

Table of Contents

	Preface	IX
	Symbols	XV
1	Principles of X-ray Diffraction	1
1.1	The Basic Phenomenon	1
1.2	The $\theta/2\theta$ Scan	11
1.3	Intensity of Bragg Reflections	14
1.3.1	Atomic Form Factors	17
1.3.2	Structure Factor	19
1.3.3	Multiplicity	24
1.3.4	Geometry Factor	25
1.3.5	Preferred Orientation (Texture)	25
1.3.6	Polarization Factor	26
1.3.7	Absorption Factor	26
1.3.8	Integration of the Interference Function	29
1.4	Applications	37
	Exercises	39
	References	41
2	Identification of Chemical Phases	43
2.1	Histogram-Based Techniques	43
2.2	Linear Attenuation Coefficient μ	55
2.3	Determination and Interpretation of the μt Product	60
2.4	Analysis of Phase Mixtures	66
2.5	Amorphous Thin Films	70
2.6	Accurate Determination of Lattice Parameter	74
2.7	Applications	80
	Exercises	81
	References	83

VI | *Table of Contents*

3	Line Profile Analysis	85
3.1	Model Functions and Peak Parameters	86
3.2	Instrumental Line Profile	97
3.3	Deconvolution by Fourier Techniques	101
3.4	Reflection Broadening by Small Crystallite Size Only	107
3.4.1	Scherrer Equation	108
3.4.2	Column Height Distribution	111
3.4.3	Crystallite Shapes Other Than Cubes	112
3.4.4	Determination of the Column Height Distribution Function	115
3.4.5	Determination of the Crystallite Size Distribution Function	118
3.5	Concomitant Occurrence of Size and Strain Broadening	120
3.5.1	Analysis According to Williamson and Hall	122
3.5.2	Method of Warren and Averbach	126
3.5.3	Single-Line Analysis	129
3.5.4	Techniques of Whole-Pattern Fitting	130
3.6	Applications	134
	Exercises	136
	References	138
4	Grazing Incidence Configurations	143
4.1	Grazing Incidence X-ray Diffraction (GIXRD)	148
4.2	Penetration Depth and Information Depth	155
4.3	Depth-Dependent Properties	158
4.4	Refractive Index for X-rays	160
4.5	Total External Reflection and Critical Angle	161
4.6	X-ray Reflectivity (XRR)	165
4.6.1	Reflectivity of a Substrate	166
4.6.2	Reflectivity of a Single Layer	168
4.6.3	Reflectivity of Multilayers and Superlattices	171
4.7	Grazing Incidence Diffraction (GID)	175
4.8	Applications	177
	Exercises	179
	References	181
5	Texture and Preferred Orientation	183
5.1	Texture Factors	188
5.2	Pole Figures	191
5.3	Measurement of Pole Figures	195
5.4	Directions, Orientations and Inverse Pole Figures	200
5.5	Fiber Textures or Layer Textures	204
5.5.1	Harmonic Method	204
5.5.2	Whole Pattern Techniques	207
5.5.3	Rocking Curves (ω Scans)	211
5.6	Biaxial and Fully General Textures	216
5.6.1	Azimuthal Scans (ϕ Scans)	218
5.6.2	General Orientation Distribution	220

5.6.3	Determination of Fully General Texture	225
5.7	Depth Dependence of Thin-Film Textures	228
5.8	Applications	230
	Exercises	234
	References	235
6	Residual Stress Analysis	239
	<i>Mario Birkholz and Christoph Genzel</i>	
6.1	Ceiiinnosssttuv	241
6.2	Fundamental Equation of XSA	246
6.3	Measurement of d_{ψ} Distributions	249
6.4	Diffraction Elastic Constants (DECs) s_1 and $1/2s_2$	258
6.5	Grain Interaction Models	261
6.6	The Effect of Texture	265
6.7	Classification of Stresses	268
6.7.1	Classification by Dimension	268
6.7.2	Residual Stresses in Multiphase Materials	269
6.7.3	Origin of Residual Stresses: Extrinsic and Intrinsic Stresses	271
6.8	Effect of Residual Stress Gradients	273
6.8.1	General Considerations	273
6.8.2	The Biaxial Stress State	274
6.9	Detection of Residual Stress Gradients in Thin Films	276
6.9.1	Basic Relations	276
6.9.2	X-ray Penetration Depth for the General Case of Asymmetric Diffraction	278
6.9.3	Special Methods for X-ray Stress Gradient Analysis	281
6.9.4	Grazing-Incidence Diffraction (GID)	282
6.9.5	The Scattering Vector Method	284
6.9.6	Realization of H Mode on a Four-Circle Diffractometer	286
6.10	Applications	289
	Exercises	291
	References	291
7	High-Resolution X-ray Diffraction	297
	<i>Mario Birkholz and Paul F. Fewster</i>	
7.1	Strain, Strain Relaxation and Composition in Epitaxial Layers	303
7.2	High-Resolution Rocking Curves	306
7.3	Mosaicity and Extinction	314
7.4	Dynamical Theory of Ewald and Extensions	319
7.5	High-Resolution Rocking Curves and Profiles from Layer Structures	324
7.6	Reciprocal Space Mapping	332
7.7	Diffuse Scattering	337
7.8	Extensions to High-Resolution Diffraction	338
	Exercises	339
	References	340