

# Interdisciplinary Applied Mathematics

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## Volume 23

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Muhammad Sahimi

# Heterogeneous Materials

Nonlinear and Breakdown Properties  
and Atomistic Modeling

With 119 Illustrations



Springer

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*To children of the third world  
who have the talent but not the means to succeed  
and to  
the memory of my father, Habibollah Sahimi,  
who instilled in me, a third world child, the love of reading*

# Preface

Disorder plays a fundamental role in many natural and man-made systems that are of industrial and scientific importance. Of all the disordered systems, heterogeneous materials are perhaps the most heavily utilized in all aspects of our daily lives, and hence have been studied for a long time. With the advent of new experimental techniques, it is now possible to study the morphology of disordered materials and gain a much deeper understanding of their properties. Novel techniques have also allowed us to design materials of morphologies with the properties that are suitable for intended applications.

With the development of a class of powerful theoretical methods, we now have the ability for interpreting the experimental data and predicting many properties of disordered materials at many length scales. Included in this class are renormalization group theory, various versions of effective-medium approximation, percolation theory, variational principles that lead to rigorous bounds to the effective properties, and Green function formulations and perturbation expansions. The theoretical developments have been accompanied by a tremendous increase in the computational power and the emergence of massively parallel computational strategies. Hence, we are now able to model many materials at molecular scales and predict many of their properties based on first-principle computations.

In this two-volume book we describe and discuss various theoretical and computational approaches for understanding and predicting the effective macroscopic properties of heterogeneous materials. Most of the book is devoted to comparing and contrasting the two main classes of, and approaches to, disordered materials, namely, the continuum models and the discrete models. Predicting the effective properties of composite materials based on the continuum models, which are based on solving the classical continuum equations of transport, has a long history and goes back to at least the middle of the nineteenth century. Even a glance at the literature on the subject of heterogeneous materials will reveal the tremendous amount of work that has been carried out in the area of continuum modeling. Rarely, however, can such continuum models provide accurate predictions of the effective macroscopic properties of *strongly* disordered multiphase materials. In particular, if the contrast between the properties of a material's phases is large, and the phases form large clusters, most continuum models break down. At the same time, due to their very nature, the discrete models, which are based on a lattice representation of a material's morphology, have the ability for providing accurate predictions for the effective properties of heterogeneous materials, even when the heterogeneities are strong, while another class of discrete models, that represent a material as a collection of its constituent atoms and molecules, provides accurate predictions of

the material's properties at mesoscopic scales, and thus, in this sense, the discrete models are complementary to the continuum models. The last three decades of the twentieth century witnessed great advances in discrete modeling of materials and predicting their macroscopic properties, and one main goal of this book is to describe these advances and compare their predictions with those of the continuum models. In Volume I we consider characterization and modeling of the morphology of disordered materials, and describe theoretical and computational approaches for predicting their *linear* transport and optical properties, while Volume II focuses on nonlinear properties, and fracture and breakdown of disordered materials, in addition to describing their atomistic modeling. Some of the theoretical and computational approaches are rather old, while others are very new, and therefore we attempt to take the reader through a journey to see the history of the development of the subjects that are discussed in this book. Most importantly, we always compare the predictions with the relevant experimental data in order to gain a better understanding of the strengths and/or shortcomings of the two classes of models.

A large number of people have helped me gain deeper understanding of the topics discussed in this book, and hence have helped me to write about them. Not being able to name them all, I limit myself to a few of them who, directly or indirectly, influenced the style and contents of this book. Dietrich Stauffer has greatly contributed to my understanding of percolation theory, disordered media, and critical phenomena, some of the main themes of this book; I am deeply grateful to him. For their tireless help in the preparation of various portions of this book, I would like to thank two of my graduate students, Sushma Dhulipala and Alberto Schroth. Although they may not be aware of it, Professors Pedro Ponte Castañeda of the University of Pennsylvania and Salvatore Torquato of Princeton University provided great help by guiding me through their excellent work, which is described in this book; I would like to thank them both. Some of my own work described in this book has been carried out in collaboration with many people; I am pleased to acknowledge their great contributions, especially those of Dr. Sepehr Arbabi, my former doctoral student. The constant encouragement and support offered by many of my colleagues, a list of whom is too long to be given here, are also gratefully acknowledged. I would like particularly to express my deep gratitude to my former doctoral student Dr. Jaleh Ghassemzadeh, who provided me with critical help at all stages of preparation of this book. Several chapters of this book have been used, in their preliminary versions, in some of the courses that I teach, and I would like to acknowledge the comments that I received from my students.

My wife, Mahnoush, and son, Ali, put up with the countless hours, days, weeks, and months that I spent in preparing this book and my almost complete absence during the time that I was writing, but never denied me their love and support without which this book would have never been completed; I love and cherish them both.

Muhammad Sahimi  
Los Angeles, California, USA  
May 2002

# Contents

<b>Preface</b>	<b>vii</b>
<b>Abbreviated Contents for Volume I</b>	<b>x</b>
<b>Introduction to Volume II</b>	<b>1</b>
<b>1 Characterization of Surface Morphology</b>	<b>6</b>
1.0 Introduction . . . . .	6
1.1 Self-Similar Fractal Structures . . . . .	7
1.2 The Correlation Function . . . . .	9
1.3 Rough Surfaces: Self-affine Fractals . . . . .	10
1.4 Generation of Rough Surfaces: Fractional Brownian Motion . . . . .	11
1.4.1 The Power-Spectrum Method . . . . .	12
1.4.2 Successive Random Additions . . . . .	15
1.4.3 The Weierstrass–Mandelbrot Algorithm . . . . .	15
1.5 Scaling Properties of Rough Surfaces . . . . .	16
1.6 Modeling of Growth of Thin Films with Rough Surface . . . . .	19
1.7 Measurement of Roughness Exponent . . . . .	22
Summary . . . . .	23
<b>I Effective Properties of Heterogeneous Materials with Constitutive Nonlinearities</b>	<b>25</b>
<b>2 Nonlinear Conductivity and Dielectric Constant: The Continuum Approach</b>	<b>27</b>
2.0 Introduction . . . . .	27
2.1 Variational Principles . . . . .	29
2.2 Bounds on the Effective Energy Function . . . . .	34
2.2.1 Lower Bounds . . . . .	35
2.2.1.1 One-Point Bounds . . . . .	35
2.2.1.2 Two-Point Bounds . . . . .	36
2.2.1.3 Three-Point Bounds . . . . .	38
2.2.2 Approximate Estimates of the Effective Energy . . . . .	39
2.2.2.1 Conductor– Superconductor Composites . . . . .	39
2.2.2.2 Conductor–Insulator Composites . . . . .	40



2.2.3	Upper Bounds and Estimates . . . . .	40
2.3	Exact Results for Laminates . . . . .	42
2.4	Effective Dielectric Constant of Strongly Nonlinear Materials . . . . .	45
2.4.1	Inclusions with Infinite Dielectric Constant . . . . .	46
2.4.2	Inclusions with Zero Dielectric Constant . . . . .	47
2.5	Effective Conductivity of Nonlinear Materials . . . . .	47
2.5.1	Materials with Nonlinear Isotropic Phases . . . . .	48
2.5.2	Strongly Nonlinear Materials with Isotropic Phases . . . . .	50
2.6	Second-Order Exact Results . . . . .	53
2.6.1	Strongly Nonlinear Isotropic Materials . . . . .	55
2.6.1.1	The Maxwell–Garnett Estimates . . . . .	56
2.6.1.2	Effective-Medium Approximation Estimates . . . . .	57
2.6.2	Conductor–Superconductor Composites . . . . .	58
2.6.3	Conductor–Insulator Composites . . . . .	58
2.6.4	General Two-Phase Materials . . . . .	60
	Summary . . . . .	62

**3 Nonlinear Conductivity, Dielectric Constant, and  
Optical Properties: The Discrete Approach 64**

3.0	Introduction . . . . .	64
3.1	Strongly Nonlinear Composites . . . . .	64
3.1.1	Exact Solution for Bethe Lattices . . . . .	66
3.1.1.1	Microscopic Versus Macroscopic Conductivity . . . . .	68
3.1.1.2	Effective-Medium Approximation for Bethe Lattices . . . . .	71
3.1.2	Effective-Medium Approximation for Three-Dimensional Materials . . . . .	71
3.1.3	The Decoupling Approximation . . . . .	75
3.1.4	Perturbation Expansion . . . . .	76
3.1.5	Variational Approach . . . . .	76
3.1.6	Exact Duality Relations . . . . .	77
3.1.7	Scaling Properties . . . . .	79
3.1.7.1	Series Expansion Analysis . . . . .	81
3.1.7.2	Field-Theoretic Approach . . . . .	82
3.1.8	Resistance Noise, Moments of Current Distribution, and Scaling Properties . . . . .	83
3.2	Nonlinear Transport Caused by a Large External Field . . . . .	85
3.3	Weakly Nonlinear Composites . . . . .	89
3.3.1	Effective-Medium Approximation . . . . .	90

3.3.2	Resistance Noise, Moments of Current Distribution, and Scaling Properties . . . . .	93
3.3.3	Crossover from Linear to Weakly Nonlinear Conductivity . . . . .	97
3.3.4	Exact Duality Relations . . . . .	99
3.3.5	Comparison with the Experimental Data . . . . .	101
3.4	Dielectric Constant of Weakly Nonlinear Composites . . . . .	103
3.4.1	Exact Results . . . . .	104
3.4.2	Effective-Medium Approximation . . . . .	105
3.4.3	The Maxwell–Garnett Approximation . . . . .	105
3.5	Electromagnetic Field Fluctuations and Optical Nonlinearities . . . . .	106
3.5.1	Scaling Properties of Moments of the Electric Field . . . . .	109
3.5.1.1	Distribution of Electric Fields in Strongly Disordered Composites . . . . .	110
3.5.1.2	Moments of the Electric Field . . . . .	116
3.5.1.3	Field Fluctuations at Frequencies Below the Resonance . . . . .	118
3.5.1.4	Computer Simulation . . . . .	122
3.5.1.5	Comparison with the Experimental Data . . . . .	124
3.5.2	Anomalous Light Scattering from Semicontinuous Metal Films . . . . .	125
3.5.2.1	Rayleigh Scattering . . . . .	126
3.5.2.2	Scaling Properties of the Correlation Function . . . . .	128
3.5.3	Surface-Enhanced Raman Scattering . . . . .	130
3.5.3.1	General Formulation . . . . .	131
3.5.3.2	Raman and Hyper-Raman Scattering in Metal–Dielectric Composites . . . . .	133
3.5.3.3	Comparison with the Experimental Data . . . . .	135
3.5.4	Enhancement of Optical Nonlinearities in Metal–Dielectric Composites . . . . .	135
3.5.4.1	Kerr Optical Nonlinearities . . . . .	135
3.5.4.2	Enhancement of Nonlinear Scattering from Strongly Disordered Films . . . . .	139
3.5.4.3	Comparison with the Experimental Data . . . . .	143
3.6	Electromagnetic Properties of Solid Composites . . . . .	143
3.6.1	Effective-Medium Approximation . . . . .	144
3.7	Beyond the Quasi-static Approximation: Generalized Ohm’s Law	149
3.8	Piecewise Linear Transport Processes . . . . .	157
3.8.1	Computer Simulation . . . . .	159

3.8.2	Scaling Properties . . . . .	160
3.8.3	Effective-Medium Approximation . . . . .	160
	Summary . . . . .	163

**4 Nonlinear Rigidity and Elastic Moduli:**

	<b>The Continuum Approach</b>	<b>164</b>
4.0	Introduction . . . . .	164
4.1	Constitutive Relations and Potentials . . . . .	165
4.2	Formulation of the Problem . . . . .	169
4.3	The Classical Variational Principles . . . . .	170
	4.3.1 One-Point Bounds . . . . .	172
	4.3.2 Two-Point Bounds: The Talbot–Willis Method . . . . .	172
4.4	Variational Principles Based on a Linear Comparison Material . . . . .	175
	4.4.1 Materials with Isotropic Phases . . . . .	176
	4.4.2 Strongly Nonlinear Materials . . . . .	178
	4.4.3 Materials with Anisotropic Phases . . . . .	178
	4.4.3.1 Polycrystalline Materials . . . . .	179
	4.4.3.2 Strongly Nonlinear Materials . . . . .	180
	4.4.3.3 Materials with Isotropic and Strongly Nonlinear Phases . . . . .	181
	4.4.3.4 Strongly Nonlinear Polycrystalline Materials . . . . .	181
	4.4.3.5 Ideally Plastic Materials . . . . .	182
4.5	Bounds with Piecewise Constant Elastic Moduli . . . . .	182
	4.5.1 Materials with Isotropic Phases . . . . .	183
	4.5.2 Polycrystalline Materials . . . . .	184
4.6	Second-Order Exact Results . . . . .	186
	4.6.1 Weak-Contrast Expansion . . . . .	186
	4.6.2 Strong-Contrast Expansion . . . . .	188
4.7	Applications of Second-Order Exact Results . . . . .	192
	4.7.1 Porous Materials . . . . .	192
	4.7.1.1 Two-Point Bounds . . . . .	193
	4.7.1.2 Three-Point Bounds . . . . .	194
	4.7.2 Rigidly Reinforced Materials . . . . .	195
	4.7.2.1 Two-Point Bounds . . . . .	196
	4.7.2.2 Three-Point Bounds and Estimates . . . . .	197
	4.7.3 Completely Plastic Materials . . . . .	198
4.8	Other Theoretical Methods . . . . .	202
4.9	Critique of the Variational Procedure . . . . .	203
	Summary . . . . .	204

<b>II</b>	<b>Fracture and Breakdown of Heterogeneous Materials</b>	<b>207</b>
<b>5</b>	<b>Electrical and Dielectric Breakdown: The Discrete Approach</b>	<b>209</b>
5.0	Introduction . . . . .	209
5.1	Continuum Models of Dielectric Breakdown . . . . .	211
5.1.1	Griffith-like Criterion and the Analogy with Brittle Fracture . . . . .	212
5.1.2	Computer Simulation . . . . .	215
5.2	Discrete Models of Electrical Breakdown . . . . .	215
5.2.1	The Dilute Limit . . . . .	216
5.2.2	The Effect of Sample Size . . . . .	217
5.2.3	Electrical Failure in Strongly Disordered Materials . . . . .	218
5.2.4	Computer Simulation . . . . .	220
5.2.5	Distribution of the Failure Currents . . . . .	222
5.2.6	The Effect of Failure Thresholds . . . . .	224
5.2.7	Dynamical and Thermal Aspects of Electrical Breakdown . . . . .	226
5.2.7.1	Discrete Dynamical Models . . . . .	227
5.2.7.2	Breakdown in an AC Field: Thermal Effects . . . . .	230
5.2.7.3	Comparison with the Experimental Data . . . . .	232
5.3	Electromigration Phenomena and the Minimum Gap . . . . .	234
5.4	Dielectric Breakdown . . . . .	237
5.4.1	Exact Duality Relation . . . . .	237
5.4.2	Stochastic Models . . . . .	238
5.4.3	Deterministic Models . . . . .	241
5.4.3.1	Scaling Properties of Dielectric Breakdown . . . . .	243
5.4.3.2	Distribution of Breakdown Fields . . . . .	245
5.4.4	Comparison with the Experimental Data . . . . .	247
	Summary . . . . .	248
<b>6</b>	<b>Fracture: Basic Concepts and Experimental Techniques</b>	<b>249</b>
6.0	Introduction . . . . .	249
6.1	Historical Background . . . . .	250
6.2	Fracture of a Homogeneous Solid . . . . .	252
6.3	Introduction of Heterogeneity . . . . .	253
6.4	Brittle Versus Ductile Materials . . . . .	254
6.5	Mechanisms of Fracture . . . . .	255
6.5.1	Elastic Incompatibility . . . . .	255
6.5.2	Plastic Deformation . . . . .	255
6.5.3	Coalescence of Plastic Cavities . . . . .	256

6.5.4	Cracks Initiated by Thin Brittle Films . . . . .	256
6.5.5	Crazing . . . . .	257
6.5.6	Boundary Sliding . . . . .	257
6.6	Conventional Fracture Modes . . . . .	257
6.7	Stress Concentration and Griffith's Criterion . . . . .	258
6.8	The Stress Intensity Factor and Fracture Toughness . . . . .	261
6.9	Classification of the Regions Around the Crack Tip . . . . .	263
6.10	Dynamic Fracture . . . . .	265
6.11	Experimental Methods in Dynamic Fracture . . . . .	266
6.11.1	Application of External Stress . . . . .	266
6.11.1.1	Static Stress . . . . .	266
6.11.1.2	Initiation of Fractures . . . . .	268
6.11.1.3	Dynamic Stress . . . . .	268
6.11.2	Direct Measurement of the Stress Intensity Factor . . . . .	269
6.11.2.1	The Method of Caustics . . . . .	269
6.11.2.2	Photoelasticity . . . . .	269
6.11.3	Direct Measurement of Energy . . . . .	270
6.11.4	Measurement of Fracture Velocity . . . . .	270
6.11.4.1	High-Speed Photography . . . . .	270
6.11.4.2	Measurement of Resistivity . . . . .	271
6.11.4.3	Ultrasonic Measurements . . . . .	271
6.11.5	Measurement of the Thermal Effects . . . . .	272
6.11.6	Measurement of Acoustic Emissions of Fractures . . . . .	272
6.12	Oscillatory Fracture Patterns . . . . .	273
6.13	Mirror, Mist, and Hackle Pattern on a Fracture Surface . . . . .	275
6.14	Roughness of Fracture Surfaces . . . . .	277
6.14.1	Measurement of Roughness of Fracture Surface . . . . .	279
6.14.2	Mechanisms of Surface Roughness Generation . . . . .	283
6.14.2.1	Growth of Microcracks . . . . .	283
6.14.2.2	Plastic Deformation . . . . .	284
6.14.2.3	Macroscopic Branching and Bifurcation . . . . .	284
6.15	Cleavage of Crystalline Materials . . . . .	284
6.16	Fracture Properties of Materials . . . . .	286
6.16.1	Polymeric Materials . . . . .	287
6.16.2	Ceramics . . . . .	288
6.16.3	Metals . . . . .	289
6.16.4	Fiber-Reinforced Composites . . . . .	290
6.16.5	Metal-Matrix Composites . . . . .	290
	Summary . . . . .	291
<b>7</b>	<b>Brittle Fracture: The Continuum Approach</b>	<b>292</b>
7.0	Introduction . . . . .	292

7.1	Scaling Analysis . . . . .	294
7.1.1	Scaling Analysis of Materials Strength . . . . .	294
7.1.2	Scaling Analysis of Dynamic Fracture . . . . .	295
7.2	Continuum Formulation of Fracture Mechanics . . . . .	298
7.2.1	Dissipation and the Cohesive Zone . . . . .	298
7.2.2	Universal Singularities near the Fracture Tip . . . . .	299
7.3	Linear Continuum Theory of Elasticity . . . . .	300
7.3.1	Static Fractures in Mode III . . . . .	303
7.3.2	Dynamic Fractures in Mode I . . . . .	304
7.4	The Onset of Fracture Propagation: Griffith's Criterion . . . . .	308
7.5	The Equation of Motion for a Fracture in an Infinite Plate . . . . .	311
7.5.1	Mode III . . . . .	314
7.5.2	Mode I . . . . .	316
7.6	The Path of a Fracture . . . . .	318
7.6.1	Planar Quasi-static Fractures: Principle of Local Symmetry . . . . .	318
7.6.2	Three-Dimensional Quasi-static Fractures . . . . .	319
7.6.3	Dynamic Fractures: Yoffe's Criterion . . . . .	320
7.7	Comparison with the Experimental Data . . . . .	321
7.7.1	The Limiting Velocity of a Fracture . . . . .	323
7.8	Beyond Linear Continuum Fracture Mechanics . . . . .	325
7.8.1	The Dissipated Heat . . . . .	325
7.8.2	The Structure of Fracture Surface . . . . .	327
7.8.3	Topography of Fracture Surface . . . . .	327
7.8.4	Properties of Fracture Surface . . . . .	327
7.8.5	Conic Markings on Fracture Surface . . . . .	328
7.8.6	Riblike Patterns on Fracture Surface . . . . .	329
7.8.7	Roughness of Fracture Surface . . . . .	329
7.8.8	Modeling Rough Fracture Surfaces . . . . .	332
7.8.9	Fracture Branching at Microscopic Scales . . . . .	334
7.8.10	Multiple Fractures Due to Formation and Coalescence of Microscopic Voids . . . . .	334
7.8.11	Microscopic Versus Macroscopic Fracture Branching . . . . .	335
7.8.12	Nonuniqueness of the Stress Intensity Factor . . . . .	336
7.8.13	Dependence of the Fracture Energy on Crack Velocity . . . . .	336
7.8.14	Generalized Griffith Criterion for Fractures with Self-Affine Surfaces . . . . .	337
7.8.15	Crack Propagation Faster Than the Rayleigh Wave Speed . . . . .	340
7.9	Shortcomings of Linear Continuum Fracture Mechanics . . . . .	342

7.10	Instability in Dynamic Fracture of Isotropic Amorphous Materials . . . . .	342
7.10.1	The Onset of Velocity Oscillations . . . . .	343
7.10.2	Relation Between Surface Structure and Dynamical Instability . . . . .	344
7.10.3	Mechanism of the Dynamical Instability . . . . .	345
7.10.4	Universality of Microbranch Profiles . . . . .	347
7.10.5	Crossover from Three-Dimensional to Two-Dimensional Behavior . . . . .	347
7.10.6	Energy Dissipation . . . . .	348
7.10.7	Universality of the Dynamical Instability . . . . .	349
7.11	Models of the Cohesive Zone . . . . .	349
7.11.1	The Barenblatt–Dugdale Model . . . . .	350
7.11.2	Two-Field Continuum Models . . . . .	351
7.11.3	Finite-Element Simulation . . . . .	354
7.11.4	Fracture Propagation in Three Dimensions . . . . .	357
7.11.5	Failure of Dynamic Models of Cohesive Zone . . . . .	362
7.12	Brittle-to-Ductile Transition . . . . .	363
	Summary . . . . .	366
<b>8</b>	<b>Brittle Fracture: The Discrete Approach</b>	<b>367</b>
8.0	Introduction . . . . .	367
8.1	Quasi-static Fracture of Fibrous Materials . . . . .	371
8.1.1	Equal-Load-Sharing (Democratic) Models . . . . .	372
8.1.2	Local-Load-Sharing Models . . . . .	375
8.1.3	Computer Simulation . . . . .	381
8.1.4	Mean-Field and Effective-Medium Approximations . . . . .	384
8.2	Quasi-static Fracture of Heterogeneous Materials . . . . .	390
8.2.1	Lattice Models . . . . .	391
8.2.1.1	Shape of the Macroscopic Fracture . . . . .	397
8.2.1.2	Dependence of the Elastic Moduli on the Extent of Cracking . . . . .	400
8.2.1.3	Fracture Strength of Materials with Strong Disorder . . . . .	402
8.2.1.4	Distribution of Fracture Strength . . . . .	405
8.2.1.5	Size-Dependence of Fracture Properties . . . . .	408
8.2.2	Comparison with the Experimental Data . . . . .	412
8.2.3	Percolation Versus Quasi-static Brittle Fracture . . . . .	413
8.2.4	Universal Fixed Points in Quasi-static Brittle Fracture . . . . .	416
8.3	Dynamic Brittle Fracture . . . . .	421
8.3.1	Dynamic Fracture in Mode I . . . . .	424
8.3.2	Dynamic Fracture in Mode III . . . . .	426

8.3.2.1	Phonon Emission . . . . .	434
8.3.2.2	Forbidden Fracture Velocities . . . . .	436
8.3.2.3	Nonlinear Instabilities . . . . .	436
8.3.2.4	The Connection to the Yoffe's Criterion . . . . .	437
8.3.3	The Effect of Quenched Disorder . . . . .	438
8.3.4	Comparison with the Experimental Data . . . . .	442
8.4	Fracture of a Brittle Material by an Impact . . . . .	443
8.5	Dynamic Fracture of Materials with Annealed Disorder . . . . .	446
8.6	Fracture of Polymeric Materials . . . . .	448
8.7	Fracture of Thin Solid Films . . . . .	451
	Summary . . . . .	453

### **III Atomistic and Multiscale Modeling of Materials 455**

<b>9</b>	<b>Atomistic Modeling of Materials</b>	<b>457</b>
9.0	Introduction . . . . .	457
9.1	Density-Functional Theory . . . . .	461
9.1.1	Local-Density Approximation . . . . .	464
9.1.2	Generalized Gradient Approximation . . . . .	466
9.1.3	Nonperiodic Systems . . . . .	467
9.1.4	Pseudopotential Approximation . . . . .	467
9.2	Classical Molecular Dynamics Simulation . . . . .	471
9.2.1	Basic Principles . . . . .	472
9.2.2	Evaluation of Molecular Forces in a Periodic System . . . . .	476
9.2.3	The Verlet and Leapfrog Algorithms . . . . .	477
9.2.4	Constant-Energy Ensembles . . . . .	479
9.2.5	Constant-Temperature Ensembles . . . . .	479
9.2.6	Constant-Pressure and Temperature Ensembles . . . . .	481
9.2.7	Simulation of Rigid and Semirigid Molecules . . . . .	481
9.2.8	Ion–Ion Interactions . . . . .	486
9.3	Nonequilibrium Molecular Dynamics Simulation . . . . .	490
9.4	Quantum Molecular Dynamics Simulation: The Car–Parrinello Method . . . . .	494
9.4.1	The Equations of Motion . . . . .	495
9.4.2	The Verlet Algorithm . . . . .	496
9.4.3	The Kohn–Sham Eigenstates and Orthogonalization of the Wave Functions . . . . .	497
9.4.4	Dynamics of the Ions and the Unit Cell . . . . .	498
9.4.4.1	The Hellmann–Feynman Theorem . . . . .	499
9.4.4.2	Pulay Forces and Stresses . . . . .	500
9.4.4.3	The Structure Factor and Total Ionic Potential . . . . .	501



9.4.5	Computational Procedure for Quantum Molecular Dynamics . . . . .	502
9.4.6	Linear System-Size Scaling . . . . .	506
9.4.7	Extensions of the Car–Parrinello Quantum Molecular Dynamics Method . . . . .	506
9.4.8	Tight-Binding Methods . . . . .	507
9.5	Direct Minimization of Total Energy . . . . .	507
9.5.1	The Steepest-Descent Method . . . . .	508
9.5.2	The Conjugate-Gradient Method . . . . .	508
9.5.3	Minimizing the Total Energy by the Conjugate-Gradient Method . . . . .	509
9.6	Vectorized and Massively-Parallel Molecular Dynamics Simulation . . . . .	513
9.6.1	Vectorized Molecular Dynamics Algorithms . . . . .	513
9.6.2	Massively-Parallel Molecular Dynamics Algorithms . . . . .	514
9.6.2.1	Atom-Decomposition Algorithms . . . . .	515
9.6.2.2	Force-Decomposition Algorithms . . . . .	517
9.6.2.3	Spatial-Decomposition Algorithms . . . . .	519
9.6.2.4	Load Balance in Massively-Parallel Molecular Dynamics Simulation . . . . .	521
9.6.2.5	Selecting a Massively-Parallel Molecular Dynamics Algorithm . . . . .	522
9.7	Interatomic Interaction Potentials . . . . .	523
9.7.1	The Embedded-Atom Model . . . . .	524
9.7.2	The Stillinger–Weber Potential . . . . .	527
9.7.3	The Tersoff Potentials . . . . .	529
9.7.4	The Brenner Potentials . . . . .	533
9.7.5	Other Interaction Potentials . . . . .	537
9.8	Molecular Dynamics Simulation of Fracture Propagation . . . . .	538
9.8.1	Early Simulations . . . . .	540
9.8.2	Large Size and Scalable Molecular Dynamics Simulation of Fracture . . . . .	544
9.8.3	Comparison with the Experimental Observations . . . . .	546
9.8.3.1	Fracture Instabilities . . . . .	546
9.8.3.2	Morphology of Fracture Surface . . . . .	548
9.8.3.3	Fracture Propagation Faster Than the Rayleigh Wave Speed . . . . .	549
	Summary . . . . .	550

<b>10</b>	<b>Multiscale Modeling of Materials: Joining Atomistic Models with Continuum Mechanics</b>	<b>551</b>
10.0	Introduction . . . . .	551
10.1	Multiscale Modeling . . . . .	554

10.1.1	Sequential Multiscale Approach: Atomistically-Informed Continuum Models . . . . .	554
10.1.2	Parallel Multiscale Approach . . . . .	556
10.2	Defects in Solids: Joining Finite-Element and Atomistic Computations . . . . .	557
10.2.1	The Quasi-continuum Formulation . . . . .	559
10.2.2	Constitutive Models . . . . .	563
10.2.3	The Atomistic Model . . . . .	563
10.2.4	Field Equations and Their Spatial Discretization . . . . .	563
10.2.5	Local Quasi-continuum Formulation . . . . .	565
10.2.6	Nonlocal Quasi-continuum Formulation . . . . .	567
10.2.7	The Criterion for Nonlocality of Elements . . . . .	568
10.2.8	Application to Stacking Faults in FCC Crystals . . . . .	570
10.2.9	Application to Nanoindentation . . . . .	573
10.3	Fracture Dynamics: Joining Tight-Binding, Molecular Dynamics, and Finite-Element Computations . . . . .	576
10.3.1	The Overall Hamiltonian . . . . .	576
10.3.2	The Tight-Binding Region . . . . .	577
10.3.3	Molecular Dynamics Simulation . . . . .	578
10.3.4	Finite-Element Simulation . . . . .	579
10.3.5	Interfacing Finite-Element and Molecular Dynamics Regions . . . . .	581
10.3.6	Interfacing Molecular Dynamics and Tight-Binding Regions . . . . .	584
10.3.7	Seamless Simulation . . . . .	587
10.3.8	Multiscale Simulation of Fracture Propagation in Silicon . . . . .	587
10.4	Other Applications of Multiscale Modeling . . . . .	588
10.4.1	Atomistically Induced Stress Distributions in Composite Materials . . . . .	588
10.4.2	Chemical Vapor Deposition . . . . .	589
	Summary . . . . .	590

**References 593**

**Index 633**

# Abbreviated Contents for Volume I

Preface

Abbreviated Contents for Volume II

- 1 Introduction
- I Characterization and Modeling of the Morphology
  - 2 Characterization of Connectivity and Clustering
  - 3 Characterization and Modeling of the Morphology
- II Linear Transport and Optical Properties
  - 4 Effective Conductivity, Dielectric Constant, and Optical Properties: The Continuum Approach
  - 5 Effective Conductivity and Dielectric Constant: The Discrete Approach
  - 6 Frequency-Dependent Properties: The Discrete Approach
  - 7 Rigidity and Elastic Properties: The Continuum Approach
  - 8 Rigidity and Elastic Properties: The Discrete Approach
  - 9 Rigidity and Elastic Properties of Network Glasses, Polymers, and Composite Solids: The Discrete Approach

References

Index