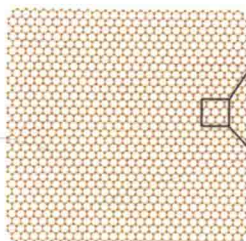
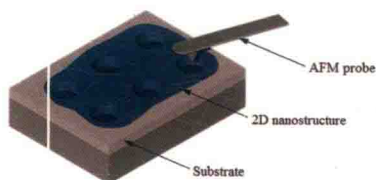


# The Wiley Microsystem and Nanotechnology Series

Ronald Pethig & Horacio Espinosa, Series Editors



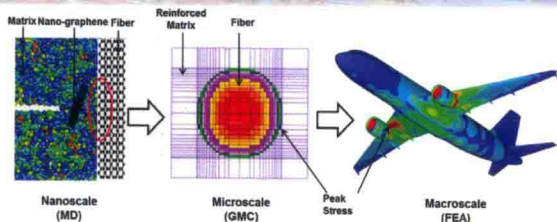
For Educational Use Only



SW defect

# Advanced Computational Nanomechanics

Editor  
NUNO SILVESTRE



WILEY

# ADVANCED COMPUTATIONAL NANOMECHANICS

Edited by

**Nuno Silvestre**

*University of Lisbon  
Portugal*

**WILEY**

This edition first published 2016  
© 2016 John Wiley & Sons Ltd

*Registered office*

John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, United Kingdom

For details of our global editorial offices, for customer services and for information about how to apply for permission to reuse the copyright material in this book please see our website at [www.wiley.com](http://www.wiley.com).

The right of the author to be identified as the author of this work has been asserted in accordance with the Copyright, Designs and Patents Act 1988.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, except as permitted by the UK Copyright, Designs and Patents Act 1988, without the prior permission of the publisher.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic books.

Designations used by companies to distinguish their products are often claimed as trademarks. All brand names and product names used in this book are trade names, service marks, trademarks or registered trademarks of their respective owners. The publisher is not associated with any product or vendor mentioned in this book.

**Limit of Liability/Disclaimer of Warranty:** While the publisher and author have used their best efforts in preparing this book, they make no representations or warranties with respect to the accuracy or completeness of the contents of this book and specifically disclaim any implied warranties of merchantability or fitness for a particular purpose. It is sold on the understanding that the publisher is not engaged in rendering professional services and neither the publisher nor the author shall be liable for damages arising herefrom. If professional advice or other expert assistance is required, the services of a competent professional should be sought

*Library of Congress Cataloging-in-Publication Data*

Advanced computational nanomechanics / edited by Nuno Silvestre.

pages cm

Includes bibliographical references and index.

ISBN 978-1-119-06893-8 (cloth)

1. Nanotechnology--Mathematics. 2. Nanoelectromechanical systems--Mathematical models.  
3. Nanostructures--Mathematical models. 4. Micromechanics--Mathematics. I. Silvestre, Nuno, editor.  
T174.7.A385 2016  
620'.5--dc23

2015035009

A catalogue record for this book is available from the British Library.

Typeset in 10/12pt TimesLTStd by SPi Global, Chennai, India

Printed and bound in Singapore by Markono Print Media Pte Ltd

# **ADVANCED COMPUTATIONAL NANOMECHANICS**

## **Microsystem and Nanotechnology Series**

Series Editors—Ron Pethig and Horacio Dante Espinosa

### **Advanced Computational Nanomechanics**

Silvestre, February 2016

### **Micro-Cutting: Fundamentals and Applications**

Cheng, Huo, August 2013

### **Nanoimprint Technology: Nanotransfer for Thermoplastic and Photocurable Polymer**

Taniguchi, Ito, Mizuno and Saito, August 2013

### **Nano and Cell Mechanics: Fundamentals and Frontiers**

Espinosa and Bao, January 2013

### **Digital Holography for MEMS and Microsystem Metrology**

Asundi, July 2011

### **Multiscale Analysis of Deformation and Failure of Materials**

Fan, December 2010

### **Fluid Properties at Nano/Meso Scale**

Dyson et al., September 2008

### **Introduction to Microsystem Technology**

Gerlach, March 2008

### **AC Electrokinetics: Colloids and Nanoparticles**

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/macroscale. 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 their 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*

# Contents

<b>List of Contributors</b>	<b>xi</b>
<b>Series Preface</b>	<b>xiii</b>
<b>Preface</b>	<b>xv</b>
<b>1 Thermal Conductivity of Graphene and Its Polymer Nanocomposites: A Review</b>	<b>1</b>
<i>Yingyan Zhang, Yu Wang, Chien Ming Wang and Yuantong Gu</i>	
1.1 Introduction	1
1.2 Graphene	1
1.2.1 Introduction of Graphene	1
1.2.2 Properties of Graphene	6
1.2.3 Thermal Conductivity of Graphene	7
1.3 Thermal Conductivity of Graphene–Polymer Nanocomposites	9
1.3.1 Measurement of Thermal Conductivity of Nanocomposites	9
1.3.2 Modelling of Thermal Conductivity of Nanocomposites	9
1.3.3 Progress and Challenge for Graphene–Polymer Nanocomposites	14
1.3.4 Interfacial Thermal Resistance	16
1.3.5 Approaches for Reduction of Interfacial Thermal Resistance	19
1.4 Concluding Remarks	22
References	22
<b>2 Mechanics of CNT Network Materials</b>	<b>29</b>
<i>Mesut Kirca and Albert C. To</i>	
2.1 Introduction	29
2.1.1 Types of CNT Network Materials	30
2.1.2 Synthesis of CNT Network Materials	31
2.1.3 Applications	35
2.2 Experimental Studies on Mechanical Characterization of CNT Network Materials	39
2.2.1 Non-covalent CNT Network Materials	40
2.2.2 Covalently Bonded CNT Network Materials	45

2.3	Theoretical Approaches Toward CNT Network Modeling	48
2.3.1	<i>Ordered CNT Networks</i>	48
2.3.2	<i>Randomly Organized CNT Networks</i>	50
2.4	Molecular Dynamics Study of Heat-Welded CNT Network Materials	55
2.4.1	<i>A Stochastic Algorithm for Modeling Heat-Welded Random CNT Network</i>	56
2.4.2	<i>Tensile Behavior of Heat-Welded CNT Networks</i>	60
	References	65
<b>3</b>	<b>Mechanics of Helical Carbon Nanomaterials</b>	<b>71</b>
	<i>Hiroyuki Shima and Yoshiyuki Suda</i>	
3.1	Introduction	71
3.1.1	<i>Historical Background</i>	71
3.1.2	<i>Classification: Helical “Tube” or “Fiber”?</i>	73
3.1.3	<i>Fabrication and Characterization</i>	74
3.2	Theory of HN-Tubes	76
3.2.1	<i>Microscopic Model</i>	76
3.2.2	<i>Elastic Elongation</i>	79
3.2.3	<i>Giant Stretchability</i>	80
3.2.4	<i>Thermal Transport</i>	82
3.3	Experiment of HN-Fibers	84
3.3.1	<i>Axial Elongation</i>	84
3.3.2	<i>Axial Compression</i>	87
3.3.3	<i>Resonant Vibration</i>	89
3.3.4	<i>Fracture Measurement</i>	92
3.4	Perspective and Possible Applications	93
3.4.1	<i>Reinforcement Fiber for Composites</i>	93
3.4.2	<i>Morphology Control in Synthesis</i>	93
	References	94
<b>4</b>	<b>Computational Nanomechanics Investigation Techniques</b>	<b>99</b>
	<i>Ghasem Ghadyani and Moones Rahmandoust</i>	
4.1	Introduction	99
4.2	Fundamentals of the Nanomechanics	100
4.2.1	<i>Molecular Mechanics</i>	101
4.2.2	<i>Newtonian Mechanics</i>	101
4.2.3	<i>Lagrangian Equations of Motion</i>	102
4.2.4	<i>Hamilton Equations of a <math>\Gamma</math>-Space</i>	104
4.3	Molecular Dynamics Method	106
4.3.1	<i>Interatomic Potentials</i>	106
4.3.2	<i>Link Between Molecular Dynamics and Quantum Mechanics</i>	112
4.3.3	<i>Limitations of Molecular Dynamics Simulations</i>	114
4.4	Tight Binding Method	115
4.5	Hartree–Fock and Related Methods	116
4.6	Density Functional Theory	118

4.7	Multiscale Simulation Methods	120
4.8	Conclusion	120
	References	120
<b>5</b>	<b>Probabilistic Strength Theory of Carbon Nanotubes and Fibers</b>	<b>123</b>
	<i>Xi F. Xu and Irene J. Beyerlein</i>	
5.1	Introduction	123
5.2	A Probabilistic Strength Theory of CNTs	124
5.2.1	<i>Asymptotic Strength Distribution of CNTs</i>	124
5.2.2	<i>Nonasymptotic Strength Distribution of CNTs</i>	127
5.2.3	<i>Incorporation of Physical and Virtual Testing Data</i>	130
5.3	Strength Upscaling from CNTs to CNT Fibers	135
5.3.1	<i>A Local Load Sharing Model</i>	136
5.3.2	<i>Interpretation of CNT Bundle Tensile Testing</i>	139
5.3.3	<i>Strength Upscaling Across CNT-Bundle-Fiber Scales</i>	141
5.4	Conclusion	145
	References	145
<b>6</b>	<b>Numerical Nanomechanics of Perfect and Defective Hetero-junction CNTs</b>	<b>147</b>
	<i>Ali Ghavamian, Moones Rahmandoust and Andreas Öchsner</i>	
6.1	Introduction	147
6.1.1	<i>Literature Review: Mechanical Properties of Homogeneous CNTs</i>	147
6.1.2	<i>Literature Review: Mechanical Properties of Hetero-junction CNTs</i>	150
6.2	Theory and Simulation	152
6.2.1	<i>Atomic Geometry and Finite Element Simulation of Homogeneous CNTs</i>	152
6.2.2	<i>Atomic Geometry and Finite Element Simulation of Hetero-junction CNTs</i>	153
6.2.3	<i>Finite Element Simulation of Atomically Defective Hetero-junction CNTs</i>	155
6.3	Results and Discussion	156
6.3.1	<i>Linear Elastic Properties of Perfect Hetero-junction CNTs</i>	156
6.3.2	<i>Linear Elastic Properties of Atomically Defective Hetero-junction CNTs</i>	162
6.4	Conclusion	164
	References	171
<b>7</b>	<b>A Methodology for the Prediction of Fracture Properties in Polymer Nanocomposites</b>	<b>175</b>
	<i>Samit Roy and Avinash Akepati</i>	
7.1	Introduction	175
7.2	Literature Review	175
7.3	Atomistic <i>J</i> -Integral Evaluation Methodology	176
7.4	Atomistic <i>J</i> -Integral at Finite Temperature	181
7.5	Cohesive Contour-based Approach for <i>J</i> -Integral	184



7.6	Numerical Evaluation of Atomistic $J$ -Integral	185
7.7	Atomistic $J$ -Integral Calculation for a Center-Cracked Nanographene Platelet	187
7.8	Atomistic $J$ -Integral Calculation for a Center-Cracked Nanographene Platelet at Finite Temperature ( $T = 300$ K)	190
7.9	Atomistic $J$ -Integral Calculation for a Center-Cracked Nanographene Platelet Using ReaxFF	192
7.10	Atomistic $J$ -Integral Calculation for a Center-Cracked EPON 862 Model	194
7.11	Conclusions and Future Work	197
	Acknowledgment	198
	References	199
<b>8</b>	<b>Mechanical Characterization of 2D Nanomaterials and Composites</b>	<b>201</b>
	<i>Ruth E. Roman, Nicola M. Pugno and Steven W. Cranford</i>	
8.1	Discovering 2D in a 3D World	201
8.2	2D Nanostructures	203
	8.2.1 <i>Graphene</i>	203
	8.2.2 <i>Graphynes and Graphene Allotropes</i>	204
	8.2.3 <i>Silicene</i>	205
	8.2.4 <i>Boron Nitride</i>	206
	8.2.5 <i>Molybdenum Disulfide</i>	207
	8.2.6 <i>Germanene, Stanene, and Phosphorene</i>	208
8.3	Mechanical Assays	210
	8.3.1 <i>Experimental</i>	210
	8.3.2 <i>Computational</i>	211
8.4	Mechanical Properties and Characterization	212
	8.4.1 <i>Defining Stress</i>	213
	8.4.2 <i>Uniaxial Stress, Plane Stress, and Plane Strain</i>	214
	8.4.3 <i>Stiffness</i>	216
	8.4.4 <i>Effect of Bond Density</i>	218
	8.4.5 <i>Bending Rigidity</i>	219
	8.4.6 <i>Adhesion</i>	222
	8.4.7 <i>Self-Adhesion and Folding</i>	225
8.5	Failure	227
	8.5.1 <i>Quantized Fracture Mechanics</i>	228
	8.5.2 <i>Nanoscale Weibull Statistics</i>	231
8.6	Multilayers and Composites	233
8.7	Conclusion	236
	Acknowledgment	236
	References	237
<b>9</b>	<b>The Effect of Chirality on the Mechanical Properties of Defective Carbon Nanotubes</b>	<b>243</b>
	<i>Keka Talukdar</i>	
9.1	Introduction	243
9.2	Carbon Nanotubes, Their Molecular Structure and Bonding	245
	9.2.1 <i>Diameter and Chiral Angle</i>	245