

Contents

Preface	xi
1 Introduction	1
1.1 Potential of Nanoscale Engineering	1
1.2 Motivation for Multiple Scale Modeling	2
1.3 Educational Approach	5
2 Classical Molecular Dynamics	7
2.1 Mechanics of a System of Particles	7
2.1.1 Generalized Coordinates	8
2.1.2 Mechanical Forces and Potential Energy	8
2.1.3 Lagrange Equations of Motion	10
2.1.4 Integrals of Motion and Symmetric Fields	12
2.1.5 Newtonian Equations	13
2.1.6 Examples	14
2.2 Molecular Forces	17
2.2.1 External Fields	18
2.2.2 Pair-Wise Interaction	20
2.2.3 Multibody Interaction	24
2.2.4 Exercises	26
2.3 Molecular Dynamics Applications	28
3 Lattice Mechanics	37
3.1 Elements of Lattice Symmetries	37
3.1.1 Bravais Lattices	38
3.1.2 Basic Symmetry Principles	40
3.1.3 Crystallographic Directions and Planes	42
3.2 Equation of Motion of a Regular Lattice	42
3.2.1 Unit Cell and the Associate Substructure	43
3.2.2 Lattice Lagrangian and Equations of Motion	45
3.2.3 Examples	47
3.3 Transforms	49
3.3.1 Fourier Transform	50
3.3.2 Laplace Transform	51
3.3.3 Discrete Fourier Transform	53

3.4	Standing Waves in Lattices	54
3.4.1	Normal Modes and Dispersion Branches	55
3.4.2	Examples	57
3.5	Green's Function Methods	58
3.5.1	Solution for a Unit Pulse	59
3.5.2	Free Lattice with Initial Perturbations	61
3.5.3	Solution for Arbitrary Dynamic Loads	61
3.5.4	General Inhomogeneous Solution	62
3.5.5	Boundary Value Problems and the Time History Kernel	62
3.5.6	Examples	65
3.6	Quasi-Static Approximation	66
3.6.1	Equilibrium State Equation	66
3.6.2	Quasi-Static Green's Function	67
3.6.3	Multiscale Boundary Conditions	67
4	Methods of Thermodynamics and Statistical Mechanics	79
4.1	Basic Results of the Thermodynamic Method	80
4.1.1	State Equations	81
4.1.2	Energy Conservation Principle	84
4.1.3	Entropy and the Second Law of Thermodynamics	86
4.1.4	Nernst's Postulate	88
4.1.5	Thermodynamic Potentials	89
4.2	Statistics of Multiparticle Systems in Thermodynamic Equilibrium	91
4.2.1	Hamiltonian Formulation	92
4.2.2	Statistical Description of Multiparticle Systems	93
4.2.3	Microcanonical Ensemble	97
4.2.4	Canonical Ensemble	101
4.2.5	Maxwell–Boltzmann Distribution	104
4.2.6	Thermal Properties of Periodic Lattices	107
4.3	Numerical Heat Bath Techniques	111
4.3.1	Berendsen Thermostat	112
4.3.2	Nosé–Hoover Heat Bath	118
4.3.3	Phonon Method for Solid–Solid Interfaces	119
5	Introduction to Multiple Scale Modeling	123
5.1	MAAD	124
5.2	Coarse-Grained Molecular Dynamics	126
5.3	Quasi-Continuum Method	126
5.4	CADD	128
5.5	Bridging Domain	129
6	Introduction to Bridging Scale	131
6.1	Bridging Scale Fundamentals	131
6.1.1	Multiscale Equations of Motion	133
6.2	Removing Fine Scale Degrees of Freedom in Coarse Scale Region	136
6.2.1	Relationship of Lattice Mechanics to Finite Elements	137
6.2.2	Linearized MD Equation of Motion	139

6.2.3	Elimination of Fine Scale Degrees of Freedom	141
6.2.4	Commentary on Reduced Multiscale Formulation	143
6.2.5	Elimination of Fine Scale Degrees of Freedom: 3D Generalization	143
6.2.6	Numerical Implementation of Impedance Force	150
6.2.7	Numerical Implementation of Coupling Force	151
6.3	Discussion on the Damping Kernel Technique	152
6.3.1	Programming Algorithm for Time History Kernel	157
6.4	Cauchy–Born Rule	158
6.5	Virtual Atom Cluster Method	159
6.5.1	Motivations and General Formulation	159
6.5.2	General Idea of the VAC Model	163
6.5.3	Three-Way Concurrent Coupling with QM Method	164
6.5.4	Tight-Binding Method for Carbon Systems	167
6.5.5	Coupling with the VAC Model	169
6.6	Staggered Time Integration Algorithm	170
6.6.1	MD Update	170
6.6.2	FE Update	172
6.7	Summary of Bridging Scale Equations	172
6.8	Discussion on the Bridging Scale Method	173
7	Bridging Scale Numerical Examples	175
7.1	Comments on Time History Kernel	175
7.2	1D Bridging Scale Numerical Examples	176
7.2.1	Lennard-Jones Numerical Examples	176
7.2.2	Comparison of VAC Method and Cauchy–Born Rule	178
7.2.3	Truncation of Time History Kernel	179
7.3	2D/3D Bridging Scale Numerical Examples	182
7.4	Two-Dimensional Wave Propagation	184
7.5	Dynamic Crack Propagation in Two Dimensions	187
7.6	Dynamic Crack Propagation in Three Dimensions	195
7.7	Virtual Atom Cluster Numerical Examples	200
7.7.1	Bending of Carbon Nanotubes	200
7.7.2	VAC Coupling with Tight Binding	200
8	Non-Nearest Neighbor MD Boundary Condition	203
8.1	Introduction	203
8.2	Theoretical Formulation in 3D	203
8.2.1	Force Boundary Condition: 1D Illustration	207
8.2.2	Displacement Boundary Condition: 1D Illustration	210
8.2.3	Comparison to Nearest Neighbors Formulation	211
8.2.4	Advantages of Displacement Formulation	212
8.3	Numerical Examples: 1D Wave Propagation	212
8.4	Time-History Kernels for FCC Gold	213
8.5	Conclusion for the Bridging Scale Method	215
8.5.1	Bridging Scale Perspectives	220

9	Multiscale Methods for Material Design	223
9.1	Multiresolution Continuum Analysis	225
9.1.1	Generalized Stress and Deformation Measures	227
9.1.2	Interaction between Scales	231
9.1.3	Multiscale Materials Modeling	232
9.2	Multiscale Constitutive Modeling of Steels	234
9.2.1	Methodology and Approach	235
9.2.2	First-Principles Calculation	235
9.2.3	Hierarchical Unit Cell and Constitutive Model	237
9.2.4	Laboratory Specimen Scale: Simulation and Results	239
9.3	Bio-Inspired Materials	244
9.3.1	Mechanisms of Self-Healing in Materials	244
9.3.2	Shape-Memory Composites	246
9.3.3	Multiscale Continuum Modeling of SMA Composites	250
9.3.4	Issues of Modeling and Simulation	256
9.4	Summary and Future Research Directions	260
10	Bio-Nano Interface	263
10.1	Introduction	263
10.2	Immersed Finite Element Method	265
10.2.1	Formulation	265
10.2.2	Computational Algorithm of IFEM	268
10.3	Vascular Flow and Blood Rheology	269
10.3.1	Heart Model	269
10.3.2	Flexible Valve-Viscous Fluid Interaction	270
10.3.3	Angioplasty Stent	270
10.3.4	Monocyte Deposition	272
10.3.5	Platelet Adhesion and Blood Clotting	272
10.3.6	RBC Aggregation and Interaction	274
10.4	Electrohydrodynamic Coupling	280
10.4.1	Maxwell Equations	281
10.4.2	Electro-manipulation	283
10.4.3	Rotation of CNTs Induced by Electroosmotic Flow	285
10.5	CNT/DNA Assembly Simulation	287
10.6	Cell Migration and Cell-Substrate Adhesion	290
10.7	Conclusions	295
	Appendix A Kernel Matrices for EAM Potential	297
	Bibliography	301
	Index	315