## Contents

1 Crystals and crystal structures 1.1 The nature of the crystalline state 1.2 Constructing crystals from close-packed hexagonal layers of atom 1.3 Unit cells of the hcp and ccp structures 1.4 Constructing crystals from square layers of atoms	6 9 9 11 18
<ul> <li>The nature of the crystalline state</li> <li>Constructing crystals from close-packed hexagonal layers of atom</li> <li>Unit cells of the hcp and ccp structures</li> </ul>	s 5 6 9 9 11 18
<ul><li>1.2 Constructing crystals from close-packed hexagonal layers of atom</li><li>1.3 Unit cells of the hcp and ccp structures</li></ul>	s 5 6 9 9 11 18
1.3 Unit cells of the hcp and ccp structures	6 9 9 11 18
· · · · · · · · · · · · · · · · · · ·	9 9 11 18
1.4 Constructing crystals from square layers of atoms	9 11 18
- · · · · · · · · · · · · · · · · · · ·	11 18
1.5 Constructing body-centred cubic crystals	18
1.6 Interstitial structures	
1.7 Some simple ionic and covalent structures	
1.8 Representing crystals in projection: crystal plans	20
1.9 Stacking faults and twins	20
1.10 The crystal chemistry of inorganic compounds	27
1.10.1 Bonding in inorganic crystals	28
1.10.2 Representing crystals in terms of coordination polyhedro	
1.11 Introduction to some more complex crystal structures	32
1.11.1 Perovskite (CaTiO <sub>3</sub> ), barium titanate (BaTiO <sub>3</sub> ) and	22
related structures	32
1.11.2 Tetrahedral and octahedral structures—silicon carbide and alumina	34
1.11.3 The oxides and oxy-hydroxides of iron	36
1.11.4 Silicate structures	38
1.11.5 The structures of silica, ice and water	44
1.11.6 The structures of carbon	48
Exercises	54
2 Two-dimensional patterns, lattices and symmetry	56
2.1 Approaches to the study of crystal structures	56
2.2 Two-dimensional patterns and lattices	57
2.3 Two-dimensional symmetry elements	59
2.4 The five plane lattices	62
2.5 The seventeen plane groups	65
2.6 One-dimensional symmetry: border or frieze patterns	66
2.7 Symmetry in art and design: counterchange patterns	66
2.8 Layer (two-sided) symmetry and examples in woven textiles	74
2.9 Non-periodic patterns and tilings	78
Exercises	83

x Contents

3	Bravais lattices and crystal systems					
	3.1	Introduction	86			
	3.2	The fourteen space (Bravais) lattices	86			
	3.3	The symmetry of the fourteen Bravais lattices: crystal systems	90			
	3.4	The coordination or environments of Bravais lattice points:				
		space-filling polyhedra	92			
	Exerc		97			
1	C	atal				
4	Crystal symmetry: point groups, space groups,					
	symmetry-related properties and quasiperiodic					
	crys	tals	99			
	4.1	Symmetry and crystal habit	99			
	4.2	The thirty-two crystal classes	101			
	4.3	Centres and inversion axes of symmetry	102			
	4.4	Crystal symmetry and properties	106			
	4.5	Translational symmetry elements	110			
	4.6	Space groups	113			
	4.7	Bravais lattices, space groups and crystal structures	120			
	4.8	The crystal structures and space groups of organic compounds	123			
		4.8.1 The close packing of organic molecules	124			
		4.8.2 Long-chain polymer molecules	127			
	4.9	Quasicrystals (quasiperiodic crystals or crystalloids)	129			
	Exerc	ises	134			
5	Describing lattice planes and directions in crystals:					
O	- · ·					
	Miller indices and zone axis symbols					
	5.1	Introduction	135			
	5.2	Indexing lattice directions—zone axis symbols	136			
	5.3	Indexing lattice planes—Miller indices	137			
	5.4	Miller indices and zone axis symbols in cubic crystals	140			
	5.5	Lattice plane spacings, Miller indices and Laue indices	141			
	5.6	Zones, zone axes and the zone law, the addition rule	143			
		5.6.1 The Weiss zone law or zone equation	143			
		5.6.2 Zone axis at the intersection of two planes	143			
		5.6.3 Plane parallel to two directions	144			
		5.6.4 The addition rule	144			
	5.7	Indexing in the trigonal and hexagonal systems: Weber symbols				
	and Miller-Bravais indices					
	5.8	Transforming Miller indices and zone axis symbols	148			
	5.9	Transformation matrices for trigonal crystals with rhombohedral				
		lattices	151			
	5.10	A simple method for inverting a $3 \times 3$ matrix	152			
	Exercises					

Contents xi

6	The	reciprocal lattice	155		
	6.1	Introduction	155		
	6.2	Reciprocal lattice vectors	155		
	6.3	Reciprocal lattice unit cells	157		
	6.4	Reciprocal lattice cells for cubic crystals	161		
	6.5	Proofs of some geometrical relationships using reciprocal lattice			
		vectors	163		
		6.5.1 Relationships between $a$ , $b$ , $c$ and $a^*$ , $b^*$ , $c^*$	163		
		6.5.2 The addition rule	164		
		6.5.3 The Weiss zone law or zone equation	164		
		6.5.4 d-spacing of lattice planes (hkl)	165		
		6.5.5 Angle $\rho$ between plane normals $(h_1k_1l_1)$ and $(h_2k_2l_2)$	165		
		6.5.6 Definition of $a^*$ , $b^*$ , $c^*$ in terms of $a$ , $b$ , $c$	166		
		6.5.7 Zone axis at intersection of planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$	166		
		6.5.8 A plane containing two directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$	166		
	6.6	Lattice planes and reciprocal lattice planes	166		
	6.7	Summary	169		
	Exerc	ises	169		
7	The diffraction of light				
	7.1 Introduction				
	7.1	Simple observations of the diffraction of light	170 172		
	7.3	The nature of light: coherence, scattering and interference	177		
	7.4	Analysis of the geometry of diffraction patterns from gratings and	1 / /		
	7.4	nets	180		
	7.5	The resolving power of optical instruments: the telescope, camera,	100		
	7.5	microscope and the eye			
	Exercises				
	Liter		197		
8	X-ra	ay diffraction: the contributions of Max von			
	Laue, W. H. and W. L. Bragg and P. P. Ewald				
	8.1	Introduction	198		
	8.2	Laue's analysis of X-ray diffraction: the three Laue equations	199		
	8.3	Bragg's analysis of X-ray diffraction: Bragg's law	202		
	8.4	Ewald's synthesis: the reflecting sphere construction	204		
	Exerc		209		
			_0,		
9	The diffraction of X-rays				
	9.1	Introduction	210		
	9.2	The intensities of X-ray diffracted beams: the structure factor			
		equation and its applications	214		

xii Contents

	9.3	The broadening of diffracted beams: reciprocal lattice points and nodes			
		9.3.1 The Scherrer equation: reciprocal lattice points and nodes	223 223		
		9.3.2 Integrated intensity and its importance	227		
		9.3.3 Crystal size and perfection: mosaic structure and	,		
		coherence length	227		
	9.4	Fixed $\theta$ , varying $\lambda$ X-ray techniques: the Laue method	228		
	9.5 Fixed $\lambda$ , varying $\theta$ X-ray techniques: oscillation, rotation and				
		precession methods	231		
		9.5.1 The oscillation method	232		
		9.5.2 The rotation method	234		
		9.5.3 The precession method	235		
	9.6	X-ray diffraction from single crystal thin films and multilayers	239		
	9.7				
	9.8 Practical considerations: X-ray sources and recording techn		246		
		9.8.1 The generation of X-rays in X-ray tubes	247		
		9.8.2 Synchrotron X-ray generation	248		
		9.8.3 X-ray recording techniques	249		
	Exerc	ises	249		
10	X-ray diffraction of polycrystalline materials 253				
		1 0			
	10.1	Introduction	252		
	10.2	The geometrical basis of polycrystalline (powder) X-ray diffraction	253		
		techniques 10.2.1 Intensity measurement in the X-ray diffractometer	258 258		
			260		
	10.2.2 Back reflection and Debye–Scherrer powder techn 10.3 Some applications of X-ray diffraction techniques in				
		polycrystalline materials	262		
		10.3.1 Accurate lattice parameter measurements	262		
		10.3.2 Identification of unknown phases	263		
		10.3.3 Measurement of crystal (grain) size	266		
		10.3.4 Measurement of internal elastic strains	266		
	10.4	Preferred orientation (texture, fabric) and its measurement	267		
		10.4.1 Fibre textures	268		
		10.4.2 Sheet textures	269		
	10.5	X-ray diffraction of DNA: simulation by light diffraction	272		
	10.6	The Rietveld method for structure refinement	277		
	Exerc	ises	280		
11	Elec	etron diffraction and its applications	283		
	11.1	Introduction	283		
	11.2	The Ewald reflecting sphere construction for electron diffraction	284		
	11.3	The analysis of electron diffraction patterns	288		
		· , ·			

Contents	X111

	11.4	Applications of electron diffraction	290
		11.4.1 Determining orientation relationships between crystals	290
		11.4.2 Identification of polycrystalline materials	292
		11.4.3 Identification of quasiperiodic crystals (quasicrystals)	292
	11.5	Kikuchi and electron backscattered diffraction (EBSD) patterns	294
		11.5.1 Kikuchi patterns in the TEM	294
		11.5.2 Electron backscattered diffraction (EBSD) patterns in the SEM	298
	11.6	Image formation and resolution in the TEM	300
	Exerc	·	304
12	The	stereographic projection and its uses	308
	12.1	Introduction	308
	12.1	Construction of the stereographic projection of a cubic crystal	311
	12.3	Manipulation of the stereographic projection: use of the Wulff net	314
	12.3	Stereographic projections of non-cubic crystals	317
	12.5	Applications of the stereographic projection	320
	12.3	12.5.1 Representation of point group symmetry	320
		12.5.2 Representation of orientation relationships	322
		12.5.3 Representation of preferred orientation (texture or fabric)	323
		12.5.4 Trace analysis	325
	Exerc	·	328
13	Fou	rier analysis in diffraction and image formation	329
	13.1	Introduction—Fourier series and Fourier transforms	329
	13.2	Fourier analysis in crystallography	332
		13.2.1 X-ray resolution of a crystal structure	337
	13.3	The structural analysis of crystals and molecules	338
		13.3.1 Trial and error methods	339
		13.3.2 The Patterson function: Patterson or vector maps	340
		13.3.3 Interpretation of Patterson maps: heavy atom and	
		isomorphous replacement techniques	346
		13.3.4 Direct methods	348
		13.3.5 Charge flipping	349
	13.4	Analysis of the Fraunhofer diffraction pattern from a grating	350
	13.5	Abbe theory of image formation	356
14	The	physical properties of crystals and their	
		cription by tensors	362
	14.1	Introduction	362
	14.1	Second rank tensor properties	363
	17.4	become fank tensor properties	505

xiv Contents

	14.2.1	vectors	363	
	14.2.2	Simplification of second rank tensor equations: principal axes	366	
	14.2.3	Representation of second rank tensor properties: the		
14.2	NI	representation quadric	366	
14.3	14.3.1	nn's principle	368	
14.4		Pyroelectricity and ferroelectricity rank tensors that describe stress and strain	369	
14,4	14.4.1		369	
	14.4.1	The stress tensor: principal axes (eigenvectors) and principal values (eigenvalues)	260	
	14.4.2	The strain tensor, Neumann's principle, and thermal	369	
	17.7.2	expansion	372	
	14.4.3	Atomic displacement parameters (ADPs)	374	
14.5		tical properties of crystals	374	
14.6	_	- · · ·		
14.7		rank tensor properties: elasticity	379 380	
Exercis		1 1	382	
Appendix 1	Comp	outer programs, models and model-building in crystallography	385	
Appendix 2 Polyhedra in crystallography		edra in crystallography	393	
Appendix 3	Biogra	aphical notes on crystallographers and scientists mentioned		
	in the		403	
Appendix 4	Some	useful crystallographic relationships	449	
Appendix 5 A simple introduction to vectors use in crystallography		ple introduction to vectors and complex numbers and their crystallography	452	
Appendix 6	-	matic absences (extinctions) in X-ray diffraction and double ction in electron diffraction patterns	459	
Appendix 7	Group	theory in crystallography	469	
Answers to	exercise	S	481	
			497	
Index		507		
			507	