

Contents

	Preface	V
1	Complex Structures: A Symbiosis of Experiments and Numerical Studies	1
	J. H. BILGRAM and H. M. SINGER	
	Abstract	1
1.1	Introduction	1
1.2	Experimental Studies	2
1.3	Numerical Studies	5
1.4	Conclusions	6
	Acknowledgements	7
	References	7
2	Thermal Roughening of a Solid-on-Solid Model with Elastic Interaction	9
	FRANK GUTHEIM, HEINER MÜLLER-KRUMBHAAR, EFIM BRENER and CHRISTOPH PÜTTER	
2.1	Introduction	9
2.2	Step Interaction	9
2.3	Model Description	10
2.4	Results and Discussion	13
2.4.1	Height Correlation Function	13
2.4.2	Energetic Scales	14
2.4.3	Average Energy	14
2.4.4	Defect Correlations	14
2.4.5	Line Energy vs. Step Interaction	15
2.4.6	Crystal Growth	15
2.5	Conclusion	16
	References	16
3	A Phase-Field Model for Crystallization into Multiple Grain Structures	17
	HAMID ASSADI	
	Abstract	17
3.1	Introduction	17

3.2	Theoretical Background and Model Development	18
3.3	Simulations	21
3.3.1	Temperature Dependence of Interfacial Energy	22
3.3.2	Crystallization by Inoculation	22
3.3.3	Crystallization by Homogeneous Nucleation	24
	References	26
4	Scaling Relations for Dendritic Solidification in Binary Alloys	27
	HEIKE EMMERICH, MATTHIAS JURGK, RICARDO SIQUIERI	
4.1	Introduction	27
4.2	Two-scale Modeling for Binary Alloys	28
4.3	A Novel Scaling Relation Taking into Account Crystal Density	30
4.4	Numerical Investigations of the Two-scale Model	31
	Summary	32
	References	33
5	Modeling the Spatial Phase Separation Process in Hypermonotectic Alloys	34
	M. WU, A. LUDWIG, L. RATKE	
	Abstract	34
5.1	Introduction	34
5.2	Numerical Model	35
5.2.1	Phase Definition	35
5.2.2	Conservation equations	35
5.2.3	Droplet Growth and Mass Transfer	36
5.2.4	Marangoni Force and Hydrodynamic Resistance	37
5.3	Problem description	38
5.4	Results and Discussions	39
5.4.1	Without Gravity	39
5.4.2	With Gravity	40
5.5	Conclusions	42
	References	42
6	Modeling of the Solidification of Immiscible Alloys	44
	J. Z. ZHAO, Z. Q. HU, L. RATKE	
	Abstract	44
6.1	Introduction	44
6.2	Theoretical Model	45
6.3	Numerical Results and Discussions	48
6.4	Conclusions	51
	Acknowledgments	51
	References	51

7	Phase-Field Modeling of Dendritic Solidification: Verification for the Model Predictions with Latest Experimental Data	52
	P.K. GALENKO, D.M. HERLACH, O. FUNKE, G. PHANIKUMAR	
	Abstract	52
7.1	Introduction	52
7.2	Governing equations	53
7.3	Results and Discussion	55
7.3.1	Dendritic Patterns	56
7.3.2	Comparison with experimental data	57
7.4	Conclusions	58
	Acknowledgements	59
	References	59
8	Phase-Field Modeling of Phase Transitions in Ternary Alloys	61
	BRITTA NESTLER	
8.1	Introduction	61
8.2	Phase-Field Model	62
8.3	Phase Transitions of Ternary Alloys	64
8.4	Outlook	68
	Acknowledgements	69
	References	69
9	Modeling of Heat and Solute Flows during Solidification of Droplets	70
	R. HERINGER, CH.-A. GANDIN, G. LESOULT, H. HENEIN	
	Abstract	70
9.1	Introduction	70
9.2	Experimental	71
9.3	Modeling	72
9.3.1	Macroscopic Heat and Solute Flows	72
9.3.2	Front Tracking and Growth Velocity	73
9.3.3	Microsegregation and Mushy Zone Solidification	74
9.3.4	Initial and Boundary Conditions, Numerical Implementation	75
9.4	Results	76
9.5	Concluding Remarks	80
	Acknowledgements	81
	References	81
10	Thermo-physical and Physical Properties for Use in Solidification Modelling of Multi-component Alloys	82
	N. SAUNDERS, Z. GUO, A. P. MIODOWNIK and J.-PH. SCHILLÉ	
	Abstract	82
10.1	Introduction	82
10.2	Technical Background	84
10.2.1	The Scheil-Gulliver Approach with Modification for fast C and N Diffusion	84

10.2.2	Modelling of Physical Properties	87
10.3	Example Calculations	88
10.3.1	Variations in Behaviour Within an Alloy Composition Specification Range	88
10.3.2	Behaviour of the Liquid in the Mushy Zone	90
10.4	Discussion	93
10.5	Summary and Conclusions	93
	References	94
11	Determination of Solidification Curves Based on DSC Experiments with Improved Heat-transfer Model	95
	DJORDJE MIRKOVIĆ, JOACHIM GRÖBNER, RAINER SCHMID-FETZER	
11.1	Introduction	95
11.2	DSC Experiment and Heat-Transfer Model (DSC-HTM)	96
11.2.1	DSC Experiment	96
11.2.2	Heat-transfer Model	96
11.3	Solidification Curves Determined by Alternative Methods	99
11.3.1	Quenching and Image Analysis (QIA)	99
11.3.2	Thermodynamic Calculation of Solidification Curves	99
11.4	Results and Discussion	100
	Acknowledgement	102
	References	102
12	Measurement of the Surface Tension of Undercooled Melts by the Oscillating Drop Method in an Electrostatic Levitator	103
	PETER L. RYDER and NILS WARNCKE	
12.1	Introduction	103
12.2	Experimental Methods	104
12.2.1	The Levitator	104
12.2.2	The Oscillating Drop Method	105
12.2.2.1	Principle	105
12.2.2.2	Excitation and Detection of the Oscillations	105
12.3	Results	106
12.4	Summary and Conclusions	109
	Acknowledgements	109
	References	109
13	Liquid-liquid Interfacial Tension and Wetting in Immiscible Al-based Systems	110
	WALTER HOYER, IVAN KABAN, MARKUS MERKWITZ	
13.1	Introduction	110
13.2	Experimental Technique	110
13.3	Results and Discussion	113
13.4	Conclusions	117
	Acknowledgements	118

References 118

14	In-Situ Optical Determination of Fraction Solid	119
	L. RATKE, D. TSCHUSCHNER	
	Abstract	119
14.1	Introduction	119
14.2	Experimental	120
14.3	Experimental Results	121
14.4	Mathematical Analysis of the Intensity Curves	122
14.5	Fraction Solid	124
14.6	Discussion and Conclusion	125
	References	127
15	Magnetic Effects on the Nucleation in Undercooled Co-Pd Melts	128
	DIRK HOLLAND-MORITZ AND FRANS SPAEPEN	
15.1	Introduction	128
15.2	Classical Approach to Describe the Nucleation Behavior of Co-Pd Melts	129
15.3.	Extension of the Classical Nucleation Model by Magnetic Contributions	132
15.4.	Conclusions	135
	Acknowledgements	135
	References	136
16	Identification of the Substrate of Heterogeneous Nucleation in Zn-Al Alloy Inoculated with ZnTi-Based Master Alloy	137
	WITOLD K. KRAJEWSKI, A. LINDSAY GREER, THOMAS E. QUESTED, WALDEMAR WOLCZYNSKI	
	Abstract	137
16.1	Introduction	137
16.2	Experimental Methods	138
16.3	Results and Discussion	140
16.3.1	Thermal Analysis and Structure	140
16.3.2	Crystal Structure and Chemical Composition	142
16.3.3	Crystal orientation	144
16.3.3.1	TEM Examination of Thin Foils	144
16.3.3.2	SEM – EBSD Examinations	144
16.4	Conclusions	146
	Acknowledgements	147
	References	147

17	Undercooling and Solidification of Liquid Silicon	148
	C. PANOFEN, R. P. LIU, D. HOLLAND-MORITZ, T. VOLKMANN, D.M. HERLACH	
17.1	Abstract	148
17.2	Introduction	148
17.3	Experimental	149
17.4	Results & Discussion	151
17.4.1	Surface Morphologies and Solidification Mode	151
17.4.2	Growth Velocity Results	153
17.5	Conclusion	155
	Acknowledgements	155
	References	155
18	Two-Phase Equilibrium in Binary Alloy Nano Particles	157
	P. BUNZEL, G. WILDE, H. RÖSNER, J. WEISSMÜLLER	
18.1	Introduction	157
18.2	Idealized Model System	158
18.2.1	The Model Alloy	158
18.2.2	Particle Shape and Properties of the Phase Boundary	159
18.2.3	Surface Area of the Phase Boundary	159
18.2.4	Molar Free Energies	160
18.3	Size-dependent Alloy Phase Diagrams	161
18.4	Conclusion	164
	Acknowledgement	165
	References	165
19	Three-dimensional Reconstruction of Experimentally Grown Xenon Dendrites	166
	H.M. SINGER and J.H. BILGRAM	
19.1	Introduction	166
19.2	Experimental Setup	167
19.3	Analytical Models vs. Simulations	168
19.4	Reconstruction	169
19.5	Results and Discussion	172
	References	173
20	Mechanically Deformed Primary Dendritic Structures Observed During the Solidification of Undercooled Melts	175
	ANDREW M. MULLIS, KALIN DRAGNEVSKI, & ROBERT F. COCHRANE	
20.1	Introduction	175
20.2	Experimental Method	177
20.3	Experimental Evidence for Deformed Dendritic Structures	178
20.4	Discussion	179
20.5	Summary & Conclusions	183
	References	183

21 Effect of Hydrodynamics on Microstructure Evolution of Nd-Fe-B Alloys 185

R. HERMANN, G. GERBETH, O. FILIP, J. PRIEDE, V. SHATROV

Abstract 185

21.1 Introduction 185

21.2 Experimental 186

21.3 Results 187

21.3.1 Levitation 187

21.3.2 Magnetic Two-phase Stirrer 190

21.4 Conclusions 192

Acknowledgements 193

References 193

22 Effect of the Fluid Convection Driven by a Rotating Magnetic Field on the Solidification of a PbSn Alloy 194

B. WILLERS, S. ECKERT, U. MICHEL, G. ZOUHAR

22.1 Introduction 194

22.2 Experimental Procedure 195

22.3 Discussion of the Results 197

22.3.1 Thermal analysis 197

22.3.2 UDV Measurements 199

22.3.3 Microstructure 200

22.4 Discussion, Conclusions 202

Acknowledgement 202

References 203

23 Grain Sedimentation and Melt Convection Phenomena During Globular Equiaxed Solidification 204

M. WU, A. LUDWIG and A. BÜHRIG-POLACZEK

23.1 Introduction 204

23.2 Brief Description of the Numerical Model 205

23.3 Experimental procedure 207

23.4 Results and discussions 208

23.5 Conclusions and outlook 211

Acknowledgments 212

References 212

24 Metastable Primary Solidification Modes in the Fe-Cr-Ni System During Laser Welding 213

H. SCHOBERT, TH. BÖLLINGHAUS, M. WOLF

Abstract 213

24.1 Introduction 213

24.2 Ferrite – Austenite Type of Primary Solidification Change 214

24.3 Geometric Analysis of Solidification Structures 218

24.4 Metastable States and Epitaxial Effects at the Fusion Line 222

24.5 Metastable Ferritic Solidification 223

24.6	Conclusions	225
	References	226
25	Crystallization of the $\text{Nd}_2\text{Fe}_{14}\text{B}$ Peritectic Phase from the Undercooled Melt by Containerless Processing	227
	SHUMPEI OZAWA, MINGJUN LI, SUGURU SUGIYAMA, ITARU JIMBO and KAZUHIKO KURIBAYASHI	
25.1	Introduction	227
25.2	Experimental Procedure	228
25.3	Results	228
25.3.1	$\text{Nd}_{11.8}\text{Fe}_{82.3}\text{B}_{5.9}$ ($\text{Nd}_2\text{Fe}_{14}\text{B}$) Alloy	228
25.3.2	$\text{Nd}_{14}\text{Fe}_{79}\text{B}_7$ Alloy	231
25.4	Discussions	234
25.5	Conclusion	237
	Acknowledgements	237
	References	238
26	Thermomagnetic Analyses of Nd-Fe-B Bulk Alloys Solidified from the Undercooled Melt	239
	S. REUTZEL, T. VOLKMANN, J. GAO, J. STROHMENGER, D.M. HERLACH	
	Abstract	239
26.1	Introduction	239
26.2	Experimental	240
26.3	Results and Discussion	241
26.4	Summary	248
	Acknowledgements	248
	References	249
27	Analysis of the Solidification Microstructure of Multi-component Gamma Titanium Aluminide Alloys	250
	VIOLA KÜSTNER, MICHAEL OEHRING, ANITA CHATTERJEE, HELMUT CLEMENS, FRITZ APPEL	
27.1	Introduction	250
27.2	Experiments	251
27.3	Results	251
27.4	Discussion	255
27.5	Conclusions	257
	Acknowledgements	257
	References	257
28	Formation of Eutectic Cells in Ternary Al-Cu-Ag Alloys	259
	ULRIKE HECHT, VICTOR WITUSIEWICZ, ANNE DREVERMANN, STEPHAN REX	
28.1	Introduction	259
28.2	Experimental Procedure	260
28.2.1	Sample Material	260

28.2.2	Solidification Process and Sample Analysis	260
28.3	Experimental Results	261
28.3.1	Planar Coupled Growth	262
28.3.2	Cellular Coupled Growth: Elongated and Regular Cells	264
28.4	Discussion of the Process of Cell Formation	267
28.5	Summary and Outlook	269
	Acknowledgements	270
	References	270
29	Lamellar Pattern Formation during 2D-Directional Solidification of Ternary Eutectic Alloys	271
	MARKUS APEL, BERND BÖTTGER, VICTOR WITUSIEWICZ, ULRIKE HECHT, INGO STEINBACH	
29.1	Introduction	271
29.2	Phase Field Model	271
29.2.1	Material Data	273
29.2.2	Numerical Aspects and Simulation Procedure	274
29.3	Simulation Results	275
29.3.1	The Basic State and Tilted Growth	275
29.3.2	Higher Order Stacking Sequences and Axisymmetric Growth	277
29.4	Discussion and Summary	277
	Acknowledgement	278
	References	279
30	Simulation of Stray Grain Formation in Investment Cast Turbine Blades	280
	X. L. YANG, H. B. DONG, W. WANG and P. D. LEE	
	Abstract	280
30.1	Introduction	280
30.2	Model Description	281
30.3	Simulation Parameters	282
30.4	Results and Discussion	283
30.4.1	Effect of Withdrawal Velocity and Isothermal Conditions on Undercooling	283
30.4.2	Dendritic Growth and Stray Grain Formation	284
30.4.3	Effect of Withdrawal Velocity on Stray Grain Formation	286
30.4.4	Effect of Inclination Angle of Isotherms on Stray Grain Formation	287
30.5	Conclusions	288
	Acknowledgements	288
	References	288
31	Laser Cladding Applications to Combinatorial Materials Science	290
	R. VILAR, P. CARVALHO, R. COLAÇO	
	Abstract	290
31.1	Introduction	290

31.2	Laser Assisted Synthetic Methods	292
31.3	Examples of Application	293
31.3.1	Structure and Properties of Ni-Al-Co Alloys	293
31.3.2	Metal-matrix-composites for Wear-resistant Coatings	295
31.4	Conclusions	298
	References	298

32 Control of Morphological Features in Micropatterned Ultrathin Films 300

E. MEYER, H.-G. BRAUN

Abstract 300

32.1	Introduction	300
32.2	Experimental	301
32.3	Results and Discussion	301
32.4	Perspectives	307
	Acknowledgement	308
	References	308

Author Index 311

Subject Index 313