

# *Contents*

## *Part I. Basics*

### *Chapter 1. X-Rays and Diffraction*

1.1.	X-Rays . . . . .	3
1.2.	The Production of X-Rays . . . . .	5
1.3.	Diffraction . . . . .	14
1.4.	A Very Brief Historical Perspective . . . . .	18

### *Chapter 2. Lattices and Crystal Structures*

2.1.	Types of Solid and Order . . . . .	21
2.2.	Point Lattices and the Unit Cell . . . . .	23
2.3.	Crystal Systems and Bravais Lattices . . . . .	24
2.4.	Crystal Structures . . . . .	27
2.4.1.	One Atom per Lattice Point . . . . .	27
2.4.2.	Two Atoms of the Same Kind per Lattice Point	31
2.4.3.	Two Different Atoms per Lattice Point . . .	36
2.4.4.	More than Two Atoms per Lattice Point . . .	40
2.5.	Notation for Crystal Structures . . . . .	41
2.6.	Miller Indices . . . . .	43
2.7.	Diffraction from Crystalline Materials—Bragg's Law	50
2.8.	The Structure Factor . . . . .	52
2.9.	Diffraction from Amorphous Materials . . . . .	60

### *Chapter 3. Practical Aspects of X-Ray Diffraction*

3.1.	Geometry of an X-Ray Diffractometer . . . . .	63
------	---	----

3.2.	Components of an X-Ray Diffractometer . . . . .	65
3.2.1.	The X-Ray Source . . . . .	65
3.2.2.	The Specimen . . . . .	66
3.2.3.	The Optics . . . . .	68
3.2.4.	The Detector . . . . .	72
3.3.	Examination of a Standard X-Ray Diffraction Pattern	80
3.4.	Sources of Information . . . . .	85
3.5.	X-Ray Safety . . . . .	91
3.6.	Introduction to the Experimental Modules . . . . .	93

## *Part II. Experimental Modules*

<i>Module 1. Crystal Structure Determination. I: Cubic Structures</i> . . . . .	97
<i>Module 2. Crystal Structure Determination. II: Hexagonal Structures</i> . . . . .	125
<i>Module 3. Precise Lattice Parameter Measurements</i> . . . . .	153
<i>Module 4. Phase Diagram Determination</i> . . . . .	167
<i>Module 5. Detection of Long-Range Ordering</i> . . . . .	193
<i>Module 6. Determination of Crystallite Size and Lattice Strain</i> . . . . .	207
<i>Module 7. Quantitative Analysis of Powder Mixtures</i> . . . . .	223
<i>Module 8. Identification of an Unknown Specimen</i> . . . . .	237

## *Appendices*

<i>Appendix 1. Plane-Spacing Equations and Unit Cell Volumes</i> . . . . .	251
<i>Appendix 2. Quadratic Forms of Miller Indices for the Cubic System</i> . . . . .	254

<i>Appendix 3. Atomic and Ionic Scattering Factors of Some Selected Elements</i> . . . . .	255
<i>Appendix 4. Summary of Structure Factor Calculations</i> . . . . .	256
<i>Appendix 5. Mass Absorption Coefficients <math>\mu/\rho</math> (<math>\text{cm}^2/\text{g}</math>) and Densities <math>\rho</math> (<math>\text{g}/\text{cm}^3</math>) of Some Selected Elements</i> . . . . .	257
<i>Appendix 6. Multiplicity Factors</i> . . . . .	258
<i>Appendix 7. Lorentz–Polarization Factor</i> $\left( \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right)$ . . . . .	259
<i>Appendix 8. Physical Constants and Conversion Factors</i> . . . . .	261
<i>Appendix 9. JCPDS–ICDD Card Numbers for Some Common Materials</i> . . . . .	262
<i>Appendix 10. Crystal Structures and Lattice Parameters of Some Selected Materials</i> . . . . .	263
<i>Bibliography</i> . . . . .	265
<i>Index</i> . . . . .	271