

Contents

	<i>Foreword</i>	<i>page xv</i>
	<i>by G. B. Olson</i>	
	<i>Preface</i>	xvii
	<i>Acknowledgments</i>	xix
1	Introduction	1
	1.1 Definition of a Few Terms Used in Computational Design of Materials	2
	1.2 The Past and Present Development of Computational Design of Engineering Materials	3
	1.3 The Structure of the Book	7
	References	9
2	Fundamentals of Atomistic Simulation Methods	12
	2.1 Density Functional Theory	13
	2.1.1 The Many-Body Schrödinger Equation	13
	2.1.2 The Hartree Approximation	15
	2.1.3 Kohn–Sham Equation	15
	2.1.4 Pseudopotential Method	20
	2.2 Molecular Dynamics	22
	2.2.1 The Basic Mechanical Quantities in MD	22
	2.2.2 Periodic Boundary Conditions	26
	2.2.3 Time Integration Algorithm	28
	2.2.4 Ensemble	29
	2.2.5 Procedure of MD Simulation	30
	2.2.6 Ab Initio Molecular Dynamics	31
	2.3 Some Quantities Obtained from First-Principles Calculations	33
	2.3.1 Lattice Parameter	33
	2.3.2 Thermodynamic Properties above 0 K	35
	2.3.3 Elastic Properties	36
	2.3.4 Defect Properties	39
	2.4 A Case Study: Design of an Ultra-lightweight Mg–Li Alloys Using First-Principles Calculations	41
	References	44

3	Fundamentals of Mesoscale Simulation Methods	46
3.1	Mesoscale Simulation	47
3.2	Phase-Field Method	48
3.2.1	History of the Phase-Field Method	48
3.2.2	Principles of the Phase-Field Method	50
3.2.2.1	Diffuse Interface	50
3.2.2.2	Order Parameter	51
3.2.2.3	Free-Energy Functional	51
3.2.2.4	Dynamic Equations	52
3.2.2.5	Anisotropy	53
3.2.3	Phase-Field Model for Solidification of a Pure Substance	54
3.2.4	Phase-Field Model for Alloy Solidification	55
3.2.4.1	WBM Model	55
3.2.4.2	KKS Model	56
3.2.5	Multiphase-Field Model	58
3.2.6	Phase-Field Crystal Model	60
3.2.7	Microscopic Phase-Field Models	63
3.2.8	Applications of the Phase-Field Method	65
3.3	Cellular Automaton Method	66
3.3.1	Historical Background	67
3.3.2	Principles of the Cellular Automaton Method	67
3.3.3	Classical Cellular Automaton Model	68
3.3.3.1	Nucleation Model	69
3.3.3.2	Grain Growth Model	69
3.3.4	Modified Cellular Automation Model	71
3.3.4.1	Growth Kinetics and Orientation	71
3.3.4.2	Solute Redistribution	72
3.3.4.3	Thermal Transport	72
3.3.4.4	Interface Curvature	72
3.3.5	Discussion Regarding Grid Anisotropy	73
3.3.6	Applications of the Cellular Automation Method	74
3.4	Other Mesoscale Simulation Methods	74
3.4.1	Front-Tracking Method	75
3.4.2	Level-Set Method	76
3.4.3	Comparisons among Different Mesoscale Simulation Methods	77
3.5	Integration of the Phase-Field Method with Other Simulation Approaches	79
3.5.1	PF Modeling with Atomic Simulations	79
3.5.2	PF Modeling with Crystal Plasticity	82
3.5.3	PF Modeling with Macro Transport Equations	84
3.5.4	PF Modeling with CALPHAD	86
3.5.5	PF Modeling with Machine Learning	87

	Contents	ix
3.6	A Case Study: Phase-Field Design of High-Energy-Density Polymer Nanocomposites	89
	References	90
4	Fundamentals of Crystal Plasticity Finite Element Method	95
4.1	Crystal Plasticity and Its General Features	95
4.2	Basic Concepts and Equations of Continuum Mechanics	96
4.2.1	Definition of a Few Basic Terms in Continuum Mechanics	96
4.2.2	Three Coordinate Systems and the Deformation Gradient	97
4.2.3	Isochoric/Volumetric Split of the Deformation Gradient	98
4.2.4	Polar Decomposition	99
4.2.5	Eulerian and Lagrangian Finite Strain Tensors	99
4.3	Mechanical Constitutive Laws of Crystal Plasticity	100
4.3.1	Dislocation-Based Constitutive Models	101
4.3.2	Constitutive Models for Displacive Transformation	102
4.4	Brief Introduction to the Finite Element Method	103
4.5	Software and Procedure for the Crystal Plasticity Finite Element Simulation	105
4.5.1	Brief Introduction to Several FEM Software Packages	105
4.5.2	Procedure for the Crystal Plasticity Finite Element Method	107
4.6	A Case Study: Plastic Deformation-Induced Surface Roughening in Al Polycrystals	108
	References	111
5	Fundamentals of Computational Thermodynamics and the CALPHAD Method	113
5.1	Introduction	114
5.2	Overview of the CALPHAD Method	115
5.2.1	Origins and Development of the CALPHAD Method	115
5.2.2	Principles of the CALPHAD Method	116
5.2.3	Overview of Commercial and Open-Source CALPHAD-Based Software	122
5.3	Thermodynamic Modeling of Gibbs Energy	123
5.3.1	Phases with Fixed Composition	123
5.3.1.1	Pure Elements	123
5.3.1.2	Magnetic Contribution	125
5.3.1.3	Pressure Contribution	127
5.3.1.4	Stoichiometric Compounds	129
5.3.2	Solution Phases	133
5.3.2.1	Substitutional Solution	133
5.3.2.2	Gas Phase	138
5.3.2.3	Associate Solution	140
5.3.2.4	Quasichemical Model	143
5.3.2.5	Comparison of Models for Ordered Liquid Solutions	145
5.3.2.6	Sublattice Model for Solid Solution Phases	146

x	Contents	
	5.4 Establishment of Thermodynamic CALPHAD Databases	155
	5.5 Alloy Design Applications Using Solely Thermodynamic CALPHAD Databases	159
	5.5.1 Overview	159
	5.5.2 Applications Based on Equilibrium Calculations	160
	5.5.2.1 Stable Phase Diagram Calculations	162
	5.5.2.2 Metastable Phase Diagram Calculations	166
	5.5.2.3 Property Diagram Calculations	168
	5.5.3 Applications Based on Scheil Simulations	170
	5.6 Alloy Design Applications Using Extended CALPHAD-Type Databases	178
	5.6.1 Overview	178
	5.6.2 Simulation of Solidification	179
	5.6.3 Simulation of Heat Treatment	181
	5.7 A Case Study: CALPHAD Design of Al Alloys with High Resistance to Hot Tearing	184
	References	189
6	Fundamentals of Thermophysical Properties	198
	6.1 Definition of Thermophysical Properties	199
	6.2 Diffusion Coefficient	200
	6.2.1 Fick's Laws of Diffusion and Various Diffusion Coefficients	200
	6.2.2 Atomic Mechanism of Diffusion	204
	6.2.2.1 Interstitial Mechanism	205
	6.2.2.2 Direct Exchange and Ring Mechanisms	205
	6.2.2.3 Vacancy Mechanism	205
	6.2.2.4 Indirect Interstitial Mechanism	205
	6.2.2.5 Diffusion in Ordered Phase	206
	6.2.3 Interdiffusion in Binary, Ternary, and Multicomponent Systems	207
	6.2.3.1 Interdiffusion in Binary Systems	207
	6.2.3.2 Interdiffusion in Ternary Systems	210
	6.2.3.3 Interdiffusion in Multicomponent Systems	217
	6.2.4 Diffusion in Phases with Narrow Homogeneity Ranges	219
	6.2.4.1 Wagner's Approach	219
	6.2.4.2 Du and Schuster Approach	220
	6.2.5 Short-Circuit Diffusion	223
	6.2.5.1 A-Type Kinetic Regime	224
	6.2.5.2 B-Type Kinetic Regime	225
	6.2.5.3 C-Type Kinetic Regime	226
	6.2.6 Computational Methods for Calculations of Diffusivity	227
	6.2.6.1 Atomistic Description of Diffusion	227
	6.2.6.2 MD Simulation	232
	6.2.6.3 Semi-Empirical Methods	233
	6.2.6.4 Diffusion Simulations Using DICTRA Software	236

6.3	Interfacial Energy	239
6.4	Viscosity	243
6.5	Volume	245
6.6	Thermal Conductivity	247
6.7	Some Other Thermophysical Properties	251
6.8	Establishment of Thermophysical Property Databases	252
6.9	A Case Study: Precipitation and Age Hardening in an AA6005 Al Alloy	253
	References	257
7	Case Studies on Steel Design	264
7.1	Brief Introduction about Steel	264
7.2	Ultrahigh-Strength and Corrosion-Resistant Ferrium S53 Steel	268
7.2.1	Strategy for the Systems Design of Ferrium S53	269
7.2.2	Design of Strength, Toughness, and Fatigue Resistance	269
7.2.2.1	Martensitic Transformation Behavior	271
7.2.2.2	Precipitation of Coherent M ₂ C Carbides	273
7.2.2.3	Solidification Microsegregation and Castability	275
7.2.3	Design of Resistance to General Corrosion and Stress Corrosion Cracking	277
7.2.4	Hydrogen Embrittlement	279
7.2.5	Prototype and Applications of Ferrium S53	279
7.3	AISI H13 Hot-Work Tool Steel	281
7.3.1	Simulations of Microstructure Evolution, Yield Stress, Flow Curve, and Creep	282
7.3.1.1	Simulation of Microstructure	282
7.3.1.2	Simulation of Yield Stress	284
7.3.1.3	Simulation of the Flow Curve	285
7.3.1.4	Simulation of Creep	286
7.3.2	Simulation of Heat Transfer, Phase Transformation, and Stress Relaxation	287
7.3.2.1	Simulation of Heat Transfer	287
7.3.2.2	Simulation of Phase Transformations	288
7.3.2.3	Simulation of Stress Relaxation	289
	References	291
8	Case Studies on Light Alloy Design	295
8.1	Introduction	295
8.2	Aluminum Alloys	296
8.2.1	Cast Al Alloy A356: Solidification Simulation and Microsegregation	297
8.2.2	Wrought Al Alloy 7xxx: Heat Treatment Simulation and Precipitation Kinetics	302
8.3	Magnesium Alloys	304

8.3.1	Selection of Cast Mg Alloy Composition and Optimized Heat Treatment	306
8.3.1.1	Selected Case Studies for New Creep-Resistant Mg Alloys	306
8.3.1.2	Solidification Path and T6 Heat Treatment of AZ Series Alloys	307
8.3.1.3	Computational Design and Development of New Mg–Al–Sn-Based (AT) Cast Alloys	310
8.3.2	Biomedical Mg Alloy Implants	312
8.4	Summary	318
8.4.1	Alloy Design Applications Using Solely Thermodynamic CALPHAD Databases	318
8.4.2	Alloy Design Applications Using Extended CALPHAD-Type Databases and Kinetic Simulations	318
	References	319
9	Case Studies on Superalloy Design	323
9.1	Introduction	323
9.2	Ni-Based Single-Crystal Superalloys	325
9.2.1	Model Description	328
9.2.1.1	Thermodynamic Properties	328
9.2.1.2	Density	328
9.2.1.3	Misfit	329
9.2.1.4	Creep-Rupture Lifetime	329
9.2.1.5	Design Criteria	329
9.2.2	Alloy Design Procedure	330
9.2.2.1	Surrogate Models	331
9.2.2.2	Optimization Algorithm	331
9.2.3	Alloy Design and Experimental Validation	331
9.3	Ni–Fe-Based Superalloys for Advanced Ultrasupercritical Units	333
9.3.1	Model Description	334
9.3.2	Alloy Design Procedure	335
9.3.3	Alloy Design and Experimental Validation	338
	References	340
10	Case Studies on Cemented Carbide Design	342
10.1	Brief Introduction to Cemented Carbides	342
10.2	Ultrafine Cemented Carbides	344
10.2.1	Segregation of the (Ta,W)C Cubic Phase in Ultrafine Cemented Carbides	345
10.2.2	Optimization of Composition, Sintering Temperature, and Inhibitors	347
10.3	Cemented Carbides with Composite Binder Phases of Co and γ' -Ni ₃ Al	351

	Contents	xiii
10.3.1	Optimization of Composition and Sintering Temperature	353
10.3.2	Morphology Control of the Composite Binder Phases and WC Grains	355
10.4	Gradient Cemented Carbides	360
10.4.1	Computational Design of Gradient Microstructure	361
10.4.2	A Microstructure-Based Hardness Model for Gradient Cemented Carbides	362
	References	367
11	Case Studies on Hard Coating Design	370
11.1	Introduction to Cutting Tools and Hard Coatings	370
11.2	PVD Hard Coating	372
11.2.1	Cathodic Arc Evaporation and Magnetron Sputtering	372
11.2.2	Metastable Phase Formation and TiN–AlN Phase Diagrams	375
11.2.3	Spinodal Decomposition	378
11.2.4	Multilayer Hard Coating	379
11.3	CVD Hard Coating	383
11.3.1	Experimental Setup	383
11.3.2	Through-Process Modeling of CVD MT–Ti(C,N) Hard Coating	385
	References	398
12	Case Studies on Energy Materials Design	402
12.1	Case Study for Design of Hydrogen Storage Materials	403
12.1.1	Overview of Hydrogen Storage Materials	403
12.1.2	Complex Light Metal Hydride LiBH ₄	404
12.1.2.1	Overview of LiBH ₄ Properties	404
12.1.2.2	Strategy for Understanding Dehydrogenation of LiBH ₄	406
12.1.2.3	Thermodynamics of LiBH ₄	408
12.1.2.4	Point Defects in LiBH ₄ : Understand the Dehydrogenation of LiBH ₄	414
12.1.2.5	Structural Evolution and Diffusivity of LiBH ₄	417
12.2	Case Study for Design of Li–Ion Batteries	419
12.2.1	Overview of Li–Ion Batteries	419
12.2.2	Relationship among Phase Diagram, Thermodynamics, and Electrochemical Properties	421
12.2.3	Li–Mn–O Spinel Cathode Material	422
12.2.3.1	Phase Diagrams	423
12.2.3.2	Evaluation of Cyclability	425
12.2.3.3	Evaluation of Safety	428
12.2.3.4	Evaluation of Energy Density	429
12.2.3.5	Optimization of the Composition Based on Comprehensive Consideration	430
	References	431

13	Summary and Future Development of Materials Design	433
	13.1 Brief Summary of This Book	434
	13.2 Highlighting Computational Design of Other Engineering Materials and Processes	437
	13.2.1 Highlighting the Design of Mo ₂ BC Thin Film	438
	13.2.2 Highlighting the Design of Nanocurvature-Enhanced Fabrication of Cu ₃ Sn	438
	13.2.3 Highlighting the Design of Steel Production Process	441
	13.2.4 Highlighting the Design of Slag as Recycled Material	442
	13.3 Future Orientations and Challenges for Computational Design of Engineering Materials	443
	13.3.1 General Aspects of Computational Design of Engineering Materials, ICME, MGI, and CDMD	443
	13.3.2 Advancement of Models and Approaches for More Quantitative Simulation in Materials Design	444
	13.3.2.1 Heterointerface and Homointerface Thermodynamics	444
	13.3.2.2 Thermodynamics under External Fields	447
	13.3.2.3 More Quantitative Phase-Field Models	448
	13.3.3 Databases and Materials Informatics	449
	13.3.3.1 Scientific Databases	449
	13.3.3.2 Materials Informatics	449
	13.3.4 Enhanced Simulation Software Packages	450
	13.3.5 Concurrent Design of Materials and Products	451
	13.3.6 ICME and MGI as Well as Their Correlations to CDMP	453
	References	454
	<i>Appendix A Ancillary Materials</i>	457
	<i>Appendix B Notations</i>	461
	<i>Index</i>	469

Colour plates are to be found between pages 460 and 461.