

# Contents

---

## Part I Background

---

### 1 Prehistory of Quasicrystals

Jens-Boie Suck .....	3
1.1 Introduction .....	3
1.2 Mathematics .....	4
1.3 Crystallography .....	6
1.4 Incommensurate Structures .....	9
1.5 Structure Models of Amorphous Solids .....	11
1.6 Supercooled Liquids .....	12
References .....	14

### 2 A Guide to Mathematical Quasicrystals

Michael Baake .....	17
2.1 Introduction .....	17
2.2 Non-Crystallographic Symmetries .....	19
2.3 Diffraction .....	20
2.4 Quasiperiodicity and the Projection Method .....	24
2.5 Minimal Embedding and Further Examples .....	27
2.6 LI Classes and Symmetry .....	31
2.7 Parametrization of LI Classes .....	32
2.8 Local Derivability and MLD Classes .....	34
2.9 Local Equivalence and Limit Translation Module .....	36
2.10 Local Derivability and Symmetry Preservation .....	37
2.11 Inflation Symmetries and Matching Rules .....	38
2.12 A Summary of the Perfect World .....	41
2.13 Alternatives: Disorder and Random Tilings .....	41
2.14 Concluding Remarks .....	45
References .....	46

### 3 Aperiodic Tilings on the Computer

Uwe Grimm, Michael Schreiber .....	49
3.1 Introduction .....	49
3.2 How to Construct Quasiperiodic Tilings .....	50

3.3	A Small Example Program: Inflating the Chair Tiling .....	51
3.4	Once Again: The Ubiquitous Fibonacci Chain .....	55
3.5	The Octagonal Tiling: Projection and Inflation .....	59
3.6	De Bruijn's Ingenuity: The Dualization Method .....	61
3.7	Giving It a Trial: A Penrose-Tiling Puzzle .....	63
3.8	Concluding Remarks .....	64
	References .....	65

---

## Part II Atomic Structure and Growth

---

### 4 Quasicrystallography

	Ted Janssen .....	69
4.1	Introduction .....	69
4.2	Symmetry .....	70
4.3	Embedding .....	71
4.4	Superspace Groups .....	74
4.5	The Icosahedral Groups .....	76
4.6	Dihedral Groups .....	78
4.7	Wyckoff Positions .....	80
4.8	Diffraction .....	80
	References .....	81

### 5 Experimental Determination of the Structure of Quasicrystalline Alloys: Experimental Techniques and Modeling

	Michel Boudard .....	82
5.1	Introduction .....	82
5.2	X-Ray and Neutron Diffraction .....	83
5.3	Quasicrystallography or How to Extract Information about the Structure from the Diffraction Data .....	87
5.4	An Example: The Structure of the i-AlPdMn Icosahedral Phase ..	94
5.5	Further Ideas for Building Models .....	108
	References .....	113

### 6 Electron Microscopy and Surface Investigations of Quasicrystals

	Hans-Ude Nissen, Conradin Beeli .....	115
6.1	Introduction .....	115
6.2	High-Resolution Electron Micrographs and Their Interpretation ..	121
6.3	Decagonal Quasicrystals .....	126
6.4	Icosahedral Quasicrystal Structures .....	139
6.5	Dodecagonal, Octagonal, and Cubic Quasicrystals .....	148
6.6	Special Electron Diffraction Techniques Applied to Quasicrystals ..	152

6.7	Surface-Sensitive Techniques Applied to Quasicrystals.....	155
	References .....	161
<b>7</b>	<b>Structure of Quasicrystals via Pair Potentials</b>	
	Marek Mihalkovič .....	167
7.1	Introduction .....	167
7.2	Pair Potentials .....	168
7.3	Approaches to Structure Determination from Structural Energies ..	169
7.4	Tiling-Decoration Approach .....	171
7.5	Summary.....	181
	References .....	181
<b>8</b>	<b>Quasicrystals as Hierarchical Packing of Overlapping Clusters</b>	
	Christian Janot, Jean-Marie Dubois .....	183
8.1	Introduction .....	183
8.2	Penrose Tiling with a Single Prototile .....	185
8.3	The Jellium Model for Clusters and Quasicrystals .....	187
8.4	The Cluster Structure of AlPdMn Quasicrystals .....	191
8.5	Conclusion .....	196
	References .....	196
<b>9</b>	<b>Modeling Quasicrystal Growth</b>	
	Uwe Grimm, Dieter Joseph.....	199
9.1	Introduction .....	199
9.2	Growing Ideal Penrose Tilings .....	201
9.3	Growth in the Random Scenario .....	204
9.4	Atomistic Growth Models .....	205
9.5	Algorithmically Motivated Cluster Growth Models.....	208
9.6	Physically Motivated Cluster Growth Models .....	209
9.7	Random Tiling Growth Models .....	211
9.8	Concluding Remarks.....	214
	References .....	216

---

**Part III Production of Quasicrystalline Alloys**

---

<b>10</b>	<b>Production of Quasicrystalline Alloys and Phase Diagrams</b>	
	Reinhard Lück.....	221
10.1	Introduction .....	221
10.2	Establishing and Mapping of High-Order Phase Diagrams .....	221
10.3	Methods of Investigation .....	223
10.4	Examples of Ternary Systems .....	225
10.5	Calculation of Phase Diagrams .....	228

10.6 Using Phase Diagrams of Quasicrystal-Forming Systems . . . . . 229  
 10.7 Conclusion . . . . . 231  
 References . . . . . 231

**11 Undercooling of Quasicrystal-Forming Liquid Alloys**

Dirk Holland-Moritz . . . . . 233  
 11.1 Introduction . . . . . 233  
 11.2 Undercooling and Nucleation . . . . . 234  
 11.3 Experimental Studies on the Nucleation Behavior  
     of Quasicrystalline and Polytetrahedral Phases . . . . . 238  
 11.4 Estimation of the Energy of the Solid–Liquid Interface . . . . . 244  
 11.5 Conclusions . . . . . 246  
 References . . . . . 246

---

**Part IV Defects and Mechanical Properties**

---

**12 Phasons, Dislocations, and Cracks**

Hans-Rainer Trebin . . . . . 251  
 12.1 Introduction . . . . . 251  
 12.2 Phasons . . . . . 251  
 12.3 Plasticity . . . . . 256  
 12.4 Cracks . . . . . 259  
 12.5 Conclusion . . . . . 259  
 References . . . . . 261

**13 Defects**

Markus Wollgarten, Volker Franz, Michael Feuerbacher, Knut Urban . . 262  
 13.1 Introduction . . . . . 262  
 13.2 Observation and Characterization of Phason Defects . . . . . 262  
 13.3 Observation and Characterization of Dislocations . . . . . 268  
 13.4 Dislocation Motion and Dissociation . . . . . 275  
 References . . . . . 277

**14 Ion Channeling in Quasicrystals**

Dieter Plachke, Heinz Dieter Carstanjen . . . . . 280  
 14.1 Introduction . . . . . 280  
 14.2 Basics of Channeling . . . . . 281  
 14.3 Lindhard’s Theory of Channeling . . . . . 288  
 14.4 Experimental . . . . . 291  
 14.5 Ion Channeling in Quasicrystals . . . . . 294  
 References . . . . . 304

**15 Mechanical Properties of Quasicrystals**  
 Knut Urban, Michael Feuerbacher, Markus Wollgarten . . . . . 305

15.1 Introduction . . . . . 305  
 15.2 High-Temperature Plastic Deformation . . . . . 306  
 15.3 Discussion . . . . . 315  
 References . . . . . 317

---

**Part V Electronic Properties**

---

**16 Electronic Conductivity of Quasicrystals and Approximants**  
 Stephan Roche, Claire Berger, Didier Mayou . . . . . 321

16.1 Introduction . . . . . 321  
 16.2 Electronic Conductivity of Quasicrystals . . . . . 322  
 16.3 Localization in Quasiperiodic Systems . . . . . 325  
 16.4 Kubo–Greenwood Conductivity . . . . . 328  
 16.5 Conclusion . . . . . 334  
 References . . . . . 335

**17 Electron Densities of States in Quasicrystals and Approximants**  
 Esther Belin-Ferré . . . . . 338

17.1 Introduction . . . . . 338  
 17.2 Photoemission Spectroscopies . . . . . 338  
 17.3 X-Ray Emission and Photoabsorption Spectroscopies . . . . . 343  
 17.4 Electron Energy Loss Spectroscopy . . . . . 354  
 17.5 Optical Measurements . . . . . 356  
 17.6 Conclusion . . . . . 359  
 References . . . . . 360

**18 Electronic Transport Properties of Quasicrystalline Thin Films**  
 Roland Haberkern . . . . . 364

18.1 Introduction . . . . . 364  
 18.2 Preparation of Thin Quasicrystalline Films . . . . . 365  
 18.3 Amorphous to Quasicrystalline Transition . . . . . 367  
 18.4 Comparing the a- with the i-Phase – The Scattering Approach . . . 369  
 18.5 The Al-Pd-Re System . . . . . 373  
 18.6 Conclusion . . . . . 376  
 References . . . . . 377

**19 Electron Transport in a Magnetic Field:**

**A Landauer-Formula Approach**

Gerald Kasner, Holger Wegmann, Harald Böttger .....	379
19.1 Introduction .....	379
19.2 The Model .....	380
19.3 Density of States and Magnetoconductance .....	382
19.4 Spectra in a Magnetic Field .....	384
19.5 Conclusions .....	391
References .....	392

**20 Phonons and Electrons in Quasicrystals**

Marián Krajíč, Jürgen Hafner .....	393
20.1 Introduction .....	393
20.2 Reciprocal Quasilattice, Quasi-Brillouin Zone .....	394
20.3 Numerical Techniques for the Calculation of Spectra of Elementary Excitations in Quasicrystals .....	396
20.4 Phonons in Quasicrystals .....	402
20.5 Electrons in Quasicrystals .....	408
20.6 Conclusion .....	418
References .....	419

---

**Part VI Atomic Dynamics and Thermodynamics**

---

**21 Computer Simulations of Lattice Dynamics  
in Quasicrystals**

Ted Janssen .....	423
21.1 Introduction .....	423
21.2 Phonons in IC-Modulated Phases and IC Composites .....	424
21.3 Models for Phonons in Quasicrystals .....	427
21.4 Model Calculations .....	429
21.5 The Character of Spectra and Eigenvectors .....	432
21.6 Surface Phonons in Quasicrystals .....	433
References .....	434

**22 Experimental Determination of the Dispersion  
of Vibrations in Monodomain Quasicrystalline Alloys**

Bernard Hennion, Marguerite Quilichini .....	436
22.1 Introduction .....	436
22.2 Inelastic Neutron Scattering on Three-Axis Spectrometer .....	437
22.3 Experimental Results with Ultrasonic and Brillouin Measurements	442
22.4 Neutron Scattering Measurements on Monodomain Quasicrystals .	442
22.5 Conclusion .....	451
References .....	452

<b>23 Vibrational Density of States of Stable and Metastable Quasicrystalline Alloys</b>	
Jens-Boie Suck .....	454
23.1 Introduction .....	454
23.2 Determination of the Generalized Vibrational Density of States by Neutron Inelastic Scattering .....	456
23.3 Results for Metastable Quasicrystalline Alloys .....	460
23.4 Stable Quasicrystalline Alloys .....	462
23.5 Temperature Dependence of the GVDOS .....	466
References .....	469
<b>24 Thermodynamics of Quasicrystals</b>	
Reinhard Lück .....	472
24.1 Introduction .....	472
24.2 Molar Heat .....	473
24.3 Thermodynamic Functions of Formation .....	474
24.4 Metastable Quasicrystals and Heat of Transformation .....	477
24.5 Stability Arguments .....	478
24.6 Conclusion .....	482
References .....	483
<hr/>	
<b>Part VII Magnetic Properties</b>	
<hr/>	
<b>25 Magnetic Properties of Quasicrystals and Approximants</b>	
Guy Trambly de Laissardière, Didier Mayou .....	487
25.1 Introduction .....	487
25.2 Localized Moments on Transition Metal Impurity .....	489
25.3 One Transition Atom in a Realistic Effective Metallic Medium ...	494
25.4 Interaction Between Transition Metal Atoms .....	498
25.5 Conclusion .....	502
References .....	503
<hr/>	
<b>Part VIII Surfaces and Applications</b>	
<hr/>	
<b>26 Bulk and Surface Properties of Quasicrystalline Materials and Their Potential Applications</b>	
Jean-Marie Dubois .....	507
26.1 Introduction .....	507
26.2 Recurrent Localization of Electronic States .....	508
26.3 Phase Selection and Preparation Conditions .....	510
26.4 Potential Applications of Transport Properties .....	514
26.5 Surface Properties .....	518

XIV Contents

26.6 Strengthening of Metallic Matrices .....	527
26.7 Hydrogen Storage .....	529
26.8 At the Edge of a New Era in Quasicrystals Science .....	531
References .....	532
<b>A Further Reading: Literature on Quasicrystals</b>	
Michael Baake, Uwe Grimm .....	539
<b>Index</b> .....	545