CAMBRIDGE
Cambridge University Press & Assessment
978-1-107-01115-1 — Introduction to Computational Nanomechanics
Shaofan Li , Jun Li
Table of Contents
More Information

Contents

Preface *page* ix
Acknowledgments xi

Part I First-Principles Calculations

1 A Short Primer on Quantum Mechanics 3
1.1 Wave–Particle Duality: Law of Physics 3
1.2 Schrödinger Equation 8
1.3 Solution Examples of the Schrödinger Equation 11
1.4 Interpretations of Quantum Mechanics 28
1.5 Homework Problems 32

2 Density Functional Theory 35
2.1 Many-body Schrödinger Equation 35
2.2 Hartree–Fock Approximation 38
2.3 Hohenberg and Kohn Theorems 39
2.4 Kohn–Sham Formalism 43
2.5 Example: DFT Calculation of Silicon Band Structure 46

3 Quantum Stress 52
3.1 Quantum Stress Theory 52
3.2 Reciprocal-Space Expression for Quantum Stress 55
3.3 Quantum Stress via DFT 60
3.4 Quantum Electronic Stress 65
3.5 Higher-Order Quantum Stress Theory 69
3.6 Higher-Order Quantum Stress via DFT 70
3.7 Quantum Couple Stress via DFT 72

4 Introduction to VASP 76
4.1 Files Used by VASP 76
4.2 Example: Structural Optimization and Self-consistent Charge Density 84
4.3 Example: DFT Calculation of Si Band Structure 89
4.4 Example: DFT Modeling of Calcium Silicate Hydrate (C-S-H) Structure 94

© in this web service Cambridge University Press & Assessment www.cambridge.org

CAMBRIDGE
Cambridge University Press & Assessment
978-1-107-01115-1 — Introduction to Computational Nanomechanics
Shaofan Li , Jun Li
Table of Contents
More Information

Part II Statistical Molecular Dynamics

5 Fundamentals of Statistical Mechanics 105
5.1 Lagrangian Mechanics 105
5.2 Hamiltonian Mechanics 106
5.3 Liouville Theorem 111
5.4 Canonical Transformation and Symplectic Condition 113
5.5 Laws of Thermodynamics 115
5.6 Thermodynamics States 117
5.7 Legendre Transformation 120
5.8 Statistical Ensembles 124
5.9 Homework Problems 155

6 Fundamentals of Molecular Dynamics 158
6.1 How to Derive Molecular Dynamics from Quantum Mechanics 158
6.2 Ab-Initio Molecular Dynamics 162
6.3 How to Calculate Mechanical Forces in Quantum Mechanical Systems 163
6.4 Classical Molecular Dynamics 166
6.5 Examples of Atomistic Potentials 169
6.6 Periodic Boundary Condition 180
6.7 Neighbor Lists 185
6.8 Homework Problems 187

7 Molecular Dynamics Time Integration Techniques 189
7.1 Basic Concept of Time Integration 189
7.2 Verlet Algorithms 191
7.3 Predictor–Corrector Methods 199
7.4 Symplectic Algorithm 201
7.5 Homework Problems 203

8 Temperature Control in MD Simulations 204
8.1 Velocity Scaling 204
8.2 Stochastic Thermostat 206
8.3 Nosé–Hoover Thermostat 208
8.4 How to Integrate Nosé–Hoover MD? 216
8.5 Other Thermostats 220
8.6 Homework Problems 223

9 Andersen–Parrinello–Rahman Molecular Dynamics 225
9.1 Andersen's NPH MD 225
9.2 Parrinello-Rahman Formulation 228
9.3 PR MD for NPH Ensemble 232
9.4 Physical Justification of PR MD 238

© in this web service Cambridge University Press & Assessment www.cambridge.org

CAMBRIDGE
Cambridge University Press & Assessment
978-1-107-01115-1 — Introduction to Computational Nanomechanics
Shaofan Li , Jun Li
Table of Contents
More Information

9.5 PR MD for (NσH) or (NτH) Ensemble 242
9.6 Podio-Guidugli's Interpretation 246
9.7 Homework Problems 248

10 Introduction to LAMMPS 249
10.1 How to Download and Install LAMMPS 249
10.2 How to Run LAMMPS 251
10.3 Some Basic LAMMPS Commands 253
10.4 Case Study (I): Simulation of Three-Dimensional Nano-indentation 282
10.5 Case Study (II): MD Simulation of Mechanical Properties of Cement 287
10.6 MD Visualization Software: VMD and OVITO 291
10.7 Homework Problems 312

11 Monte Carlo Methods 313
11.1 Monte Carlo Sampling for Integrations 313
11.2 Markov Chain Monte Carlo Method 325
11.3 Hamiltonian (Hybrid) Monte Carlo Method 340

12 Langevin Equations and Dissipative Particle Dynamics 345
12.1 Langevin Equation 345
12.2 LAMMPS Examples for Langevin Dynamics 353
12.3 Dissipative Particle Dynamics 358
12.4 Homework Problems 371

13 Nonequilibrium Molecular Dynamics 373
13.1 Green–Kubo Relation 373
13.2 Example: LAMMPS Simulation of Thermal Conductivity 388
13.3 Fluctuation–Dissipation Theorem (FDT) 392
13.4 Mori–Zwanzig Formalism 401

Part III Multiscale Modeling and Simulation

14 Virial Theorem and Virial Stress 409
14.1 What Is Virial? 411
14.2 Virial Stress via Tensorial Viral Theorem 413
14.3 Virial Stress via Liouville Theorem: Irving–Kirkwood Formalism 419
14.4 Hardy Stress 427
14.5 Homework Problems 432

15 Cauchy–Born Rule and Multiscale Methods 433
15.1 Cauchy–Born Rule 433
15.2 Higher-Order Cauchy–Born Rule 446
15.3 Cauchy–Born Rule for Non-Bravais Lattices 450

© in this web service Cambridge University Press & Assessment www.cambridge.org

CAMBRIDGE

Cambridge University Press & Assessment
978-1-107-01115-1 — Introduction to Computational Nanomechanics
Shaofan Li , Jun Li
Table of Contents
More Information

15.4 Cauchy–Born Rule for Amorphous Solids 453
15.5 Homework Problems 458

16 Statistical Theory of Cauchy Continuum 459
16.1 Quasi-Harmonic Approximation 459
16.2 Homework Problems 470

17 Multiscale Method (I): Multiscale Micromorphic Molecular Dynamics 472
17.1 Multiscale Partition of First-Principles MD Lagrangian 472
17.2 Multiscale Micromorphic MD 481
17.3 Numerical Examples 487
17.4 Multiscale Coupling between MMMD and PD 495
17.5 Homework Problems 505

18 Multiscale Methods (II): Multiscale Finite Element Methods 507
18.1 Multiscale Finite Element Formulation 507
18.2 MMMD/FEM Coupling Method 513
18.3 Multiscale Cohesive Interphase Zone Model 517
18.4 Higher-Order MCZM 530

Appendix A Crystal Structure 536
A.1 Lattice and Basis 536
A.2 Unit Cells 542
A.3 Miller Indices 546
A.4 Reciprocal Lattice 549
A.5 Some Common Crystal Lattice Structures 551
A.6 Bloch Theorem 557

Bibliography 559
Author Index 565
Subject Index 567

© in this web service Cambridge University Press & Assessment www.cambridge.org