

Contents

Preface v

1 The fundamentals of crystallography 1

Introduction	1
Noncrystalline and semicrystalline states	2
Lattices	4
Crystal systems	6
Unit cells	7
Coordinates of position in the unit cell	9
Indices of lattice directions and planes	10
Hexagonal indices	12
Transformations of indices	13
Matrices in crystallography	15
Zones and zone axes; crystal geometry	16
Symmetry classes and point groups	16
Space groups	22
Glide planes and screw axes	23
Space-group notation	25
Tables of equivalent points	67
Common structure types-The Strukturbericht designation	28

2 The stereographic projection 30

Reference sphere and its stereographic projection	30
Projection of great and small circles	32
Ruled globe and stereographic nets	34
Rotation with the nets	36
Angle measurement	37
Properties of stereographic projection	38
Standard projections of crystals	38
Orientation of single-crystal wires and disks	43
Applications	44
Other perspective projections	60

3 X-rays, films, and counters 51

The continuous spectrum	61
The characteristic spectrum	63
Origin of characteristic radiation and absorption	54
Dependence of line intensities on voltage	56'

viii STRUCTURE OF METALS

- Absorption of x-rays 57
- Filtering 69
- Monochromators 61
- The scattered radiation 62
- X-ray tubes 62
- Electrical equipment for diffraction tubes 64
- X-ray protection 64
- Photographic efficiency of x-rays 65
- Electrical methods of x-ray measurement 67
- Overall constancy; monitors 72

4 Diffraction of x-rays by crystals 73

- Scattering of x-rays by atoms 73
- Bragg's law 74
- The Laue equations 76
- Interplanar spacings 79
- Reinforcement of scattered waves 80
- The structure factor 82
- THE RECIPROCAL LATTICE 84
- Interplanar spacings 86
- Conditions for diffraction 86
- Ewald's sphere of reflection 88
- X-ray diffraction methods 89

5 Laue and divergent beam methods 90

- Determination of symmetry 91
- The gnomonic projection of Laue patterns 92
- Asterism 96
- Characteristics of Laue streaks 93
- Focused Laue spots 96
- Divergent beam x-ray photographs 96

6 Rotating-crystal methods 100

- Interpretation of rotation photographs 101
- The use of the reciprocal lattice 104
- Indices of spots on a diffraction pattern 107
- Oscillating-crystal photographs 108
- Weissenberg cameras 108
- The de Jong-Bouman camera and the precession camera 110
- Instruments employing counters 112
- Measuring intensities with counters 113
- Operation at low temperatures 114
- Operation at high temperatures 116
- Bond's method for precision lattice-constant determination 116

7 The powder method 118

- Powder cameras 118
- Specimen preparation 120
- Operation at high temperatures 120

Operation at low temperatures	122
Operation at elevated pressures	123
Focusing cameras	124
Monochromators	125
Undesired wavelengths from monochromators	128
Choice of radiation	128
Diffractometers	128
Sample preparation for the diffractometer	131
Intensity measurements with the diffractometer	138
Counting statistics	133
Statistics with a rate meter	136
Interpretation of powder patterns	136
Interpretation when the unit cell is unknown	138
Numerical methods for solving patterns	138
Graphical methods for solving patterns	140
Precise measurement of lattice constants	141
Minimizing errors in Debye cameras	142
Extrapolation methods for back-reflection cameras	143
Cohen's least-squares method	146
Hess's modification	147
Least-squares computer programs	147
Diffractometer correction and extrapolation procedures	148
Wavelengths and refraction	149
Chemical analysis by powder diffraction	161
Crystallite-size determination from line broadening	166
Grain-size determination from spots on Debye rings	166
Small-angle scattering of x-rays	167
Phase-diagram determination	160
Rapid cooling; "splat" and "crusher" cooling	161
8 The determination of crystal structure 163	
Determination of the symmetry class	164
Determination of the unit cell	164
Determination of space-lattice and space group	166
Number of atoms or molecules per unit cell	167
Determination of atomic positions	167
Sizes of atoms and ions	169
Example of structure determination	170
Factors governing intensities of x-ray reflections	171
Scattering by an electron	171
Scattering by an atom	173
Calculations of atomic scattering factors	174
Dispersion corrections for x-ray scattering	176
Scattering from a unit cell	176
The integrated reflection	176
The Lorentz-polarization factors	176
The absorption factor	177
The multiplicity factor p	178
The temperature factor	178
Extinction	179
Scale factor; refinement of scale and temperature factors	180
Electron density expressed by Fourier series	181

x STRUCTURE OF METALS

- The F^2 series of Patterson 184
- The Patterson-Harker F^2 series 186
- Vector sets; superposition methods 186
- Error synthesis 187
- Computer programs 188
- Other techniques 188
- Diffraction from liquids and vitreous solids 189
- The radial distribution method 189

9 Pole figures and orientation determination 193

- Detection of preferred orientations 193
- Stereographic projection of data 196
- Fiber textures 196
- Plotting of pole figures 197
- Specimens and cameras for texture studies 199
- Use of x-ray spectrometers for texture studies 200
- Inverse pole figures 203
- Plots based on orientations of individual grains 204
- The method of Harris for inverse pole figures of fiber textures 204
- The method of Jetter, McHargue, and Williams 205
- The method of Mitchell and Rowland 206
- The method of Roe and Krigbaum 207
- DETERMINING THE ORIENTATION OF INDIVIDUAL CRYSTALS 208
- The determination of orientation by etch pits 208
- Back-reflection Laue method for determining crystal orientation 211
- The transmission Laue method 217
- Crystal orienting methods using $K\alpha$ radiation 218
- Crystal orienting with a diffractometer 221
- Cutting crystals to known orientations 221

10 The structure of metals and alloys 223

- STRUCTURES OF THE ELEMENTS 224
- The 8 - N rule 228
- Polymorphism 230
- SOLID SOLUTIONS 238
- Types of solid solutions 238
- Determination of the type of solid solution 235
- Arrangement of atoms of different elements in simple metallic structures 236
- INTERMEDIATE PHASES 239
- Nomenclature of alloy phases and compounds 240
- Structures of compounds with normal valence 241
- The nickel arsenide structure ($B8_1$ and $B8_2$) 245
- Electron phases 247
- Electron phases with cubic symmetry 253
- Electron phases with hexagonal symmetry 255
- The Laves phases 256
- Interstitial phases and compounds 259
- Structure of phases formed by the transition elements, rare earths, etc. 262
- Phases with fixed stoichiometry 262
- Phases with variable composition 266
- Other complex structures 868

11 Superlattices 270

- Common types of superlattices 271
- The $L1_2$ - or Cu_3Au -type superlattice 272
- The $B2$ - or beta-brass-type superlattice 272
- The $L1_0$ - or $CuAu$ -type superlattice 273
- The $L1_1$ superlattice in $Cu-Pt$ 275
- The DO_3 and $L2_1$ superlattices 275
- The DO_{19} - or Mg_3Cd -type superlattice 277
- Less common superlattices 278
- Long-period superlattices 279
- Elements of superlattice theories 284
- Short-range order 287
- Definition of short-range order in terms of multiple parameters 289
- Alternate views on the theories of ordering 291
- The detection of order with x-rays: temperature dependence 292
- The determination of order with x-rays: other complicating factors 294
- Superlattice domains 297
- Electron diffraction from superlattices 298
- Transmission electron microscopy of antiphase boundaries 300
- Monte Carlo calculations 302
- The thermodynamic order of superlattice transitions 303

12 Electrons in metallic crystals 306

- The metallic bond 306
- Cohesive and repulsive forces in metals 306
- Metallic valence 308
- Electronic theories of metals 310
- Electron motion in a lattice 314
- Brillouin zones 317
- The occupation of energy levels 318
- Conductors, insulators, and semiconductors 319
- Energy bands 321
- The Fermi surface 321
- The revised Bloch model 323
- The mapping of Fermi surfaces 323
- Electronic structure of the noble metals Cu , Ag , and Au 328
- Electronic structure of the transition metals 329
- Charge oscillations 333
- Superconductivity 334

13 Theories of metallic phases 338

- Electrochemical factor 339
- Electron concentration in alloys 340
- Model of the band structure of an alloy 341
- Fermi surfaces and Brillouin zones in alloys 342
- Hume-Rothery rules 343
- Electronic theories of primary solid solubility of alloys based on the noble metals 346
- Stability of electron phases 348
- Stability of long-period superlattices 361
- Electron concentration as a general parameter in alloy structures 364

xii STRUCTURE OF METALS

Lattice spacings	367
Lattice spacings and zone overlaps	360
Defect structures	364
Band structures of group V semimetals and the IV-VI semiconductors	366
Atomic sizes in metals	367
Atomic sizes in solid solutions	369
Size effects in solid solutions	370
The volume size-factors	371
Deviations from Vegard's law	372
Geometrical principles	373
Limitations	378
Crystal families in alloy phases	379

14 Defects in crystals 380

Point defects	382
Development of dislocation theory	384
Edge and screw dislocations	386
Perfect and partial dislocations; stacking faults	387
Dislocation content of crystals	389
Thompson's notation for dislocations in f.c.c. crystals	389
Nodes, stacking fault energy, cross slip	390
Loops	393
Jogs, helices, and tangles	394
Dislocation nets and small-angle boundaries	396
Imperfections resulting from solidification	399
Dislocation interactions	400
Grain boundaries and grain shapes	402
The crystallography of slip, twinning, and cleavage	403
Twins	406
Deformation twins	407
Theories of the mechanism of deformation twinning	409
Shear in deformation twinning	411
The crystallographic elements of twins	412
Observed twinning elements	414
Cleavage	414
Dislocations and stress-corrosion cracking	417

15 X-ray and electron microscopy 418

X-RAY METHODS	418
X-ray topographs (reflection images)	419
The simplest, low-magnification methods	419
Berg-Barrett method	421
Bonse method	486
Lang method	425
Borrmann method	437
General characteristics of topographic methods	428
Other methods for photographing substructure	428
ELECTRON MICROSCOPY	430
Equipment	430
Orientation determinations	432
Replicas	433

Transmission microscopy with thin foils	434
Image contrast	436
The kinematic theory of image contrast	437
Amplitude-phase diagrams	439
Images of stacking faults	440
Images of dislocations and dislocation loops	443
Coherent precipitates	446
Measures of foil thickness	446
"Supervoltage" electron microscopy	446

16 Diffraction from imperfect and cold-worked metals 447

Orientation spread; asterism	447
Reciprocal lattices of deformed and imperfect crystals	448
Inhomogeneous residual strains	449
Small coherent domains	460
Stacking faults	457
Fourier analysis of particle-size and strain broadening	453
Analysis of stacking-fault broadening	459
General treatments	461
F.c.c. and c.p.h. power patterns	462
B.c.c. powder patterns	462
Relationship between stacking-fault probability α and stacking-fault energy γ	466

17 Stress measurement by x-rays 466

Characteristics of the x-ray methods	466
Elastic stress-strain relations	467
Method for sum of principal stresses ($\sigma_1 + \sigma_2$)	469
Equations for the ellipsoid of strain and of stress	471
Two-exposure method for σ_d	472
Correction for oscillation of film (two-exposure method)	474
Single-exposure method for σ_d	474
Methods for determining σ_1 and σ_2 when their directions are known	476
Method giving magnitude and direction of principal stresses	476
Values of elastic constants; anisotropy	476
Equipment for photographic stress measurement	478
Stress measurement with diffractometer equipment	480
X-ray beam penetration	482
Stress vs. depth below surface	483
Practical applications; the need for caution	483
Broadened reflections and inhomogeneous strains	484

18 Phase transformations in the solid state 486

General characteristics of martensitic transformations	487
Polymorphic changes	489
Morphology of phase transformations	49%
Lattice relationships in Widmanstätten structures	495
Plane of precipitation and shape of precipitates	496
Discontinuous precipitation and eutectoid reactions	497
Changes occurring during aging	499
Structure changes during aging in Al-Cu, Al-Ag, and Cu-Be	600
X-ray diffraction in the early stages of aging	501
Electron microscope studies of age-hardening alloys	603

The structure of "side-band" alloys 506
Spinodal decomposition 507
Massive transformations 507
Order-disorder transformations in CuAu 509
Structures in carbon steels and the decomposition of austenite 510
Martensitic shape-change, morphology, and kinetics 517
Crystallographic aspects of martensite transformations 520
Modern phenomenological theories of martensite formation 522
Deficiencies of modern theories 525
Characteristics of some nonferrous martensites 526
The "burst" phenomenon 529
Thermoelastic and superelastic martensites 539
Transformations induced by strain 531
Orientations in other reactions 532
Solid state transformations in general 533
First-order vs. second-order transformations 533

19 Orientations in castings and deposits 535

Columnar grain orientations 536
Orientations in electrodeposits 538
Evaporated and sputtered metal films 640

20 Preferred orientations resulting from cold work 541

The importance of textures 541
General principles of texture development 546
Texture of polycrystalline wires and rods 543
Textures of polyphase wires 547
Compression textures 547
Theories of tension and compression textures 549
Taylor's theory of textures 549
The effects of inhomogeneous flow and deformation bands on textures 561
Later theories of the development of fiber textures 563
The specification of rolling textures 556
Rolling textures of f.c.c. metals 556
Body-centered cubic rolling textures 568
Close-packed hexagonal rolling textures 561
Theories of rolling textures 564
Torsion textures 566
Cold-drawn tubes 585
Textures in deep drawing 566
Textures after hot working 566

21 Preferred orientations after annealing 568

Variables and mechanisms affecting textures 668
Recrystallized wires and compression specimens 569
The cube texture in f.c.c. sheets 570
Other f.c.c. annealing textures in sheets 572
Recrystallization textures in b.c.c. sheets 573
Recrystallization textures of c.p.h. sheets and alpha-uranium 576
Sheets for magnetic applications 578
Theories of annealing textures 579

A theory of the cube texture in f.c.c. metals *582*
 Theories of textures in silicon-steel *582*

22 Electron diffraction 584

Electron waves 586
 Apparatus 586
 The diffraction pattern 587
 Specimens 588
 Identification of polycrystalline materials 589
 Extra rings 590
 Diffraction by very thin crystals 591
 Penetration 596
 Oxide layers 598
 Preferred orientations 593
 Polished surfaces 594
 Thin deposits 596
 Intensity of scattering 598
 Structure determination 598
 Kikuchi lines 599
 Diffraction of atoms and molecules *601*
 Low-energy electron diffraction *601*

23 Neutron diffraction and magnetic structures 602

Equipment and methods *602*
 Neutron scattering from atomic nuclei 603
 Structure determinations with nonmagnetic substances 606
 Neutron scattering from magnetic materials 606
 Summary of types of magnetic configurations 609
 Magnetic structures of metals and alloys 609
 Magnetic structures in compounds *611*
 Inelastic scattering of neutrons *612*

Appendix 613

A-1 Physical constants and numerical factors *613*
 A-2 Crystal geometry *613*
 UNIT CELLS IN REAL AND RECIPROCAL SPACE *614*
 INTERPLANAR SPACINGS IN CRYSTALS *614*
 ANGLES BETWEEN PLANES IN A CRYSTAL *615*
 RECIPROCAL LATTICE AXES AND ANGLES *615*
 ZONE LAWS *616*
 LATTICE POINTS AND PLANES *616*
 IDENTITY DISTANCES *616*
 ANGLES BETWEEN DIRECTIONS *616*
 PERPENDICULARITY OF LINE AND PLANE *617*
 A-3 Quadratic forms *618*
 A-4 Mass absorption coefficients (p/p) for x-rays *631*
 A-5 X-ray emission and absorption wavelengths *622*
 A-6 The crystal structure of the elements 636

Name Index 633

Subject Index 648