

Contents

List of Figures XVII

List of Tables LXIII

Nomenclature LXV

Part I Introduction

1 Introduction 3

1.1 Materials Deformation and Fracture Phenomena:
Why and How Things Break 5

1.2 Strength of Materials: Flaws, Defects, and a Perfect
Material 6

1.2.1 Crystal Structures and Molecular Packing 8

1.2.2 Cracks 10

1.2.3 Dislocations 10

1.2.4 Other Defects in Crystals and Other Structures 12

1.3 Brittle vs. Ductile Material Behavior 12

1.4 The Need for Atomistic Simulations 15

1.5 Applications: Experimental and Computational Mechanics .. 18

1.5.1 Experimental Techniques 18

1.5.2 Example Applications: The Significance
of Mechanics 20

1.6 Outline of This Book 27

Part II Basics of Atomistic, Continuum and Multiscale Methods

2 Basic Atomistic Modeling 31

2.1 Introduction 31

2.2 Modeling and Simulation 32

2.2.1 Model Building and Physical Representation 34

2.2.2	The Concept of Computational Experiments	35
2.3	Basic Statistical Mechanics	36
2.4	Formulation of Classical Molecular Dynamics	37
2.4.1	Integrating the Equations of Motion	39
2.4.2	Thermodynamic Ensembles and Their Numerical Implementation	40
2.4.3	Energy Minimization	43
2.4.4	Monte Carlo Techniques	44
2.5	Classes of Chemical Bonding	46
2.6	The Interatomic Potential or Force Field: Introduction	48
2.6.1	Pair Potentials	50
2.6.2	Multibody Potentials: Embedded Atom Method for Metals	54
2.6.3	Force Fields for Biological Materials and Polymers...	56
2.6.4	Bond Order and Reactive Potentials	59
2.6.5	Limitations of Classical Molecular Dynamics	68
2.7	Numerical Implementation	69
2.7.1	Periodic Boundary Conditions	70
2.7.2	Force Calculation	71
2.7.3	Neighbor Lists and Bins	72
2.8	Property Calculation	73
2.8.1	Temperature Calculation	73
2.8.2	Pressure Calculation	74
2.8.3	Radial Distribution Function	74
2.8.4	Mean Square Displacement Function	75
2.8.5	Velocity Autocorrelation Function	76
2.8.6	Virial Stress Tensor	76
2.9	Large-Scale Computing	78
2.9.1	Historical Development of Computing Power	79
2.9.2	Parallel Computing	80
2.9.3	Discussion	82
2.10	Visualization and Analysis Methods	83
2.10.1	Energy Method	85
2.10.2	Centrosymmetry Parameter	86
2.10.3	Slip Vector	88
2.10.4	Measurement of Defect Speed	89
2.10.5	Visualization Methods for Biological Structures	89
2.10.6	Other Methods	90
2.11	Distinguishing Modeling and Simulation	90
2.12	Application of Mechanical Boundary Conditions	90
2.13	Summary	93

3	Basic Continuum Mechanics	95
3.1	Newton's Laws of Mechanics	95
3.2	Definition of Displacement, Stress, and Strain	97
3.2.1	Stress Tensor	99
3.2.2	Equilibrium Conditions	100
3.2.3	Strain Tensor	103
3.3	Energy Approach to Elasticity	105
3.4	Isotropic Elasticity	107
3.5	Nonlinear Elasticity or Hyperelasticity	108
3.6	Elasticity of a Beam	110
3.6.1	Reduction Formulas	110
3.6.2	Equilibrium Equations	111
3.6.3	Example: Solution of a Simple Beam Problem	112
3.6.4	Calculation of Internal Stress Field	113
3.6.5	Differential Beam Equations	116
3.7	The Need for Atomistic Elasticity: What's Next	119
4	Atomistic Elasticity: Linking Atoms and Continuum	121
4.1	Thermodynamics as Bridge Between Atomistic and Continuum Viewpoints	121
4.2	The Atomic and Molecular Origin of Elasticity: Entropic vs. Energetic Sources	122
4.3	The Virial Stress and Strain	123
4.4	Elasticity Due to Energetic Contributions	124
4.4.1	Cauchy-Born Rule	124
4.4.2	Elasticity of a One-Dimensional String of Atoms	126
4.4.3	Elasticity and Surface Energy of a Two-Dimensional Triangular Lattice	128
4.4.4	Elasticity and Surface Energy of a Three-Dimensional FCC Lattice	142
4.4.5	Concluding Remarks	149
4.5	Elasticity Due to Entropic Contributions	149
4.5.1	Elasticity of Single Molecules: Worm-Like-Chain Model	150
4.5.2	Elasticity of Polymers	152
4.6	Discussion	154
5	Multiscale Modeling and Simulation Methods	157
5.1	Introduction	157
5.2	Direct Numerical Simulation vs. Multiscale and Multiparadigm Modeling	158
5.3	Differential Multiscale Modeling	159
5.4	Detailed Description of Selected Multiscale Methods to Span Vast Lengthscales	160
5.4.1	Examples of Hierarchical Multiscale Coupling	160

5.4.2	Concurrent Integration of Tight-Binding, Empirical Force Fields and Continuum Theory	162
5.4.3	The Quasicontinuum Method and Related Approaches	165
5.4.4	Continuum Approaches Incorporating Atomistic Information	168
5.4.5	Hybrid ReaxFF Model: Integration of Chemistry and Mechanics	169
5.5	Advanced Molecular Dynamics Techniques to Span Vast Timescales	175
5.6	Discussion	180

Part III Material Deformation and Failure

6	Deformation and Dynamical Failure of Brittle Materials .	185
6.1	The Nature of Brittle Fracture	186
6.2	Basics of Linear Elastic Fracture Mechanics	189
6.2.1	Energy Balance Considerations: Griffith's Model of Fracture	189
6.2.2	Asymptotic Stress Field and Stress Intensity Factor . .	194
6.2.3	Crack Limiting Speed in Dynamic Fracture	196
6.3	Atomistic Modeling of Brittle Materials	197
6.4	A One-Dimensional Example of Brittle Fracture: Joint Continuum-Atomistic Approach	201
6.4.1	Introduction	202
6.4.2	Linear-Elastic Continuum Model	204
6.4.3	Hyperelastic Continuum Mechanics Model for Bilinear Stress-Strain Law	207
6.4.4	Molecular Dynamics Simulations of the One-Dimensional Crack Model: The Harmonic Case	211
6.4.5	Molecular Dynamics Simulations of the One-Dimensional Crack Model: The Supersonic Case	217
6.4.6	Discussion and Conclusions	219
6.5	Stress and Deformation Field near Rapidly Propagating Mode I Cracks in a Harmonic Lattice	223
6.5.1	Stress and Deformation Fields	225
6.5.2	Energy Flow near the Crack Tip	227
6.5.3	Limiting Velocities of Mode I Cracks in Harmonic Lattices	229
6.5.4	Summary	230

6.6	Crack Limiting Speeds of Cracks: The Significance of Hyperelasticity.....	234
6.6.1	Modeling.....	236
6.6.2	Crack Speed and Energy Flow.....	238
6.6.3	Hyperelastic Area.....	239
6.6.4	How Fast can Cracks Propagate?.....	242
6.6.5	Characteristic Energy Length Scale in Dynamic Fracture.....	244
6.6.6	Summary.....	248
6.7	Crack Instabilities and Hyperelastic Material Behavior.....	249
6.7.1	Introduction.....	251
6.7.2	Design of Computational Model.....	252
6.7.3	Computational Experiments.....	255
6.7.4	Discussion and Conclusion.....	258
6.8	Suddenly Stopping Cracks: Linking Atomistic Modeling, Theory, and Experiment.....	260
6.8.1	Introduction.....	260
6.8.2	Theoretical Background of Suddenly Stopping Cracks.....	262
6.8.3	Atomistic Simulation Setup.....	264
6.8.4	Atomistic Simulation Results of a Suddenly Stopping Mode I Crack.....	268
6.8.5	Atomistic Simulation Results of a Suddenly Stopping Mode II Crack.....	278
6.8.6	Discussion.....	286
6.9	Crack Propagation Along Interfaces of Dissimilar Materials.....	287
6.9.1	Mode I Dominated Cracks at Bimaterial Interfaces ..	289
6.9.2	Mode II Cracks at Bimaterial Interfaces.....	294
6.9.3	Summary.....	297
6.10	Dynamic Fracture Under Mode III Loading.....	299
6.10.1	Atomistic Modeling of Mode III Cracks.....	300
6.10.2	Mode III Cracks in a Harmonic Lattice – The Reference Systems.....	300
6.10.3	Mode III Crack Propagation in a Thin Stiff Layer Embedded in a Soft Matrix.....	301
6.10.4	Suddenly Stopping Mode III Crack.....	303
6.10.5	Discussion.....	303
6.11	Brittle Fracture of Chemically Complex Materials.....	304
6.11.1	Introduction.....	305
6.11.2	Hybrid Atomistic Modeling of Cracking in Silicon: Mixed Hamiltonian Gormulation.....	307
6.11.3	Atomistic Model.....	307
6.11.4	Simulation Results.....	308

6.11.5	Dynamical Fracture Mechanisms	311
6.11.6	Reactive Chemical Processes and Fracture Initiation	316
6.11.7	Summary	317
6.12	Summary: Brittle Fracture	320
6.12.1	Hyperelasticity can Govern Dynamic Fracture	323
6.12.2	Interfaces and Geometric Confinement	326
7	Deformation and Fracture of Ductile Materials	327
7.1	Introduction	327
7.2	Continuum Theoretical Concepts of Dislocations and Their Interactions	328
7.2.1	Properties of Dislocations	329
7.2.2	Forces on Dislocations	331
7.2.3	Rice-Thomson Model for Dislocation Nucleation	332
7.2.4	Rice-Peierls Model	337
7.2.5	Link with Atomistic Concepts	338
7.2.6	Generalized Stacking Fault Curves	338
7.2.7	Linking Atomistic Simulation Results to Continuum Mechanics Theories of Plasticity	339
7.3	Modeling Plasticity Using Large-Scale Atomistic Simulations	341
7.4	Case Study: Deformation Mechanics of Model FCC Copper - LJ Potential	343
7.4.1	Model Setup	343
7.4.2	Visualization Procedure	345
7.4.3	Simulation Results	345
7.4.4	Summary	355
7.5	Case Study: Deformation Mechanics of a Nickel Nanocrystal - EAM Potential	357
7.6	Case Study: Multi-Paradigm Modeling of Chemical Complexity in Mechanical Deformation of Metals	359
7.6.1	Atomistic Model and Validation	360
7.6.2	Example Application: Modeling Hybrid Metal-Organic Systems	364
8	Deformation and Fracture Mechanics of Geometrically Confined Materials	373
8.1	Introduction	373
8.2	Thin Metal Films and Nanocrystalline Metals	381
8.2.1	Constrained Diffusional Creep in Ultra-Thin Metal Films	385
8.2.2	Single Edge Dislocations in Nanoscale Thin Films ...	390

8.2.3	Rice–Thompson Model for Nucleation of Parallel Glide Dislocations	393
8.2.4	Discussion and Summary	396
8.3	Atomistic Modeling of Constrained Grain Boundary Diffusion in a Bicrystal Model	396
8.3.1	Introduction and Modeling Procedure	397
8.3.2	Formation of the Diffusion Wedge	400
8.3.3	Development of the Crack-Like Stress Field and Nucleation of Parallel Glide Dislocations	402
8.3.4	Discussion	404
8.3.5	Summary	408
8.4	Dislocation Nucleation from Grain Triple Junction	408
8.4.1	Atomistic Modeling of the Grain Triple Junction ...	409
8.4.2	Atomistic Simulation Results	410
8.4.3	Discussion	414
8.5	Atomistic Modeling of Plasticity of Polycrystalline Thin Films	414
8.5.1	Atomistic Modeling of Polycrystalline Thin Films ...	415
8.5.2	Atomistic Simulation Results	416
8.5.3	Plasticity of Nanocrystalline Bulk Materials with Twin Lamella	422
8.5.4	Modeling of Constrained Diffusional Creep in Polycrystalline Films	426
8.5.5	Discussion	428
8.5.6	Summary: Results of Modeling of Thin Films	430
8.6	Use of Atomistic Simulation Results in Hierarchical Multiscale Modeling	432
8.6.1	Mechanisms of Plastic Deformation of Ultra-thin Uncapped Copper Films	434
8.6.2	Deformation Map of Thin Films	434
8.6.3	Yield Stress in Ultra-Thin Copper Films	435
8.6.4	The Role of Interfaces and Geometric Confinement ..	436
8.7	Deformation and Fracture Mechanics of Carbon Nanotubes	438
8.7.1	Mesoscale Modeling of CNT Bundles	441
8.7.2	Mesoscale Simulation Results	444
8.7.3	Discussion	445
8.8	Flaw-Tolerant Nanomaterials: Bulk Fracture and Deformation	446
8.8.1	Strength of Brittle Nanoparticles	446
8.8.2	Simulation Results	450
8.9	Nanoscale Adhesion Systems	452
8.9.1	Strength of Fibrillar Adhesion Systems	453
8.9.2	Theoretical Considerations of Shape Optimization of Adhesion Elements	455

8.9.3	Atomistic Modeling	456
8.9.4	Simulation Results	457
8.9.5	Summary	460
References		463
Index		483