

Contents

Preface XI

1	Introduction	1
1.1	The Role of Microstructure Materials Science	1
1.2	Free Boundary Problems and Microstructure Evolution	2
1.3	Continuum versus Sharp Interface Descriptions	5
	References	7
2	Mean Field Theory of Phase Transformations	9
2.1	Simple Lattice Models	10
2.1.1	Phase Separation in a Binary Mixture	10
2.1.2	Ising Model of Magnetism	13
2.2	Introduction to Landau Theory	17
2.2.1	Order Parameters and Phase Transformations	17
2.2.2	The Landau Free Energy Functional	18
2.2.3	Phase Transitions with a Symmetric Phase Diagram	20
2.2.4	Phase Transitions with a Nonsymmetric Phase Diagram	22
2.2.5	First-Order Transition without a Critical Point	24
	References	25
3	Spatial Variations and Interfaces	27
3.1	The Ginzburg–Landau Free Energy Functional	27
3.2	Equilibrium Interfaces and Surface Tension	29
	References	32
4	Nonequilibrium Dynamics	33
4.1	Driving Forces and Fluxes	34
4.2	The Diffusion Equation	34
4.3	Dynamics of Conserved Order Parameters: Model B	35

4.4	Dynamics of Nonconserved Order Parameters: Model A	38
4.5	Generic Features of Models A and B	39
4.6	Equilibrium Fluctuations of Order Parameters	40
4.6.1	Nonconserved Order Parameters	40
4.6.2	Conserved Order Parameters	42
4.7	Stability and the Formation of Second Phases	42
4.7.1	Nonconserved Order Parameters	42
4.7.2	Conserved Order Parameters	44
4.8	Interface Dynamics of Phase Field Models (Optional)	45
4.8.1	Model A	45
4.8.2	Model B	49
4.9	Numerical Methods	50
4.9.1	Fortran 90 Codes Accompanying this Book	50
4.9.2	Model A	51
4.9.3	Model B	55
	References	56
5	Introduction to Phase Field Modeling: Solidification of Pure Materials	57
5.1	Solid Order Parameters	57
5.2	Free Energy Functional for Solidification	60
5.3	Single Order Parameter Theory of Solidification	61
5.4	Solidification Dynamics	63
5.4.1	Isothermal Solidification: Model A Dynamics	63
5.4.2	Anisotropy	65
5.4.3	Nonisothermal Solidification: Model C Dynamics	66
5.5	Sharp and Thin Interface Limits of Phase Field Models	68
5.6	Case Study: Thin Interface Analysis of Equation 5.30	69
5.6.1	Recasting Phase Field Equations	70
5.6.2	Effective Sharp Interface Model	71
5.7	Numerical Simulations of Model C	73
5.7.1	Discrete Equations	74
5.7.2	Boundary Conditions	76
5.7.3	Scaling and Convergence of Model	77
5.8	Properties of Dendritic Solidification in Pure Materials	80
5.8.1	Microscopic Solvability Theory	81
5.8.2	Phase Field Predictions of Dendrite Operating States	83
5.8.3	Further Study of Dendritic Growth	87
	References	87
6	Phase Field Modeling of Solidification in Binary Alloys	89
6.1	Alloys and Phase Diagrams: A Quick Review	89
6.2	Microstructure Evolution in Alloys	91
6.2.1	Sharp Interface Model in One Dimension	92
6.2.2	Extension of Sharp Interface Model to Higher Dimensions	93

6.3	Phase Field Model of a Binary Alloy	95
6.3.1	Free Energy Functional	95
6.3.2	General Form of $f(\phi, c, T)$	96
6.3.3	$f(\phi, c, T)$ for Isomorphous Alloys	96
6.3.4	$f(\phi, c, T)$ for Eutectic Alloys	97
6.3.5	$f(\phi, c, T)$ for Dilute Binary Alloys	98
6.4	Equilibrium Properties of Free Energy Functional	99
6.4.1	Simple Example of a “Toy” Model	100
6.4.2	Calculation of Surface Tension	101
6.5	Phase Field Dynamics	103
6.6	Thin Interface Limits of Alloy Phase Field Models	104
6.7	Case Study: Analysis of a Dilute Binary Alloy Model	106
6.7.1	Interpolation Functions for $f(\phi, c)$	106
6.7.2	Equilibrium Phase Diagram	107
6.7.3	Steady-State c_0 and ϕ_0	108
6.7.4	Dynamical Equations	109
6.7.5	Thin Interface Properties of Dilute Alloy Model	111
6.7.6	Nonvariational Version of Model (optional)	112
6.7.7	Effective Sharp Interface Parameters of Nonvariational Model (optional)	113
6.8	Numerical Simulations of Dilute Alloy Phase Field Model	116
6.8.1	Discrete Equations	116
6.8.2	Convergence Properties of Model	119
6.9	Other Alloy Phase Field Formulations	121
6.9.1	Introducing Fictitious Concentrations	122
6.9.2	Formulation of Phase Field Equations	123
6.9.3	Steady-State Properties of Model and Surface Tension	124
6.9.4	Thin Interface Limit	125
6.9.5	Numerical Determination of C_s and C_L	126
6.10	Properties of Dendritic Solidification in Binary Alloys	127
6.10.1	Geometric Models of Directional Solidification	127
6.10.2	Spacing Selection Theories of Directional Solidification	130
6.10.3	Phase Field Simulations of Directional Solidification	132
6.10.4	The Role of Surface Tension Anisotropy	137
	References	141
7	Multiple Phase Fields and Order Parameters	143
7.1	Multiorder Parameter Models	144
7.1.1	Pure Materials	144
7.1.2	Alloys	146
7.1.3	Strain Effects on Precipitation	149
7.1.4	Anisotropy	151
7.2	Multiphase Field Models	153
7.2.1	Thermodynamics	154
7.2.2	Dynamics	156

7.3	Orientational Order Parameter for Polycrystalline Modeling	157
7.3.1	Pure Materials	157
7.3.2	Alloys	162
	References	163
8	Phase Field Crystal Modeling of Pure Materials	167
8.1	Generic Properties of Periodic Systems	168
8.2	Periodic Free Energies and the Swift–Hohenberg Equation	169
8.2.1	Static Analysis of the SH Equation	173
8.2.2	Dynamical Analysis of the SH Equation	175
8.3	Phase Field Crystal Modeling	181
8.4	Equilibrium Properties in a One-Mode Approximation	185
8.4.1	Three Dimensions: BCC Lattice	186
8.4.2	Two Dimensions: Triangular Rods	190
8.4.3	One-Dimensional Planes	193
8.5	Elastic Constants of PFC Model	194
8.5.1	PFC Dynamics	195
8.5.2	Vacancy Diffusion	196
8.6	Multiscale Modeling: Amplitude Expansions (Optional)	198
8.6.1	One Dimension	201
8.6.2	Two Dimensions	202
8.6.3	Three Dimensions	204
8.6.4	Rotational Invariance	205
8.6.5	Parameter Fitting	206
	References	207
9	Phase Field Crystal Modeling of Binary Alloys	209
9.1	A Two-Component PFC Model for Alloys	209
9.1.1	Constant Density Approximation: Liquid	210
9.1.2	Constant Concentration Approximation: Solid	211
9.2	Simplification of Binary Model	212
9.2.1	Equilibrium Properties: Two Dimensions	214
9.2.2	Equilibrium Properties: Three Dimensions (BCC)	216
9.3	PFC Alloy Dynamics	218
9.4	Applications of the Alloy PFC Model	221
	References	222
	Appendices	223
	Appendix A Thin Interface Limit of a Binary Alloy Phase Field Model	225
A.1	Phase Field Model	225
A.2	Curvilinear Coordinate Transformations	227
A.3	Length and Timescales	228
A.4	Matching Conditions between Outer and Inner Solutions	229

A.5	Outer Equations Satisfied by Phase Field Model	231
A.6	Inner Expansion of Phase Field Equations	233
A.6.1	Inner Expansion of Phase Field Equation (A37) at Different Orders	235
A.6.2	Inner Expansion of Concentration Equation (A38) at Different Orders	235
A.6.3	Inner Chemical Potential Expansion	236
A.7	Analysis of Inner Equations and Matching to Outer Fields	237
A.7.1	$\mathcal{O}(1)$ Phase Field Equation (A40)	237
A.7.2	$\mathcal{O}(1)$ Diffusion Equation (A43)	238
A.7.3	$\mathcal{O}(\varepsilon)$ Phase Field Equation (A41)	239
A.7.4	$\mathcal{O}(\varepsilon)$ Diffusion Equation (A44)	241
A.7.5	$\mathcal{O}(\varepsilon^2)$ Phase Field Equation (A42)	244
A.7.6	$\mathcal{O}(\varepsilon^2)$ Diffusion Equation (A45)	247
A.8	Summary of Results of Sections A.2–A.7	251
A.8.1	Effective Sharp Interface Limit of Equations (A2)	251
A.8.2	Interpretation of Thin Interface Limit Correction Terms	252
A.9	Elimination of Thin Interface Correction Terms	253
A.9.1	Modifying the Phase Field Equations	254
A.9.2	Changes Due to the Altered Form of Bulk Chemical Potential	255
A.9.3	Changes Due to the Addition of Antitrapping Flux	256
A.9.4	Analysis of Modified $\mathcal{O}(\varepsilon)$ Inner Diffusion Equation	258
A.9.5	Analysis of Modified $\mathcal{O}(\varepsilon^2)$ Inner Phase Field Equation	258
A.9.6	Analysis of Modified $\mathcal{O}(\varepsilon^2)$ Inner Diffusion Equation	259
	References	260
Appendix B Basic Numerical Algorithms for Phase Field Equations		261
B.1	Explicit Finite Difference Method for Model A	261
B.1.1	Spatial Derivatives	262
B.1.2	Time Marching	263
B.2	Explicit Finite Volume Method for Model B	264
B.2.1	Discrete Volume Integration	265
B.2.2	Time and Space Discretization	265
B.3	Stability of Time Marching Schemes	266
B.3.1	Linear Stability of Explicit Methods	267
B.3.2	Nonlinear Instability Criterion for Δt	270
B.3.3	Nonlinear Instability Criterion for Δx	272
B.3.4	Implicit Methods	273
B.4	Semi-Implicit Fourier Space Method	274
B.5	Finite Element Method	276
B.5.1	The Diffusion Equation in 1D	276
B.5.2	The 2D Poisson Equation	281
	References	285

Appendix C Miscellaneous Derivations 287

C.1 Structure Factor: Section 4.6.1 287

C.2 Transformations from Cartesian to Curvilinear Coordinates:
Section A.2 288

C.3 Newton's Method for Nonlinear Algebraic Equations:
Section 6.9.5 291

Index 293