

Contents

Preface *XI*

List of Contributors *XIII*

Part I	General Aspects of Crystal Growth Technology	1
1	Phase Diagrams for Crystal Growth	3
	<i>Manfred Mühlberg</i>	
1.1	Introduction	3
1.2	Thermodynamics and Phase Diagrams	4
1.3	Phase Diagrams vs. Crystal Growth from Liquid Phases	13
1.4	Conclusions	23
	References	25
2	Fundamentals of Equilibrium Thermodynamics of Crystal Growth	27
	<i>Klaus Jacobs</i>	
2.1	Introduction	27
2.2	Recapitulation of Some Basic Concepts	30
2.3	Relationships Between Thermodynamics and Kinetics	36
2.4	Thermodynamics of Melt Growth	38
2.5	Thermodynamics of Solution Growth	43
2.6	Thermodynamics of Crystal Growth from the Vapor	54
2.7	Solid–Solid Equilibria	65
2.8	Thermodynamics of Nucleation and Interfaces	67
2.9	Summary	71
	References	71
3	Thermodynamics, Origin, and Control of Defects	73
	<i>Peter Rudolph</i>	
3.1	Introduction	73
3.2	Native Point Defects	74

VI | Contents

3.3	Dislocations	81
3.4	Dislocation Cells and Grain Boundaries	85
3.5	Second-Phase Particles	92
3.6	Summary and Outlook	95
	References	96
4	Thermophysical Properties of Molten Silicon	103
	<i>Taketoshi Hibiya, Hiroyuki Fukuyama, Takao Tsukada and Masahito Watanabe</i>	
4.1	Introduction	103
4.2	Density and Volumetric Thermal Expansion Coefficient	106
4.3	Isobaric Molar Heat Capacity	110
4.4	Emissivity	113
4.5	Thermal Conductivity	117
4.6	Surface Tension	117
4.7	Diffusion Constant	121
4.8	Viscosity	123
4.9	Electrical Conductivity	125
4.10	Sensitivity Analysis	127
4.11	Recommended Thermophysical Property Data for Silicon System	127
4.12	Summary	129
	References	131
Part II	Simulation of Industrial Growth Processes	137
5	Yield Improvement and Defect Control in Bridgman-Type Crystal Growth with the Aid of Thermal Modeling	139
	<i>Jochen Friedrich</i>	
5.1	Introduction	139
5.2	Principles of Thermal Modeling	141
5.3	Verification of Numerical Models	154
5.4	Yield Enhancement by Defect Control	158
5.5	Conclusions	169
	References	170
6	Modeling of Czochralski Growth of Large Silicon Crystals	173
	<i>Vladimir Kalaev, Yuri Makarov and Alexander Zhmakin</i>	
6.1	Introduction	173
6.2	Numerical Model	174
6.3	Model Validation	181
6.4	Conclusions	191
	References	192

7	Global Analysis of Effects of Magnetic Field Configuration on Melt/Crystal Interface Shape and Melt Flow in a Cz-Si Crystal Growth	195
	<i>Koichi Kakimoto and Lijun Liu</i>	
7.1	Introduction	195
7.2	Model Description and Governing Equations Under a Transverse Magnetic Field	196
7.3	Computation Results for Model Validation	197
7.4	Numerical Analysis of a TMCZ Growth	199
7.5	Conclusions	202
	References	203
8	Modeling of Semitransparent Bulk Crystal Growth	205
	<i>Vladimir Kalaev, Yuri Makarov, Valentin Yuferev and Alexander Zhmakin</i>	
8.1	Introduction	205
8.2	Numerical Model	208
8.3	An Example: Growth of Bismuth Germanate Crystals	213
8.4	Conclusions	226
	References	227
Part III	Compound Semiconductors	229
9	Recent Progress in GaAs Growth Technologies at FREIBERGER	231
	<i>Stefan Eichler, Frank Börner, Thomas Bünger, Manfred Jurisch, Andreas Köhler, Ullrich Kretzer, Max Scheffer-Czygan, Berndt Weinert and Tilo Flade</i>	
9.1	Introduction	231
9.2	Properties of GaAs	232
9.3	Growth of Large-Diameter GaAs Single Crystals	235
9.4	LEC versus VB/VGF GaAs Wafers	246
9.5	Doping	251
9.6	Summary	263
	References	263
10	Interface Stability and Its Impact on Control Dynamics	267
	<i>Frank J. Bruni</i>	
10.1	Introduction	267
10.2	Diameter Control	268
10.3	Interface Transitions	271
10.4	Factors Influencing the Shape of the Solid/Liquid Interface	276
10.5	Conclusions and Discussion	280
	References	281

VIII | Contents

- 11 Use of Forced Mixing via the Accelerated Crucible Rotation Technique (ACRT) in Bridgman Growth of Cadmium Mercury Telluride (CMT) 283**
Peter Capper
- 11.1 Introduction 283
- 11.2 Elemental Purification (Mercury and Tellurium) 284
- 11.3 Bridgman Growth of CMT 285
- 11.4 Accelerated Crucible Rotation Technique (ACRT) 289
- 11.5 Uses in IR Devices 301
- 11.6 Summary 304
References 306
- 12 Crystal-Growth Technology for Ternary III-V Semiconductor Production by Vertical Bridgman and Vertical Gradient Freezing Methods with Accelerated Crucible Rotation Technique 307**
Partha S. Dutta
- 12.1 Introduction 307
- 12.2 Fundamental Crystal Growth Challenges for Ternary Compounds 308
- 12.3 Key Requirements for Ternary Substrates and Crystal-Growth Process 312
- 12.4 Optimization of Growth Parameters for Radially Homogeneous Crystals 314
- 12.5 Controlled Solute-Feeding Process for Axially Homogeneous Crystals 319
- 12.6 Steps in Ternary Crystal Production 327
- 12.7 Current Status of Ternary Substrates 332
- 12.8 Conclusion 332
References 333
- 13 X-Ray Diffraction Imaging of Industrial Crystals 337**
Keith Bowen, David Jacques, Petra Feichtinger and Matthew Wormington
- 13.1 Introduction 337
- 13.2 Digital X-Ray Diffraction Imaging 338
- 13.3 Applications Examples 341
- 13.4 Summary 349
References 349
- Part IV Scintillator Crystals 351**
- 14 Continuous Growth of Large Halide Scintillation Crystals 353**
Alexander Gektin, Valentine Goriletskiy and Borys Zaslavskiy
- 14.1 Introduction 353
- 14.2 Physical Principles Underlying Continuous Single-Crystal Growth 355

- 14.3 Technological Platform for Family of Continuous Crystal Growth Hardware 360
- 14.4 State-of-the-Art Crystal Performance for Continuous-Growth Techniques 367
- 14.5 Crystal Press Forging for Large Scintillator Development 376
- References 378

Part V Oxides 379

- 15 Phase Equilibria and Growth of Langasite-Type Crystals 381**
Satoshi Uda, Shou-Qi Wang, Hiromitsu Kimura and Xinming Huang
 - 15.1 Introduction – What is Langasite? 381
 - 15.2 Structure of Langasite-Type Crystals 382
 - 15.3 Study of Equilibrium Phase Diagram Around Langasite 384
 - 15.4 Study of Equilibrium Phase Diagram Around Langatate 391
 - 15.5 Conversion of Melting State of Langasite from Incongruent to Congruent 395
 - 15.6 Direct Growth of Langasite from the Melt 398
 - 15.7 Optimal Composition for the Growth of Langasite via the Czochralski Method 401
 - 15.8 Growth Technology of Four-Inch Langasite Along $[01\bar{1}1]$ 403
 - 15.9 Growth of Langasite by the Bridgman Technique 406
 - References 413
- 16 Flame-Fusion (Verneuil) Growth of Oxides 415**
Hans J. Scheel and Leonid Lytvynov
 - 16.1 Introduction 415
 - 16.2 Historical Background 416
 - 16.3 Impact of Verneuil's Principles 419
 - 16.4 Apparatus 420
 - 16.5 Powder Preparation and Feeding Control 423
 - 16.6 Thermal Conditions 427
 - 16.7 Growth of Compounds with Volatile Constituents 431
 - 16.8 Conclusions 432
 - References 433

Part VI Crystal Growth for Sustaining Energy 435

- 17 Saving Energy and Renewable Energy Through Crystal Technology 437**
Hans J. Scheel
 - 17.1 Introduction 437
 - 17.2 Storage, Transport and Saving of Energy 440
 - 17.3 World Energy Consumption and Conventional Energy Sources 441

x | Contents

- 17.4 Future Energy Sources 444
- 17.5 Costs and Risks of Conventional and of Future Energy Sources 447
- 17.6 Crystal Technology and its Role for Energy 449
- 17.7 Future Technologies for Mankind 451
- References 452

Part VII Crystal Machining 455

18 Crystal Sawing Technology 457

Hans J. Möller

- 18.1 Introduction 457
- 18.2 Multiwire Wafering Technique 457
- 18.3 Basic Sawing Mechanism 459
- 18.4 Experimental Results 470
- 18.5 Summary 472
- References 474

19 Plasma Chemical Vaporization Machining and Elastic Emission Machining 475

Yasuhisa Sano, Kazuya Yamamura, Hidekazu Mimura, Kazuto Yamauchi and Yuzo Mori

- 19.1 Introduction 475
- 19.2 Plasma Chemical Vaporization Machining (PCVM) 475
- 19.3 Elastic Emission Machining 482
- 19.4 Catalyst-Referred Etching 488
- References 493

Index 497