

Springer  
**Handbook** *of*  
**Crystal  
Growth**



DVD  
ROM

*Dhanaraj  
Byrappa  
Prasad  
Dudley  
Editors*



Springer

## Contents

|                             |      |
|-----------------------------|------|
| List of Abbreviations ..... | XXXI |
|-----------------------------|------|

## Part A Fundamentals of Crystal Growth and Defect Formation

|                                                                                             |    |
|---------------------------------------------------------------------------------------------|----|
| <b>1 Crystal Growth Techniques and Characterization: An Overview</b>                        |    |
| <i>Govindhan Dhanaraj, Kullaiah Byrappa, Vishwanath (Vish) Prasad, Michael Dudley</i> ..... | 3  |
| 1.1 Historical Developments .....                                                           | 3  |
| 1.2 Theories of Crystal Growth .....                                                        | 4  |
| 1.3 Crystal Growth Techniques .....                                                         | 6  |
| 1.4 Crystal Defects and Characterization .....                                              | 11 |
| <b>References</b> .....                                                                     | 15 |
| <b>2 Nucleation at Surfaces</b>                                                             |    |
| <i>Ivan V. Markov</i> .....                                                                 | 17 |
| 2.1 Equilibrium Crystal–Ambient Phase .....                                                 | 18 |
| 2.2 Work for Nucleus Formation .....                                                        | 24 |
| 2.3 Rate of Nucleation .....                                                                | 28 |
| 2.4 Saturation Nucleus Density .....                                                        | 35 |
| 2.5 Second-Layer Nucleation in Homoepitaxy .....                                            | 38 |
| 2.6 Mechanism of Clustering in Heteroepitaxy .....                                          | 43 |
| 2.7 Effect of Surfactants on Nucleation .....                                               | 45 |
| 2.8 Conclusions and Outlook .....                                                           | 48 |
| <b>References</b> .....                                                                     | 48 |
| <b>3 Morphology of Crystals Grown from Solutions</b>                                        |    |
| <i>Francesco Abbona, Dino Aquilano</i> .....                                                | 53 |
| 3.1 Equilibrium Shape .....                                                                 | 55 |
| 3.2 The Theoretical Growth Shape .....                                                      | 64 |
| 3.3 Factors Influencing the Crystal Habit .....                                             | 71 |
| 3.4 Surface Structure .....                                                                 | 72 |
| 3.5 Crystal Defects .....                                                                   | 73 |
| 3.6 Supersaturation – Growth Kinetics .....                                                 | 73 |
| 3.7 Solvent .....                                                                           | 75 |
| 3.8 Impurities .....                                                                        | 78 |
| 3.9 Other Factors .....                                                                     | 84 |
| 3.10 Evolution of Crystal Habit .....                                                       | 85 |
| 3.11 A Short Conclusion .....                                                               | 86 |
| 3.A Appendix .....                                                                          | 86 |
| <b>References</b> .....                                                                     | 87 |

|          |                                                                    |     |
|----------|--------------------------------------------------------------------|-----|
| <b>4</b> | <b>Generation and Propagation of Defects During Crystal Growth</b> |     |
|          | <i>Helmut Klapper</i> .....                                        | 93  |
| 4.1      | Overview .....                                                     | 94  |
| 4.2      | Inclusions .....                                                   | 95  |
| 4.3      | Striations and Growth Sectors .....                                | 101 |
| 4.4      | Dislocations .....                                                 | 107 |
| 4.5      | Twinning .....                                                     | 120 |
| 4.6      | Perfection of Crystals Grown Rapidly from Solution .....           | 125 |
|          | <b>References</b> .....                                            | 127 |
| <b>5</b> | <b>Single Crystals Grown Under Unconstrained Conditions</b>        |     |
|          | <i>Ichiro Sunagawa</i> .....                                       | 133 |
| 5.1      | Background .....                                                   | 134 |
| 5.2      | Smooth and Rough Interfaces: Growth Mechanism and Morphology ..... | 136 |
| 5.3      | Surface Microtopography .....                                      | 139 |
| 5.4      | Growth Forms of Polyhedral Crystals .....                          | 143 |
| 5.5      | Internal Morphology .....                                          | 146 |
| 5.6      | Perfection of Single Crystals .....                                | 152 |
|          | <b>References</b> .....                                            | 156 |
| <b>6</b> | <b>Defect Formation During Crystal Growth from the Melt</b>        |     |
|          | <i>Peter Rudolph</i> .....                                         | 159 |
| 6.1      | Overview .....                                                     | 159 |
| 6.2      | Point Defects .....                                                | 163 |
| 6.3      | Dislocations .....                                                 | 176 |
| 6.4      | Second-Phase Particles .....                                       | 188 |
| 6.5      | Faceting .....                                                     | 191 |
| 6.6      | Twinning .....                                                     | 193 |
| 6.7      | Summary .....                                                      | 194 |
|          | <b>References</b> .....                                            | 195 |

## Part B Crystal Growth from Melt Techniques

|          |                                                                                               |     |
|----------|-----------------------------------------------------------------------------------------------|-----|
| <b>7</b> | <b>Indium Phosphide: Crystal Growth and Defect Control by Applying Steady Magnetic Fields</b> |     |
|          | <i>David F. Bliss</i> .....                                                                   | 205 |
| 7.1      | Historical Overview .....                                                                     | 205 |
| 7.2      | Magnetic Liquid-Encapsulated Growth .....                                                     | 206 |
| 7.3      | Magnetic Field Interactions with the Melt .....                                               | 209 |
| 7.4      | Dislocation Density .....                                                                     | 216 |
| 7.5      | Magnetic Field Effects on Impurity Segregation .....                                          | 220 |
| 7.6      | Optical Characterization of InP:Fe .....                                                      | 224 |
| 7.7      | Summary .....                                                                                 | 226 |
|          | <b>References</b> .....                                                                       | 227 |

|           |                                                                                                                                     |     |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------|-----|
| <b>8</b>  | <b>Czochralski Silicon Single Crystals for Semiconductor and Solar Cell Applications</b>                                            |     |
|           | <i>Koichi Kakimoto</i> .....                                                                                                        | 231 |
| 8.1       | Silicon Single Crystals for LSIs and Solar Applications .....                                                                       | 232 |
| 8.2       | Control of Crystal Defects in Czochralski Silicon .....                                                                             | 237 |
| 8.3       | Growth and Characterization of Silicon Multicrystal for Solar Cell Applications .....                                               | 239 |
| 8.4       | Summary .....                                                                                                                       | 240 |
|           | <b>References</b> .....                                                                                                             | 241 |
| <b>9</b>  | <b>Czochralski Growth of Oxide Photorefractive Crystals</b>                                                                         |     |
|           | <i>Ernesto Diéguéz, Jose Luis Plaza, Mohan D. Aggarwal, Ashok K. Batra</i> .....                                                    | 245 |
| 9.1       | Background .....                                                                                                                    | 246 |
| 9.2       | Crystal Growth .....                                                                                                                | 246 |
| 9.3       | Design and Development of Czochralski Growth System .....                                                                           | 247 |
| 9.4       | Growth of Lithium Niobate Crystals and Its Characteristics .....                                                                    | 252 |
| 9.5       | Other Oxide Photorefractive Crystals .....                                                                                          | 262 |
| 9.6       | Growth of Sillenite Crystals and Its Characteristics .....                                                                          | 264 |
| 9.7       | Conclusions .....                                                                                                                   | 273 |
|           | <b>References</b> .....                                                                                                             | 273 |
| <b>10</b> | <b>Bulk Crystal Growth of Ternary III–V Semiconductors</b>                                                                          |     |
|           | <i>Partha S. Dutta</i> .....                                                                                                        | 281 |
| 10.1      | III–V Ternary Semiconductors .....                                                                                                  | 282 |
| 10.2      | Need for Ternary Substrates .....                                                                                                   | 283 |
| 10.3      | Criteria for Device-Grade Ternary Substrates .....                                                                                  | 284 |
| 10.4      | Introduction to Bridgman Crystal Growth Techniques .....                                                                            | 286 |
| 10.5      | Overview of III–V Binary Crystal Growth Technologies .....                                                                          | 292 |
| 10.6      | Phase Equilibria for Ternary Compounds .....                                                                                        | 300 |
| 10.7      | Alloy Segregation in Ternary Semiconductors .....                                                                                   | 302 |
| 10.8      | Crack Formation in Ternary Crystals .....                                                                                           | 304 |
| 10.9      | Single-Crystalline Ternary Seed Generation Processes .....                                                                          | 308 |
| 10.10     | Solute Feeding Processes for Homogeneous Alloy Growth .....                                                                         | 311 |
| 10.11     | Role of Melt–Solid Interface Shapes .....                                                                                           | 318 |
| 10.12     | Conclusion .....                                                                                                                    | 321 |
|           | <b>References</b> .....                                                                                                             | 321 |
| <b>11</b> | <b>Growth and Characterization of Antimony–Based Narrow–Bandgap III–V Semiconductor Crystals for Infrared Detector Applications</b> |     |
|           | <i>Vijay K. Dixit, Handady L. Bhat</i> .....                                                                                        | 327 |
| 11.1      | Importance of Antimony–Based Semiconductors .....                                                                                   | 329 |
| 11.2      | Phase Diagrams .....                                                                                                                | 330 |
| 11.3      | Crystal Structure and Bonding .....                                                                                                 | 331 |
| 11.4      | Material Synthesis and Purification .....                                                                                           | 333 |

|           |                                                                                                                    |     |
|-----------|--------------------------------------------------------------------------------------------------------------------|-----|
| 11.5      | Bulk Growth of InSb .....                                                                                          | 334 |
| 11.6      | Structural Properties of InSb, InAs <sub>x</sub> Sb <sub>1-x</sub> , and InBi <sub>x</sub> Sb <sub>1-x</sub> ..... | 340 |
| 11.7      | Physical Properties of InSb, InAs <sub>x</sub> Sb <sub>1-x</sub> , and InBi <sub>x</sub> Sb <sub>1-x</sub> .....   | 346 |
| 11.8      | Applications .....                                                                                                 | 357 |
| 11.9      | Concluding Remarks and Future Outlook .....                                                                        | 359 |
|           | <b>References</b> .....                                                                                            | 360 |
| <b>12</b> | <b>Crystal Growth of Oxides by Optical Floating Zone Technique</b>                                                 |     |
|           | <i>Hanna A. Dabkowska, Antoni B. Dabkowski</i> .....                                                               | 367 |
| 12.1      | Historical Notes .....                                                                                             | 367 |
| 12.2      | Optical Floating Zone Technique – Application for Oxides .....                                                     | 368 |
| 12.3      | Optical Floating Zone<br>and Traveling Solvent Crystal Growth Techniques .....                                     | 369 |
| 12.4      | Advantages and Limitations of the Floating Zone Techniques .....                                                   | 370 |
| 12.5      | Optical Floating Zone Furnaces .....                                                                               | 371 |
| 12.6      | Experimental Details of Ceramics and Rod Preparation for OFZT .....                                                | 372 |
| 12.7      | Stable Growth of Congruently and Incongruently Melting Oxides .....                                                | 373 |
| 12.8      | Constitutional Supercooling and Crystallization Front Stability .....                                              | 375 |
| 12.9      | Crystal Growth Termination and Cooling .....                                                                       | 377 |
| 12.10     | Characterization of Crystals Grown by the OFZ Technique .....                                                      | 377 |
| 12.11     | Determination of Defects in Crystals – The Experimental Approach ..                                                | 380 |
| 12.12     | Details of Conditions for Growth of Selected Oxide Single Crystals<br>by OFZ and TSFZ Methods .....                | 383 |
| 12.13     | Conclusions .....                                                                                                  | 386 |
|           | <b>References</b> .....                                                                                            | 386 |
| <b>13</b> | <b>Laser-Heated Pedestal Growth of Oxide Fibers</b>                                                                |     |
|           | <i>Marcello R.B. Andreeta, Antonio Carlos Hernandez</i> .....                                                      | 393 |
| 13.1      | Fiber-Pulling Research .....                                                                                       | 394 |
| 13.2      | The Laser-Heated Pedestal Growth Technique .....                                                                   | 399 |
| 13.3      | Fundamentals .....                                                                                                 | 402 |
| 13.4      | Fiber Growth Aspects .....                                                                                         | 409 |
| 13.5      | Conclusions .....                                                                                                  | 418 |
|           | <b>References</b> .....                                                                                            | 419 |
| <b>14</b> | <b>Synthesis of Refractory Materials by Skull Melting Technique</b>                                                |     |
|           | <i>Vyacheslav V. Osiko, Mikhail A. Borik, Elena E. Lomonova</i> .....                                              | 433 |
| 14.1      | Overview .....                                                                                                     | 433 |
| 14.2      | Techniques for Growth of Single Crystals in a Cold Crucible .....                                                  | 435 |
| 14.3      | Growth of Single Crystals Based on Zirconium Dioxide .....                                                         | 443 |
| 14.4      | Glass Synthesis by Skull Melting in a Cold Crucible .....                                                          | 465 |
| 14.5      | Conclusion .....                                                                                                   | 469 |
|           | <b>References</b> .....                                                                                            | 469 |

|                                                                                                      |     |
|------------------------------------------------------------------------------------------------------|-----|
| <b>15 Crystal Growth of Laser Host Fluorides and Oxides</b>                                          |     |
| <i>Hongjun Li, Jun Xu</i> .....                                                                      | 479 |
| 15.1 Crystal Growth of Laser Fluorides and Oxides from Melt.....                                     | 479 |
| 15.2 Laser Crystal Defects .....                                                                     | 487 |
| 15.3 Crystal Growth Techniques Characterization .....                                                | 501 |
| <b>References</b> .....                                                                              | 503 |
| <br><b>16 Shaped Crystal Growth</b>                                                                  |     |
| <i>Vitali A. Tatartchenko</i> .....                                                                  | 509 |
| 16.1 Definitions and Scope of Discussion: SCG by CST .....                                           | 510 |
| 16.2 DSC – Basis of SCG by CST.....                                                                  | 512 |
| 16.3 SA and SCG by CZT .....                                                                         | 517 |
| 16.4 SA and SCG by VT .....                                                                          | 519 |
| 16.5 SA and SCG by FZT .....                                                                         | 522 |
| 16.6 TPS Capillary Shaping.....                                                                      | 522 |
| 16.7 TPS Sapphire Growth .....                                                                       | 539 |
| 16.8 TPS Silicon Growth .....                                                                        | 546 |
| 16.9 TPS Metals Growth .....                                                                         | 551 |
| 16.10 TPS Peculiarities .....                                                                        | 552 |
| <b>References</b> .....                                                                              | 552 |
| <br><b>Part C Solution Growth of Crystals</b>                                                        |     |
| <br><b>17 Bulk Single Crystals Grown from Solution on Earth and in Microgravity</b>                  |     |
| <i>Mohan D. Aggarwal, Ashok K. Batra, Ravindra B. Lal, Benjamin G. Penn, Donald O. Frazier</i> ..... | 559 |
| 17.1 Crystallization: Nucleation and Growth Kinetics .....                                           | 561 |
| 17.2 Low-Temperature Solution Growth .....                                                           | 566 |
| 17.3 Solution Growth by Temperature Lowering .....                                                   | 567 |
| 17.4 Triglycine Sulfate Crystal Growth: A Case Study .....                                           | 574 |
| 17.5 Solution Growth of Triglycine Sulfate Crystals in Microgravity .....                            | 582 |
| 17.6 Protein Crystal Growth .....                                                                    | 592 |
| 17.7 Concluding Remarks .....                                                                        | 594 |
| <b>References</b> .....                                                                              | 594 |
| <br><b>18 Hydrothermal Growth of Polyscale Crystals</b>                                              |     |
| <i>Kullaiah Byrappa</i> .....                                                                        | 599 |
| 18.1 History of Hydrothermal Growth of Crystals.....                                                 | 603 |
| 18.2 Thermodynamic Basis of the Hydrothermal Growth of Crystals.....                                 | 606 |
| 18.3 Apparatus Used in the Hydrothermal Growth of Crystals .....                                     | 615 |
| 18.4 Hydrothermal Growth of Some Selected Crystals.....                                              | 620 |
| 18.5 Hydrothermal Growth of Fine Crystals.....                                                       | 634 |

|           |                                                                                                  |     |
|-----------|--------------------------------------------------------------------------------------------------|-----|
| 18.6      | Hydrothermal Growth of Nanocrystals .....                                                        | 637 |
| 18.7      | Concluding Remarks .....                                                                         | 640 |
| 18.A      | Appendix .....                                                                                   | 641 |
|           | <b>References</b> .....                                                                          | 646 |
| <b>19</b> | <b>Hydrothermal and Ammonothermal Growth of ZnO and GaN</b>                                      |     |
|           | <i>Michael J. Callahan, Qi-Sheng Chen</i> .....                                                  | 655 |
| 19.1      | Overview of Hydrothermal and Ammonothermal Growth<br>of Large Crystals .....                     | 657 |
| 19.2      | Requirements for Growth of Large, Low-Defect Crystals .....                                      | 661 |
| 19.3      | Physical and Mathematical Models .....                                                           | 666 |
| 19.4      | Process Simulations .....                                                                        | 669 |
| 19.5      | Hydrothermal Growth of ZnO Crystals .....                                                        | 674 |
| 19.6      | Ammonothermal GaN .....                                                                          | 681 |
| 19.7      | Conclusion .....                                                                                 | 685 |
|           | <b>References</b> .....                                                                          | 685 |
| <b>20</b> | <b>Stoichiometry and Domain Structure<br/>of KTP-Type Nonlinear Optical Crystals</b>             |     |
|           | <i>Michael Roth</i> .....                                                                        | 691 |
| 20.1      | Background .....                                                                                 | 691 |
| 20.2      | Stoichiometry and Ferroelectric Phase Transitions .....                                          | 697 |
| 20.3      | Growth-Induced Ferroelectric Domains .....                                                       | 703 |
| 20.4      | Artificial Domain Structures .....                                                               | 708 |
| 20.5      | Nonlinear Optical Crystals .....                                                                 | 713 |
|           | <b>References</b> .....                                                                          | 716 |
| <b>21</b> | <b>High-Temperature Solution Growth:<br/>Application to Laser and Nonlinear Optical Crystals</b> |     |
|           | <i>Joan J. Carvajal, Maria Cinta Pujol, Francesc Díaz</i> .....                                  | 725 |
| 21.1      | Basics .....                                                                                     | 726 |
| 21.2      | High-Temperature Solution Growth .....                                                           | 731 |
| 21.3      | Growth of Bulk Laser and NLO Single Crystals by the TSSG Method ....                             | 736 |
| 21.4      | Liquid-Phase Epitaxy:<br>Growth of Epitaxial Films of Laser and NLO Materials .....              | 746 |
|           | <b>References</b> .....                                                                          | 752 |
| <b>22</b> | <b>Growth and Characterization of KDP and Its Analogs</b>                                        |     |
|           | <i>Sheng-Lai Wang, Xun Sun, Xu-Tang Tao</i> .....                                                | 759 |
| 22.1      | Background .....                                                                                 | 759 |
| 22.2      | Mechanism and Kinetics of Crystallization .....                                                  | 761 |
| 22.3      | Growth Techniques for Single Crystals .....                                                      | 769 |
| 22.4      | Effect of Growth Conditions on Defects of Crystals .....                                         | 776 |
| 22.5      | Investigations on Crystal Quality .....                                                          | 783 |
|           | <b>References</b> .....                                                                          | 789 |

## Part D Crystal Growth from Vapor

|                                                                              |     |
|------------------------------------------------------------------------------|-----|
| <b>23 Growth and Characterization of Silicon Carbide Crystals</b>            |     |
| <i>Govindhan Dhanaraj, Balaji Raghothamachar, Michael Dudley</i> .....       | 797 |
| 23.1 Silicon Carbide – Background and History .....                          | 797 |
| 23.2 Vapor Growth .....                                                      | 799 |
| 23.3 High-Temperature Solution Growth .....                                  | 801 |
| 23.4 Industrial Bulk Growth by Seed Sublimation .....                        | 802 |
| 23.5 Structural Defects and Their Configurations .....                       | 805 |
| 23.6 Concluding Remarks .....                                                | 816 |
| <b>References</b> .....                                                      | 817 |
| <b>24 AlN Bulk Crystal Growth by Physical Vapor Transport</b>                |     |
| <i>Rafael Dalmau, Zlatko Sitar</i> .....                                     | 821 |
| 24.1 PVT Crystal Growth .....                                                | 822 |
| 24.2 High-Temperature Materials Compatibility .....                          | 825 |
| 24.3 Self-Seeded Growth of AlN Bulk Crystals .....                           | 827 |
| 24.4 Seeded Growth of AlN Bulk Crystals .....                                | 829 |
| 24.5 Characterization of High-Quality Bulk Crystals .....                    | 832 |
| 24.6 Conclusions and Outlook .....                                           | 839 |
| <b>References</b> .....                                                      | 839 |
| <b>25 Growth of Single-Crystal Organic Semiconductors</b>                    |     |
| <i>Christian Kloc, Theo Siegrist, Jens Pflaum</i> .....                      | 845 |
| 25.1 Basics .....                                                            | 845 |
| 25.2 Theory of Nucleation and Crystal Growth .....                           | 847 |
| 25.3 Organic Materials of Interest for Semiconducting Single Crystals .....  | 848 |
| 25.4 Pregrowth Purification .....                                            | 850 |
| 25.5 Crystal Growth .....                                                    | 854 |
| 25.6 Quality of Organic Semiconducting Single Crystals .....                 | 862 |
| 25.7 Organic Single-Crystalline Field-Effect Transistors .....               | 863 |
| 25.8 Conclusions .....                                                       | 864 |
| <b>References</b> .....                                                      | 865 |
| <b>26 Growth of III-Nitrides with Halide Vapor Phase Epitaxy (HVPE)</b>      |     |
| <i>Carl Hemmingsson, Bo Monemar, Yoshinao Kumagai, Akinori Koukitu</i> ..... | 869 |
| 26.1 Growth Chemistry and Thermodynamics .....                               | 869 |
| 26.2 HVPE Growth Equipment .....                                             | 872 |
| 26.3 Substrates and Templates for Bulk GaN Growth .....                      | 875 |
| 26.4 Substrate Removal Techniques .....                                      | 879 |
| 26.5 Doping Techniques for GaN in HVPE .....                                 | 882 |
| 26.6 Defect Densities, Dislocations, and Residual Impurities .....           | 883 |
| 26.7 Some Important Properties of HVPE-Grown Bulk GaN Material .....         | 887 |
| 26.8 Growth of AlN by HVPE: Some Preliminary Results .....                   | 888 |
| 26.9 Growth of InN by HVPE: Some Preliminary Results .....                   | 890 |
| <b>References</b> .....                                                      | 891 |

|                                                                    |     |
|--------------------------------------------------------------------|-----|
| <b>27 Growth of Semiconductor Single Crystals from Vapor Phase</b> |     |
| <i>Ramasamy Dhanasekaran</i> .....                                 | 897 |
| 27.1 Classifications of Vapor Growth .....                         | 899 |
| 27.2 Chemical Vapor Transport – Transport Kinetics .....           | 901 |
| 27.3 Thermodynamic Considerations .....                            | 905 |
| 27.4 Growth of II–VI Compound Semiconductors by CVT .....          | 912 |
| 27.5 Growth of Nanomaterial from Vapor Phase .....                 | 916 |
| 27.6 Growth of I–III–VI <sub>2</sub> Compounds .....               | 917 |
| 27.7 Growth of GaN by VPE .....                                    | 925 |
| 27.8 Conclusion .....                                              | 929 |
| <b>References</b> .....                                            | 930 |

## Part E Epitaxial Growth and Thin Films

|                                                                            |     |
|----------------------------------------------------------------------------|-----|
| <b>28 Epitaxial Growth of Silicon Carbide by Chemical Vapor Deposition</b> |     |
| <i>Ishwara B. Bhat</i> .....                                               | 939 |
| 28.1 Polytypes of Silicon Carbide .....                                    | 941 |
| 28.2 Defects in SiC .....                                                  | 942 |
| 28.3 Epitaxial Growth of Silicon Carbide .....                             | 944 |
| 28.4 Epitaxial Growth on Patterned Substrates .....                        | 952 |
| 28.5 Conclusions .....                                                     | 961 |
| <b>References</b> .....                                                    | 961 |

|                                                                |     |
|----------------------------------------------------------------|-----|
| <b>29 Liquid-Phase Electroepitaxy of Semiconductors</b>        |     |
| <i>Sadik Dost</i> .....                                        | 967 |
| 29.1 Background .....                                          | 967 |
| 29.2 Early Theoretical and Modeling Studies .....              | 971 |
| 29.3 Two-Dimensional Continuum Models .....                    | 977 |
| 29.4 LPEE Growth Under a Stationary Magnetic Field .....       | 978 |
| 29.5 Three-Dimensional Simulations .....                       | 981 |
| 29.6 High Growth Rates in LPEE: Electromagnetic Mobility ..... | 992 |
| <b>References</b> .....                                        | 996 |

|                                                                              |      |
|------------------------------------------------------------------------------|------|
| <b>30 Epitaxial Lateral Overgrowth of Semiconductors</b>                     |      |
| <i>Zbigniew R. Zytkeiwicz</i> .....                                          | 999  |
| 30.1 Overview .....                                                          | 1000 |
| 30.2 Mechanism of Epitaxial Lateral Overgrowth from the Liquid Phase .....   | 1002 |
| 30.3 Dislocations in ELO Layers .....                                        | 1011 |
| 30.4 Strain in ELO Layers .....                                              | 1016 |
| 30.5 Recent Progress in Lateral Overgrowth of Semiconductor Structures ..... | 1026 |
| 30.6 Concluding Remarks .....                                                | 1034 |
| <b>References</b> .....                                                      | 1035 |

**31 Liquid-Phase Epitaxy of Advanced Materials**

|                                                                                          |      |
|------------------------------------------------------------------------------------------|------|
| <i>Christine F. Klemenz Rivenbark</i> .....                                              | 1041 |
| 31.1 Historical Development of LPE .....                                                 | 1042 |
| 31.2 Fundamentals of LPE and Solution Growth .....                                       | 1042 |
| 31.3 Requirements for Liquid-Phase Epitaxy.....                                          | 1044 |
| 31.4 Developing New Materials:<br>On the Choice of the Epitaxial Deposition Method ..... | 1044 |
| 31.5 LPE of High-Temperature Superconductors .....                                       | 1046 |
| 31.6 LPE of Calcium Gallium Germanates.....                                              | 1055 |
| 31.7 Liquid-Phase Epitaxy of Nitrides .....                                              | 1059 |
| 31.8 Conclusions.....                                                                    | 1063 |
| <b>References</b> .....                                                                  | 1064 |

**32 Molecular-Beam Epitaxial Growth of HgCdTe**

|                                                                                        |      |
|----------------------------------------------------------------------------------------|------|
| <i>James W. Garland, Sivalingam Sivananthan</i> .....                                  | 1069 |
| 32.1 Overview.....                                                                     | 1070 |
| 32.2 Theory of MBE Growth .....                                                        | 1073 |
| 32.3 Substrate Materials.....                                                          | 1076 |
| 32.4 Design of the Growth Hardware .....                                               | 1088 |
| 32.5 In situ Characterization Tools<br>for Monitoring and Controlling the Growth ..... | 1090 |
| 32.6 Nucleation and Growth Procedure.....                                              | 1101 |
| 32.7 Dopants and Dopant Activation.....                                                | 1104 |
| 32.8 Properties of HgCdTe Epilayers Grown by MBE .....                                 | 1107 |
| 32.9 HgTe/CdTe Superlattices .....                                                     | 1112 |
| 32.10 Architectures of Advanced IR Detectors .....                                     | 1115 |
| 32.11 IR Focal-Plane Arrays (FPAs) .....                                               | 1118 |
| 32.12 Conclusions.....                                                                 | 1119 |
| <b>References</b> .....                                                                | 1121 |

**33 Metalorganic Vapor-Phase Epitaxy of Diluted Nitride and Arsenide Quantum Dots**

|                                                 |      |
|-------------------------------------------------|------|
| <i>Udo W. Pohl</i> .....                        | 1133 |
| 33.1 Principle of MOVPE.....                    | 1133 |
| 33.2 Diluted Nitride InGaAsN Quantum Wells..... | 1137 |
| 33.3 InAs/GaAs Quantum Dots.....                | 1142 |
| 33.4 Concluding Remarks .....                   | 1148 |
| <b>References</b> .....                         | 1148 |

**34 Formation of SiGe Heterostructures and Their Properties**

|                                                     |      |
|-----------------------------------------------------|------|
| <i>Yasuhiro Shiraki, Akira Sakai</i> .....          | 1153 |
| 34.1 Background .....                               | 1153 |
| 34.2 Band Structures of Si/Ge Heterostructures..... | 1154 |
| 34.3 Growth Technologies .....                      | 1156 |
| 34.4 Surface Segregation .....                      | 1157 |
| 34.5 Critical Thickness .....                       | 1161 |
| 34.6 Mechanism of Strain Relaxation .....           | 1163 |

|                                                          |                                                                                                 |      |
|----------------------------------------------------------|-------------------------------------------------------------------------------------------------|------|
| 34.7                                                     | Formation of Relaxed SiGe Layers .....                                                          | 1165 |
| 34.8                                                     | Formation of Quantum Wells, Superlattices, and Quantum Wires .....                              | 1173 |
| 34.9                                                     | Dot Formation .....                                                                             | 1177 |
| 34.10                                                    | Concluding Remarks and Future Prospects .....                                                   | 1184 |
|                                                          | <b>References</b> .....                                                                         | 1184 |
| <b>35</b>                                                | <b>Plasma Energetics in Pulsed Laser and Pulsed Electron Deposition</b>                         |      |
|                                                          | <i>Mikhail D. Strikovski, Jeonggoo Kim, Solomon H. Kolagani</i> .....                           | 1193 |
| 35.1                                                     | Energetic Condensation in Thin Film Deposition .....                                            | 1193 |
| 35.2                                                     | PLD and PED Techniques .....                                                                    | 1194 |
| 35.3                                                     | Transformations of Atomic Energy in PLD and PED .....                                           | 1195 |
| 35.4                                                     | Optimization of Plasma Flux for Film Growth .....                                               | 1204 |
| 35.5                                                     | Conclusions .....                                                                               | 1208 |
|                                                          | <b>References</b> .....                                                                         | 1209 |
| <br><b>Part F Modeling in Crystal Growth and Defects</b> |                                                                                                 |      |
| <b>36</b>                                                | <b>Convection and Control in Melt Growth of Bulk Crystals</b>                                   |      |
|                                                          | <i>Chung-Wen Lan</i> .....                                                                      | 1215 |
| 36.1                                                     | Physical Laws for Transport Processes .....                                                     | 1217 |
| 36.2                                                     | Flow Structures in the Melt .....                                                               | 1219 |
| 36.3                                                     | Flow Control by External Forces .....                                                           | 1228 |
| 36.4                                                     | Outlook .....                                                                                   | 1238 |
|                                                          | <b>References</b> .....                                                                         | 1238 |
| <b>37</b>                                                | <b>Vapor Growth of III Nitrides</b>                                                             |      |
|                                                          | <i>Dang Cai, Lili Zheng, Hui Zhang</i> .....                                                    | 1243 |
| 37.1                                                     | Overview of Vapor Growth of III Nitrides .....                                                  | 1244 |
| 37.2                                                     | Mathematical Models for AlN/GaN Vapor Deposition .....                                          | 1248 |
| 37.3                                                     | Characteristics of AlN/GaN Vapor Deposition .....                                               | 1251 |
| 37.4                                                     | Modeling of GaN IVPE Growth – A Case Study .....                                                | 1258 |
| 37.5                                                     | Surface Evolution of GaN/AlN Film Growth from Vapor .....                                       | 1274 |
| 37.6                                                     | Concluding Remarks .....                                                                        | 1275 |
|                                                          | <b>References</b> .....                                                                         | 1276 |
| <b>38</b>                                                | <b>Continuum-Scale Quantitative Defect Dynamics<br/>in Growing Czochralski Silicon Crystals</b> |      |
|                                                          | <i>Milind S. Kulkarni</i> .....                                                                 | 1281 |
| 38.1                                                     | The Discovery of Microdefects .....                                                             | 1283 |
| 38.2                                                     | Defect Dynamics in the Absence of Impurities .....                                              | 1284 |
| 38.3                                                     | Czochralski Defect Dynamics in the Presence of Oxygen .....                                     | 1304 |
| 38.4                                                     | Czochralski Defect Dynamics in the Presence of Nitrogen .....                                   | 1313 |
| 38.5                                                     | The Lateral Incorporation of Vacancies in Czochralski Silicon Crystals .....                    | 1321 |
| 38.6                                                     | Conclusions .....                                                                               | 1328 |
|                                                          | <b>References</b> .....                                                                         | 1332 |

|                                                                                              |      |
|----------------------------------------------------------------------------------------------|------|
| <b>39 Models for Stress and Dislocation Generation in Melt Based Compound Crystal Growth</b> |      |
| <i>Vishwanath (Vish) Prasad, Srinivas Pendurti</i> .....                                     | 1335 |
| 39.1 Overview .....                                                                          | 1335 |
| 39.2 Crystal Growth Processes .....                                                          | 1336 |
| 39.3 Dislocations in Semiconductors Materials .....                                          | 1337 |
| 39.4 Models for Dislocation Generation .....                                                 | 1339 |
| 39.5 Diamond Structure of the Crystal .....                                                  | 1343 |
| 39.6 Deformation Behavior of Semiconductors .....                                            | 1346 |
| 39.7 Application of the Haasen Model to Crystal Growth .....                                 | 1350 |
| 39.8 An Alternative Model .....                                                              | 1351 |
| 39.9 Model Summary and Numerical Implementation .....                                        | 1360 |
| 39.10 Numerical Results .....                                                                | 1362 |
| 39.11 Summary .....                                                                          | 1374 |
| <b>References</b> .....                                                                      | 1375 |
| <b>40 Mass and Heat Transport in BS and EFG Systems</b>                                      |      |
| <i>Thomas F. George, Stefan Balint, Liliانا Braescu</i> .....                                | 1379 |
| 40.1 Model-Based Prediction of the Impurity Distribution – Vertical BS System .....          | 1380 |
| 40.2 Model-Based Prediction of the Impurity Distribution – EFG System ..                     | 1389 |
| <b>References</b> .....                                                                      | 1400 |

## Part G Defects Characterization and Techniques

|                                                                               |      |
|-------------------------------------------------------------------------------|------|
| <b>41 Crystalline Layer Structures with X-Ray Diffractometry</b>              |      |
| <i>Paul F. Fewster</i> .....                                                  | 1405 |
| 41.1 X-Ray Diffractometry .....                                               | 1406 |
| 41.2 Basic Direct X-Ray Diffraction Analysis from Layered Structures .....    | 1407 |
| 41.3 Instrumental and Theoretical Considerations .....                        | 1412 |
| 41.4 Examples of Analysis from Low to High Complexity .....                   | 1413 |
| 41.5 Rapid Analysis .....                                                     | 1419 |
| 41.6 Wafer Micromapping .....                                                 | 1420 |
| 41.7 The Future .....                                                         | 1421 |
| <b>References</b> .....                                                       | 1422 |
| <b>42 X-Ray Topography Techniques for Defect Characterization of Crystals</b> |      |
| <i>Balaji Raghothamachar, Michael Dudley, Govindhan Dhanaraj</i> .....        | 1425 |
| 42.1 Basic Principles of X-Ray Topography .....                               | 1426 |
| 42.2 Historical Development of the X-Ray Topography Technique .....           | 1428 |
| 42.3 X-Ray Topography Techniques and Geometry .....                           | 1430 |
| 42.4 Theoretical Background for X-Ray Topography .....                        | 1435 |
| 42.5 Mechanisms for Contrast on X-Ray Topographs .....                        | 1440 |

|           |                                                                                          |      |
|-----------|------------------------------------------------------------------------------------------|------|
| 42.6      | Analysis of Defects on X-Ray Topographs .....                                            | 1445 |
| 42.7      | Current Application Status and Development .....                                         | 1449 |
|           | <b>References</b> .....                                                                  | 1450 |
| <b>43</b> | <b>Defect-Selective Etching of Semiconductors</b>                                        |      |
|           | <i>Jan L. Weyher, John J. Kelly</i> .....                                                | 1453 |
| 43.1      | Wet Etching of Semiconductors: Mechanisms .....                                          | 1454 |
| 43.2      | Wet Etching of Semiconductors: Morphology and Defect Selectivity ..                      | 1459 |
| 43.3      | Defect-Selective Etching Methods .....                                                   | 1461 |
|           | <b>References</b> .....                                                                  | 1473 |
| <b>44</b> | <b>Transmission Electron Microscopy Characterization of Crystals</b>                     |      |
|           | <i>Jie Bai, Shixin Wang, Lu-Min Wang, Michael Dudley</i> .....                           | 1477 |
| 44.1      | Theoretical Basis of TEM Characterization of Defects .....                               | 1477 |
| 44.2      | Selected Examples of Application of TEM to Semiconductor Systems ..                      | 1493 |
| 44.3      | Concluding Remarks: Current Application Status and Development ..                        | 1514 |
|           | <b>References</b> .....                                                                  | 1515 |
| <b>45</b> | <b>Electron Paramagnetic Resonance Characterization of Point Defects</b>                 |      |
|           | <i>Mary E. Zvanut</i> .....                                                              | 1521 |
| 45.1      | Electronic Paramagnetic Resonance .....                                                  | 1522 |
| 45.2      | EPR Analysis .....                                                                       | 1524 |
| 45.3      | Scope of EPR Technique .....                                                             | 1534 |
| 45.4      | Supplementary Instrumentation and Supportive Techniques .....                            | 1538 |
| 45.5      | Summary and Final Thoughts .....                                                         | 1545 |
|           | <b>References</b> .....                                                                  | 1546 |
| <b>46</b> | <b>Defect Characterization in Semiconductors with Positron Annihilation Spectroscopy</b> |      |
|           | <i>Filip Tuomisto</i> .....                                                              | 1551 |
| 46.1      | Positron Annihilation Spectroscopy .....                                                 | 1552 |
| 46.2      | Identification of Point Defects and Their Charge States .....                            | 1560 |
| 46.3      | Defects, Doping, and Electrical Compensation .....                                       | 1565 |
| 46.4      | Point Defects and Growth Conditions .....                                                | 1569 |
| 46.5      | Summary .....                                                                            | 1576 |
|           | <b>References</b> .....                                                                  | 1576 |

## Part H Special Topics in Crystal Growth

|           |                                                                                 |      |
|-----------|---------------------------------------------------------------------------------|------|
| <b>47</b> | <b>Protein Crystal Growth Methods</b>                                           |      |
|           | <i>Andrea E. Gutiérrez-Quezada, Roberto Arreguín-Espinosa, Abel Moreno</i> .... | 1583 |
| 47.1      | Properties of Biomacromolecular Solutions .....                                 | 1584 |
| 47.2      | Transport Phenomena and Crystallization .....                                   | 1587 |
| 47.3      | Classic Methods of Crystal Growth .....                                         | 1587 |
| 47.4      | Protein Crystallization by Diffusion-Controlled Methods .....                   | 1588 |

|      |                                                                      |      |
|------|----------------------------------------------------------------------|------|
| 47.5 | New Trends in Crystal Growth (Crystal Quality Enhancement) .....     | 1591 |
| 47.6 | 2-D Characterization via Atomic Force Microscopy (Case Study).....   | 1595 |
| 47.7 | 3-D Characterization via X-Ray Diffraction and Related Methods ..... | 1598 |
|      | <b>References</b> .....                                              | 1599 |

#### 48 Crystallization from Gels

|       |                                                                  |      |
|-------|------------------------------------------------------------------|------|
|       | <i>S. Narayana Kalkura, Subramanian Natarajan</i> .....          | 1607 |
| 48.1  | Gel Growth in Crystal Deposition Diseases.....                   | 1608 |
| 48.2  | Experimental Methods.....                                        | 1609 |
| 48.3  | Pattern Formation in Gel Systems.....                            | 1610 |
| 48.4  | Crystals Grown Using Gel Technique .....                         | 1611 |
| 48.5  | Application in Crystal Deposition Diseases .....                 | 1614 |
| 48.6  | Crystal-Deposition-Related Diseases .....                        | 1616 |
| 48.7  | Calcium Oxalate.....                                             | 1617 |
| 48.8  | Calcium Phosphates .....                                         | 1619 |
| 48.9  | Hydroxyapatite (HAP).....                                        | 1620 |
| 48.10 | Dicalcium Phosphate Dihydrate (DCPD) .....                       | 1620 |
| 48.11 | Calcium Sulfate .....                                            | 1623 |
| 48.12 | Uric Acid and Monosodium Urate Monohydrate.....                  | 1623 |
| 48.13 | L-Cystine .....                                                  | 1624 |
| 48.14 | L-Tyrosine, Hippuric Acid, and Ciprofloxacin .....               | 1625 |
| 48.15 | Atherosclerosis and Gallstones .....                             | 1625 |
| 48.16 | Crystallization of Hormones: Progesterone and Testosterone ..... | 1628 |
| 48.17 | Pancreatitis.....                                                | 1628 |
| 48.18 | Conclusions.....                                                 | 1629 |
|       | <b>References</b> .....                                          | 1630 |

#### 49 Crystal Growth and Ion Exchange in Titanium Silicates

|      |                                                                                 |      |
|------|---------------------------------------------------------------------------------|------|
|      | <i>Aaron J. Celestian, John B. Parise, Abraham Clearfield</i> .....             | 1637 |
| 49.1 | X-Ray Methods.....                                                              | 1637 |
| 49.2 | Equipment for Time-Resolved Experiments .....                                   | 1642 |
| 49.3 | Detectors .....                                                                 | 1642 |
| 49.4 | Software .....                                                                  | 1644 |
| 49.5 | Types of In Situ Cells .....                                                    | 1645 |
| 49.6 | In-Situ Studies of Titanium Silicates (Na-TS) with Sitalakite<br>Topology ..... | 1649 |
| 49.7 | Discussion of In Situ Studies.....                                              | 1658 |
| 49.8 | Summary .....                                                                   | 1660 |
|      | <b>References</b> .....                                                         | 1660 |

#### 50 Single-Crystal Scintillation Materials

|      |                                                          |      |
|------|----------------------------------------------------------|------|
|      | <i>Martin Nikl, Anna Vedda, Valentin V. Laguta</i> ..... | 1663 |
| 50.1 | Background .....                                         | 1663 |
| 50.2 | Scintillation Materials.....                             | 1670 |
| 50.3 | Future Prospects.....                                    | 1689 |
| 50.4 | Conclusions.....                                         | 1691 |
|      | <b>References</b> .....                                  | 1691 |

|                                                                        |      |
|------------------------------------------------------------------------|------|
| <b>51 Silicon Solar Cells: Materials, Devices, and Manufacturing</b>   |      |
| <i>Mohan Narayanan, Ted Ciszek</i> .....                               | 1701 |
| 51.1 Silicon Photovoltaics.....                                        | 1701 |
| 51.2 Crystal Growth Technologies for Silicon Photovoltaics.....        | 1704 |
| 51.3 Cell Fabrication Technologies.....                                | 1711 |
| 51.4 Summary and Discussion.....                                       | 1715 |
| <b>References</b> .....                                                | 1716 |
| <br>                                                                   |      |
| <b>52 Wafer Manufacturing and Slicing Using Wiresaw</b>                |      |
| <i>Imin Kao, Chunhui Chung, Roosevelt Moreno Rodriguez</i> .....       | 1719 |
| 52.1 From Crystal Ingots to Prime Wafers.....                          | 1721 |
| 52.2 Slicing: The First Postgrowth Process in Wafer Manufacturing..... | 1726 |
| 52.3 Modern Wiresaw in Wafer Slicing.....                              | 1730 |
| 52.4 Conclusions and Further Reading.....                              | 1733 |
| <b>References</b> .....                                                | 1733 |
| <br>                                                                   |      |
| <b>Acknowledgements</b> .....                                          | 1737 |
| <b>About the Authors</b> .....                                         | 1741 |
| <b>Detailed Contents</b> .....                                         | 1759 |
| <b>Subject Index</b> .....                                             | 1791 |