

Contents

Preface IX

1	Introduction	1
2	Bulk Crystals: Three-Dimensional Lattices	5
2.1	Basic Definitions	5
2.2	Representation of Bulk Crystals	9
2.2.1	Alternative Descriptions Conserving the Lattice Representation	10
2.2.2	Alternative Descriptions Affecting the Lattice Representation	12
2.2.2.1	Cubic, Hexagonal, and Trigonal Lattices	13
2.2.2.2	Superlattices	21
2.2.2.3	Linear Transformations of Lattices	23
2.2.3	Centered Lattices	26
2.3	Periodicity Cells of Lattices	29
2.4	Lattice Symmetry	33
2.5	Neighbor Shells	44
2.6	Quasicrystals	55
2.7	Exercises	61
3	Crystal Layers: Two-Dimensional Lattices	65
3.1	Basic Definitions, Miller Indices	65
3.2	Reciprocal Lattice	68
3.3	Netplane-Adapted Lattice Vectors	71
3.4	Symmetrically Appropriate Lattice Vectors: Minkowski Reduction	74
3.5	Miller Indices for Cubic Lattices	75
3.6	Alternative Definition of Miller Indices: Hexagonal Miller–Bravais Indices	77
3.7	Symmetry Properties of Netplanes	80
3.7.1	Centered Netplanes	81

3.7.2	Inversion	84
3.7.3	Rotation	86
3.7.4	Mirror Lines	91
3.7.5	Glide Reflection	103
3.7.6	Symmetry Groups	111
3.8	Crystal Systems and Bravais Lattices in Two Dimensions	115
3.9	Crystallographic Classification of Netplanes	121
3.9.1	Oblique Netplanes	122
3.9.2	Primitive Rectangular Netplanes	123
3.9.3	Centered Rectangular Netplanes	127
3.9.4	Square Netplanes	128
3.9.5	Hexagonal Netplanes	130
3.9.6	Classification Overview	134
3.10	Exercises	135
4	Ideal Single Crystal Surfaces	139
4.1	Basic Definitions, Termination	139
4.2	Morphology of Surfaces, Stepped and Kinked Surfaces	143
4.3	Miller Index Decomposition	146
4.4	Chiral Surfaces	156
4.5	Exercises	166
5	Real Crystal Surfaces	169
5.1	Surface Relaxation	169
5.2	Surface Reconstruction	170
5.3	Faceting	182
5.4	Exercises	186
6	Adsorbate Layers	191
6.1	Definition and Classification	191
6.2	Wood Notation of Surface Geometry	199
6.3	Symmetry and Domain Formation	205
6.4	Exercises	214
7	Experimental Analysis of Real Crystal Surfaces	219
7.1	Experimental Methods	219
7.2	The NIST Surface Structure Database	221
7.3	Exercises	224
8	Nanotubes	225
8.1	Basic Definition	225
8.2	Nanotubes and Symmetry	229
8.3	Complex Nanotubes	233
8.4	Exercises	235

Appendix A: Mathematics of the Wood Notation 237

Appendix B: Mathematics of the Minkowski Reduction 243

Appendix C: Some Details of Number Theory 247

C.1 Basic Definitions 247

C.2 Euclid's Algorithm 250

C.3 Linear Diophantine Equations 251

C.4 Quadratic Diophantine Equations 254

Appendix D: Some Details of Vector Calculus and Linear Algebra 261

Appendix E: Parameter Tables of Crystals 265

Appendix F: Relevant Web Sites 267

References 269

Glossary and Abbreviations 273

Index 283

