

## Index

Page numbers in italics refer to figures.

$\mu$ t product 28, 60–66, 153, 318

### **a**

abscissa transformation 103  
 absorption 55  
 absorption coefficient 167, 214  
 absorption edges 56  
 absorption effects 26  
 absorption factor 26, 28, 57, 196  
   – exponent 156  
   – GIXRD 153, 154  
   –  $\omega$  scan 212  
 absorption index 161  
 acceleration voltage, x-ray tubes 30  
 accuracy 79  
   – loss 76  
   – phase mixture 67  
 aerosols 118  
 American Society for Testing and Materials (ASTM) 52  
 amorphous fraction 74  
 amorphous phases 70  
 amorphous silicon 70  
 amorphous substances 52  
 amorphous thin films 70–74  
 angle of rotation 191, 279  
 angle of the incident beam, GIXRD 144  
 anisotropy 115  
   – growth 124  
 anode materials, x-ray tubes 30  
 anode rotation 176  
 anomalous dispersion corrections 320  
 anti-site domains 92  
 apertures 44  
 ASTM *see* American Society for Testing and Materials  
 asymmetric diffraction 278  
   – geometry 278  
   – penetration depth 280  
   – scheme 279  
 asymmetry  
   – bragg peaks 321

  – *see also* symmetry  
 atomic form factors 17–18, 161  
 atomic mass 55  
 atomic number 50, 55  
 atomic radius 21  
 attenuation 55  
   – coefficient 67, 143  
   – x-rays 277  
 Aurivillius phases 135  
 average contrast factors 125  
 average density 67  
 average information depth 156, 158  
 average RS values 270  
 average size parameter 119  
 average stress, of sample 261  
 averaging, over full grain ensemble 119  
 axis, naming convention 221  
 axisymmetric texture 204  
 azimuthal scans 218–220

### **b**

background, x-ray 30, 46  
 background correction 197  
 background function 96, 128, 208  
 ball milling 131  
 band gap engineering 300  
 band gaps 48  
 bandwidth, monochromator 326  
 barrier coatings 37  
 Bartels monochromator 313  
 Ba<sub>0.7</sub>Sr<sub>0.3</sub>TiO<sub>3</sub> film (BST) 214  
 bcc *see* body-centered cubic structure  
 Be windows, x-ray tubes 34  
 beam angle 12  
 beam attenuator 146  
 beam broadening 194  
 beam conditioning  
   – crystals 325  
   – techniques 144

## 344 | Index

- beam divergence 69, 144–145, 220, 325–326
    - axial 78, 132
    - definition 44–46
    - finite 29
    - planes 132
  - beam length 146
  - beam mask 46
  - beam optics, parallel 144
  - beam shaping 46
    - elements 44
  - bending, thin samples 251
  - Bertaut's column theorem 111
  - biaxial residual stress state of rotational symmetry 275, 284
  - biaxial stress model 248
  - biaxial stress state 274–276
  - biaxial textures 216–228
  - blocking layer 173
  - body-centered cubic structure (bcc) 20, 91
  - bonding spheres 70
  - Bragg angle
    - aluminum 24
    - definition 9
    - distinct 151
    - with beam refraction 164
  - Bragg equation 9–10
    - film thickness 170, 310
    - limits 335
    - selection rule 261
    - single-layer system 174
    - vector form 320
  - Bragg line profiles, crystallite shapes 114
  - Bragg mirrors 173
  - Bragg peaks
    - asymmetry 330
    - epitaxial film 334
    - line profile 109
    - monitoring 229
    - position shift 165
    - splitting *see* splitting
  - Bragg reflection 9
    - crystallite number 194
    - crystallite orientation 189
    - enhancement 183
    - experimental diffractogram 52
    - high scattering angles 249
    - intensity 14–37
    - lattice orientation 191
    - number of 289
    - principles 14–37
    - reduction 153
    - rutile structure 149
    - shift 321
    - splitting 304
    - structural information 297
    - width 85
  - Bragg–Brentano geometry 15
  - brass substrate 129
  - Bremsstrahlung 30
  - BST *see* Ba<sub>0,7</sub>Sr<sub>0,3</sub>TiO<sub>3</sub> film
  - bulk elastic constants 289
  - Burgers vector 90, 124
- c**
- Caglioti formula 100
  - Cambridge Crystallographic Data Center (CCDC) 52
  - Cambridge Structure Database (CSD) 52
  - carbon 48
  - carbon layers, amorphous 134
  - Cauchy function 92, 93, 129, 136
  - c-axis
    - alignment 218
    - layer texture 232
  - CCC *see* channel-cut crystal monochromator
  - CCDC *see* Cambridge Crystallographic Data Center, *see* charge-coupled devices
  - CCP14 *see* Collaborative Computational Project #14
  - central beam, diffractometer 16, 44
  - centroid determination 250
  - centroid peak 86
  - channel-cut crystal (CCC) monochromator 327
  - characteristic radiation 30
  - charge-coupled devices (CCD) 256
  - chemical composition 57, 60
  - chemical phases, identification 42–84
  - chemical vapor deposition (CVD) 53, 299
  - chi-square function 88
  - cluster, atomic 71–72
  - coatings
    - fluorescing 45
    - molybdenum 61
    - protective 241
    - razor edge 135
    - technology 242
    - thin hard 287
  - CoFe<sub>2</sub>O<sub>4</sub> nanoparticles 136
  - coherency, cessation 17
  - coherently diffracting domains 85
  - coherently scattering domains 107
  - Collaborative Computational Project #14 (CCP14) 89
  - column height distribution 111–112
    - determination 115–117

- column theorem 111
  - columnar honeycomb structure 316
  - complex refractive index, x-rays 161
  - composition
    - epitaxial electronic films 306
    - epitaxial layers 303
  - composition-relaxation net 312
  - Compton scattering 2
  - configuration factor 151, 196
  - configurations, diffractometer 325
  - contaminants 60
  - contrast factor 132
  - convolution 136
  - coplanar geometry 211
    - HRXRD 312
  - correlation length 117
  - counting statistics 257
  - count-mean diameter 119
  - counts per second (cps) 253
  - cps *see* counts per second
  - cracking 239
  - critical angle 161–165, 280
    - GIXRD 150
    - sequence 168
  - critical temperatue 51
  - cross-section 55
    - x-rays 56
  - crystal truncation rod (CTR) 337
  - crystalline lattice faults 90–92
  - crystalline matter, elastic behavior 239
  - crystallite group method, strong texture 268
  - crystallite orientations 183
  - crystallite shapes 112–115
  - crystallite size 107–120, 134
    - area averaged 120
    - distribution function 118–120
    - volume averaged 119–120
  - crystallite subsets, selective perception 13
  - crystallographic lattice planes 9
  - crystallographic lattice planes 25
  - crystallographic structures 43
  - crystallographic unit cell 9, 19, 21
  - crystals 325
    - cubic 193, 197, 223
    - imperfections 323, 337
    - lattice 4
    - monochromators 46, 297
    - reference frame 223, 258
    - structure 48
    - symmetry 193
    - tetragonal 149
  - CSD *see* Cambridge Structure Database
  - CTR *see* crystal truncation rod
  - Cu  $K_{\alpha}$  emission line 97
  - cubic crystals 193, 197, 223
  - cubic group IV alloys 299
  - cubic III–V compounds 300
  - cuprous oxide 134
  - Curie temperatures 185
  - CVD *see* chemical vapor deposition
  - cylinders 113
  - Czochralski-grown silicon wafers (CZ-Si) 62
- d**
- damping
    - thin-film analysis 36
    - within the crystal 316
  - damping terms 172
  - Darwin treatment 314
  - data reduction 86
  - database, diffraction patterns 47
  - Debye scattering equation 70, 72
  - Debye–Waller factor 168, 172
  - DEC *see* diffraction elastic constants
  - deconvolution 101–107
  - defect incorporation, thin films 272, 275
  - defect, lattice 90
  - defocusing 196, 213, 252
    - correction 196
  - deposition process 43, 190
    - optimization 43, 226
  - depth dependence, phase dispersion 80
  - depth monitoring 229
  - depth-dependent properties, x-ray beams 158–159
  - depth-resolved XSA, methods 282
  - depth-variable 27
  - detector mode, open 197
  - detector slits 220
  - detectors 44
    - x-ray 253–258
  - deviation parameter, line profiles 322
  - device structures analysis 331
  - dial gauge 77
  - diamond structure 48–49, 299
  - diamond-like carbon (DLC) 134
  - dielectric displacement vectors 320
  - dielectric susceptibility 161
  - diesel engine technologies 135
  - differential equilibrium conditions 273, 275
  - diffracted-beam monochromators 325
  - diffraction
    - experiment 259
    - high-resolution 297–342, 338
    - x-ray 1–41

## 346 | Index

- diffraction elastic constants (DECs) 239, 258–260
  - nitrides 264
- diffraction gratings 7
- diffraction histogram 47
- diffraction pattern 13, 43
  - ball milled Ni sample 133
  - comparison 226
  - epilayer–substrate material systems 297
  - GID 175
  - nanocrystalline powder sample 105
  - simulation 324
  - symmetric 219
  - W-C:H films 135
  - YBCO 218
  - ZNO 188
- diffraction-reflection technique 175
- diffractometer,  $\theta/2\theta$  11, 15–17
  - Eta 285
  - four-circle 193, 286
  - triple-crystal 337
- diffractometer configuration
  - GIXRD 152
  - XRR 165
- diffuse scattering 337–338
- diffusion 37
- disarmament 40
- dislocation
  - contrast factors 124–125, 128
  - core 90
  - density 91
  - edge 124
  - glide 91
  - lattice 121
  - networks 107
  - pile-ups 134
  - screw 90, 124
- dislocation density 124, 126
- dislocation-free crystals 323
- dispersion correction 160
- dispersive elements 46
- displacement field 120, 126
- distortion broadening 121
- d distribution
  - definition 247
  - measurement 249–258
- distribution function
  - column height 111–112, 116, 127
  - crystallite size 115–116, 118–120
  - monodisperse 119
  - size coefficients 127
- divergence *see* beam divergence
- divergence slits (DS) 44–45
- divergent beam optics 44–47
- DLC *see* diamond-like carbon
- double-crystal configuration 326
- doublet resolution 32
- DS *see* divergence slits
- DuMond diagram 326
- dynamical theory 37, 62, 319–324
- e**
- edge dislocation 90
- edge filters 33
- EKK *see* Eshelby, Kröner and Kneer (EKK)
- elastic constants 124
- elastic modulus 241
- elastic strain 241, 271
- electric field vectors 161
- electroacoustic devices 188
- electrodeposition 134
- electron microscopy 62, 85, 107
- electron radius, classical 3
- electronic diode solid-state detectors 253
- electroplating 37
- elementary metals 21
- emission, x-ray 31–35
- emission spectrum 30
  - laboratory x-ray tube 98
- energy resolution, proportional detector 255–256
- epitaxial films
  - bragg reflection 305
  - composition 303
  - structural features 312
  - thin 297, 299
- epitaxy 303
- equal area projection 192
- equilibrium conditions 275
- error margin 88
- error propagation 226
- Eshelby, Kröner and Kneer (EKK) 263
- Eta diffractometer 285
- Euler angles 200
- Euler cradle 146, 184, 193, 287
- Euler plane 23
- Euler space 201, 220
- Ewald's dynamical theory 319–324
- excitation errors 321
- extended x-ray absorption fine structure spectroscopy (EXAFS) 57
- extinction 314
  - coefficient 319
  - conditions 20, 49, 149
  - length 319, 323
  - mosaic crystal 317
- extrinsic stresses 271

**f**

face-centered cubic structure (fcc) 20, 91  
 Fachinformationszentrum (FIZ) 52  
 fcc *see* face-centered cubic structure  
 FeRAM *see* ferroelectric random access memory  
 ferroelectric random access memory (FeRAM) 198  
 fiber axis 184  
 fiber textures 184, 200, 204–215
 

- ODF 201, 205
- volume fraction 207

 films
 

- aluminum 13, 178
- amorphous 70–74
- CrN 266
- deposition 275
- epitaxial 297, 299, 303, 305, 312
- magnetic 177
- metal 37, 80
- nanocrystalline 102
- optical 177
- piezoelectric 188
- polycrystalline 36, 54
- polycrystalline 183
- Pr<sub>2</sub>O<sub>3</sub> 177
- silicon 61
- thickness 156, 170–171, 275, 309, 318
- TiN 247
- TiO<sub>2</sub> 154
- titanium 38
- W-C:H 135

 film–substrate composite, stress 245  
 filters 97
 

- materials 30

 fine structure 57  
 first scattering peak (FSP) 72  
 fitting parameters 95  
 FIZ *see* Fachinformationszentrum  
 flat sample 77  
 fluctuations, x-ray beam 338  
 fluorescence, x-ray 30  
 focus modes, x-ray tubes 34  
 food packaging 37  
 four-circle diffractometer 286  
 Fourier coefficients 117  
 Fourier length 103  
 Fourier transform 89, 102, 127
 

- discrete 23, 104

 Fourier-conjugated variable 103  
 Fraunhofer diffraction 6  
 Fresnel diffraction 6  
 fringes 170, 310, 330

FSP *see* first scattering peak  
 full width at half maximum (FWHM) 86  
 fundamental parameter approach 100, 132, 136  
 FWHM *see* full width at half maximum

**g**

GaAs (001) substrates 318  
 GaN buffer layer 332  
 gases, scattering equation 70  
 gate oxides 176  
 Gauss function 92, 93, 129, 136
 

- three-dimensional 221

 Gaussian concentration profile 329  
 general orientation distribution 220  
 general textures 216–228  
 geometry factor 25
 

- $\omega$  scan 212

 GIABD *see* grazing incidence asymmetric Bragg diffraction  
 giant magnetoresistance effect (GMR) 177  
 GID *see* grazing incidence diffraction  
 GIXRD *see* grazing incidence x-ray diffraction  
 glass
 

- fiber 161
- substrate 53, 61, 71

 GMR *see* giant magnetoresistance effect  
 goniometer 15, 184
 

- radius 45

 graded multilayer mirrors 77  
 grain boundary migration 241  
 grain growth 241  
 grain interaction models 261–264  
 grain orientation, preferred 126  
 graphite 48  
 grazing incidence 143–182  
 grazing incidence asymmetric Bragg diffraction (GIABD) 154  
 grazing incidence diffraction (GID) 175, 282  
 grazing incidence x-ray diffraction (GIXRD) 143, 148–155  
 growth parameters, thin films 65, 275

**h**  
 H Mode 286  
 half population tilt 207  
 hard nitride coatings 233  
 harmonic analysis 222  
 harmonic method, texture factors 204–207  
 harmonic oscillators, damped 160  
 harmonic reflections 63–64  
 HBT *see* heterojunction bipolar transistor

## 348 | Index

- hcp *see* hexagonal close-packed structure  
 height misalignment 76  
 HEMT *see* high-electron-mobility transistor, *see* homogeneous elastic matrix models  
 heteroepitaxy 303  
 heterojunction bipolar transistor (HBT) 299, 300, 310  
 hexagonal close-packed structure (hcp) 20  
 hexagonal Group III nitrides 301  
 hidden elastic stresses 268  
 high-electron-mobility transistor (HEMT) 331  
 highly oriented pyrolytic graphite (HOPG) 46  
 high-resolution rocking curve 306–313  
 – Ge epilayers 308  
 high-resolution x-ray diffraction (HRXRD) 297–339  
 high-temperature superconducting films 231, 233  
 high-temperature superconductors (HTSC) 184, 187  
 histogram based techniques 43–55  
 homogeneous elastic matrix (HEM) models 261  
 Hooke's law 241  
 HOPG *see* highly oriented pyrolytic graphite  
 HRXRD *see* high-resolution x-ray diffraction  
 HTSC *see* high-temperature superconductors  
 hybrid technique, GID 175  
 hydrogen concentration 70  
 hydrogenated amorphous carbon layers 134
- i**  
 IBAD *see* ion beam-assisted deposition  
 ICDD *see* International Center for Diffraction Data  
 ideal components, method of 228  
 impact ionization 31  
 incidence angle, grazing incidence 148  
 incident beam, multilayer system 171  
 information depth 155–158  
 – variation 229  
 INLT *see* inverse numerical Laplace transform  
 Inorganic Structure Data Base (ISDB) 52–53  
 in-plane stress 247  
 instrumental calibration, stoichiometry determinations 75  
 instrumental effects, XRR scan 167  
 instrumental errors 76  
 instrumental line profile 97–101  
 instrumental parameters 79  
 instrumental peak shifts 79  
 integral breadth 110  
 – diffraction line 92–93  
 – model functions 96  
 – sample broadened profile 130  
 – total 123  
 integral intensities, x-ray diffraction 29, 35, 61, 64, 110  
 intensity damping 155  
 intensity loss, incoming beam 314  
 intensity oscillations 168  
 interactions between x-rays and matter 1  
 interatomic distances 5  
 interface roughness 174  
 interference  
 – constructive 1  
 – destructive 1, 20, 50  
 interference function 7, 29–37, 108, 112, 116  
 interlayer stresses 275  
 International Center for Diffraction Data (ICDD) 52  
 International Union of Crystallography (IUCr) 53  
 intralayer stresses 275  
 intrinsic stresses 271  
 inverse numerical Laplace transform (INLT) 277  
 inverse pole figure 202  
 – thin CrN film 266  
 inverse problem, thin-film analysis 87  
 ion beam-assisted deposition (IBAD) 217, 289  
 iron powder  
 – reflections 121  
 – Williamson-Hall plot 123  
 iron pyrite 80  
 ISDB *see* Inorganic Structure Data Base  
 IUCr *see* International Union of Crystallography
- j**  
 JCPDS *see* Joint Committee on Powder Diffraction Standards  
 Joint Committee on Powder Diffraction Standards (JCPDS) 52

**k**

- Kiessig oscillations 168
- kinematical theory 37, 314, 319
- kinetic energy, particles 275

**l**

- LaB<sub>6</sub> standard 136
- laboratory reference frame 24, 260
- ladder of complexity 240
- Lambert-Beer law 26
- La-modified PbTiO<sub>3</sub> films 203
- Laplace transform 89, 159, 164, 277
- large area electronic 61
- laser diodes (LDs) 301
- laterally graded multilayer mirror (LGMM) 145, 151
- lattice
  - bcc 20, 91
  - crystal 4
  - fcc 20, 91
  - simple cubic 9
- lattice constants, YBCO 219
- lattice distortion 120
- lattice faults 90–92
- lattice mismatch 305
  - strain 271
- lattice parameters
  - determination 74
  - dislocation 132
- lattice planes 191
  - angular relations 208
  - crystallographic 9
  - vertically tilted 147
- lattice vector 4, 319
- Laue conditions 8, 10, 108
- Laue equation 74
- Laue function 110
- layer peak, interpretation 309
- layer period 145
- layer properties 158
- layer structure profiles 324–332
- layer textures 204–215
- layers
  - blocking 173
  - carbon 134
  - epitaxial 303, 307
  - fully strained 305
  - GaN buffer 332
  - Ge epi- 308
  - III–V compound 298
  - inter- 275
  - multi- *see* multilayers
  - nickel 129

- semiconducting 232
- silver top 228
- single 168–171, 174
- superlattice 332
- ZNO:Al 232
- *see also* thin films
- LD *see* laser diodes
- least square minimization 96
- LED *see* light-emitting diodes
- Levenberg–Marquardt algorithm 88
- LGMM *see* laterally graded multilayer mirrors
- light-emitting diodes (LEDs) 301
- line broadening 74
- line focus 45, 66, 146
- line profile analysis (LPA) 85–142
  - standard sample 100
  - x-ray 134
- line profiles
  - instrumental 97–101, 133
  - standard 101
- linear absorption coefficient 60, 278
- linear attenuation coefficient 27, 55–60, 58
- liquids, model systems 70
- load test 259
- logarithmic normal function 118
- Lorentz factor 26, 35, 249
- Loschmidt's number 3
- LPA *see* line profile analysis

**m**

- macroresidual stress fields, variations 273
- macroscopic equilibrium conditions 275
- macroscopic relaxation 337
- macrostress 240, 268, 270
- magnetic thin films 177
- March function 208–209
- masks, diffractometer 44
- mass absorption coefficient 27, 57–58
  - chemical elements 59
- mass attenuation coefficient, average 66
- mass density 55
- mathematical fit 96
- MAUD program, Rietveld refinement 132
- Maxwell's equation 320
- MBE *see* molecular beam epitaxy
- mean quadratic deviation 23
- measurement geometry, x-ray diffractometer 15
- mechanical anisotropy 260
- mechanical relaxation phenomena 304
- mechanical stress 241
  - thin films 239
- medium-range order (MRO) 72

- metal lattices, atomic form factor 23
  - metallic atoms, form factors 18
  - metallic films 80
  - metallic interconnect 37, 230
    - copper 38
  - metallic ribbons 227
  - metal-organic chemical vapor deposition (MOCVD) 301
  - metals 37
    - full texture analysis 227
    - hexagonal close-packed (hcp) 21
  - microcavities 64
  - microscopic structural features 313
  - microstrain 85–86, 127, 134
  - microstress 240, 269–270
  - microstructural reorganization 241
  - microstructure
    - single crystals 315
    - solids 107
    - thin films 134, 136
  - Miller indices 9, 262
    - pole figures 225
  - mirrors
    - Bragg 173
    - graded 77
    - multilayer 145, 151
    - x-ray 175
  - misalignment, superconducting material 217
  - misfit dislocations 299
  - mismatch, epitaxial layers 303
  - misorientation, epitaxial thin films 315
  - MOCVD *see* metal-organic chemical vapor deposition
  - model functions 208
    - profile analysis 86–97
  - model patterns 54
  - model simulation 96
  - modeling, structural 87
  - molecular beam epitaxy (MBE) 299
  - molecules, in gases and liquids 71
  - moments
    - distribution function 116
    - statistical 117, 127
  - momentum transfer
    - GID 175
    - plane of 333
    - vector 6
  - monochromators 97, 325
    - $\alpha_1$ - $\alpha_2$  99
    - crystal 46, 144, 297
    - graphite 47
    - secondary 44, 47, 98
  - monodisperse distribution 111
  - mosaicity, single crystals 314–319
  - MRO *see* medium-range order
  - multilayer mirrors
    - graded 77
    - laterally graded 145, 151
  - multilayers 62, 68
    - magnetic 177
    - periodic 173
    - reflectivity 171–175
  - multiphase materials, residual stresses 270
  - multiple-crystal diffractometer 307, 328
  - multiplicity 24
- n**
- nanocrystallites, palladium 117
  - nanoparticles,  $\text{CoFe}_2\text{O}_4$  136
  - National Institute of Standards and Technology (NIST) 53
  - Neerfeld–Hill approximation 263
  - nickel layer 129
  - NIST *see* National Institute of Standards and Technology
  - nitride coatings 242
    - hard 233
  - non-coplanar configuration 195
  - Non-Proliferation Treaty, nuclear arms 40
  - normal function, logarithmic 118
  - nuclear fission bombs 40
  - numerical data analysis 87–89
- o**
- octahedrons 113
  - ODF *see* orientation distribution function
  - one-elemental metals, crystal structures 22
  - optical coatings, properties 169
  - optical films 177
  - optoelectronic devices 301
  - optoelectronic thin-film applications, texture 231
  - orientation, crystallites 183–238, 200
  - orientation densities, representation 202
  - orientation distribution function (ODF) 25, 183, 201, 220
    - coefficients 223
    - epitaxial films 315
    - expansion 205
    - normalization 225
    - sections 228
    - XSA 267
  - Ostwald’s rule of stages 80
  - outer cut-off radius 90, 132
  - overlap 102, 106
    - bragg peaks 68
    - peak 128

**p**

- pair distribution function 73
- pair production 56
- palladium nanocrystallites 117
- parafocusing geometry 194, 252
- parafocusing mode 16
- parallel beam configurations 176
- parallel beam geometry 77, 194
- parallel beam mode, diffractometer 151
- parallel beam optics 144
- parallel plate collimator (PPC) 144
- pattern decomposition 131, 132
- $\text{Pb}_{0.88}\text{La}_{0.08}\text{TiO}_3$  (PLT) 203
- PDF *see* powder diffraction file
- PSD *see* position-sensitive detectors
- peak asymmetries 97
- peak intensity measurement 198
- peak parameters, profile analysis 86–97
- peak shift 244
  - GID 176
- peak splitting 98
- Pearson function 95, 130
- PECVD *see* plasma-enhanced CVD
- peeling 239
- penetration depth 27, 59, 155–158, 162, 164, 280
  - solids 60
  - variations 253
  - x-ray 278
- perovskite structure 135, 185
  - notations 187
- perpendicular projection 192
- phase composition 43
- phase difference
  - beams 169
  - derivation 170
- phase factor 162
- phase mixtures 66–69
- phase problem 23
- phase shift 2, 6
- phase system comparison 199
- phases
  - amorphous 70
  - Aurivillius 135
  - chemical 42–84
  - metastable 53
  - nonequilibrium 53
- PHD *see* pulse height distribution
- photoelectrons 56
- photoionization 1, 55
- physical vapor deposition (PVD) 37, 60
- piezoelectrical fields 302
- piezoelectricity 188
- plane stacking 22
- plane wave propagation 162
- plasma-enhanced CVD (PECVD) 60
- plastic deformation 91, 271, 309
- PLT *see*  $\text{Pb}_{0.88}\text{La}_{0.08}\text{TiO}_3$  (PLT)
- PMS *see* pseudo macrostresses
- point focus 66
  - x-ray tubes 31
- Poisson ratio 241, 248, 304
- polarizability, spatially dependent 319
- polarization 3
- polarization factor 26, 321
- pole figures 184, 191–195, 193
  - Ag 228
  - diamond 233
  - incomplete 197
  - inverse 200–203
  - measurements 195–200
  - visualization 192
  - YBCO 219
- polonium 40
- polycapillary lenses 146, 147
- polycrystalline films 81, 216
  - residual stress 271
  - residual stress distribution 282
- polycrystals
  - elastic constants 263
  - textured 325
- porosity 60, 65, 239
- position-sensitive detectors (PSDs) 257
- postoxidation 241
- powder cell 53
- powder diffraction 47
- powder diffraction file (PDF) 52
- powder diffractometers 15
- powder pattern 125
- powder reflection, intensity 189
- PPC *see* parallel plate collimator (PPC)
- precision
  - cell edge determination 76
  - difference to accuracy 79
  - instrumental 249
- preferred orientation 25, 68
  - derivation 207
  - second axis 216
- primary extinction correction 317
- profilometry 62
- property profiles, thin films 159
- proportional counter 253–254
- protective coatings 241
- pseudo macrostresses (PMS) 270
- pseudomorphic growth 303
  - breakdown 305
- pseudo-Voigt function 95, 130

## 352 | Index

- pulse height distribution (PHD) 255
- pulse height distribution (PHD) discrimination 255
- PVD *see* physical vapor deposition
- pyroelectricity 186
  
- q**
- quartz glass 82, 166
- quartz rocks, deformed 208
  
- r**
- R values 88
- Rachinger correction 99, 104
- radial scan 334
- rank of harmonic expansion, ODF 226
- RRefSim *see* rocking curve and reflectivity simulations
- real-time multiple strip (RTMS) 258
- reciprocal space map 298, 332–337
  - SiGe(C)/Si(C) superlattice structure 336
- reference frame, crystal 111, 120
  - laboratory 111
  - transformation matrices 17
- reflection broadening 107–120, 107–120
- reflection centroids, shift 164
- reflection coefficients 172
  - multilayer system 171
- reflection intensity 67
- reflection profile 89
- reflection splitting, Ge films 308
- reflective coatings 37
- reflectivity 171–175
  - single layer 168–171
  - substrate 166–168
- refractive index 147, 160–161, 165
  - imaginary part 280
- regression, nonlinear 88, 96
- relaxation
  - determination 311
  - onset 338
  - strain 303
- relaxation parameter 304
- residual stress 134, 270
  - origin 271
- residual stress analysis (RSA) 239–296
  - depth-dependant properties 159
  - with texture 265
- residual stress evaluation, scattering vector method 286
- residual stress fields, nonuniform 278
- residual stress gradients 273–276
- residual stress measurement, x-ray diffraction 240
- residual stress state, biaxial 275, 284
- residual stress tensor, off-diagonal components 251
- resistivity, ZNO:Al layers 232
- resolution
  - divergent beam optics 45–46
  - energy 255–256
  - epitaxial layer investigations 307
  - high 297–339
  - instrumental line profile 97–98
  - spectrum 103
- Reuss approach 262
- Rietveld fitting schemes 208
- Rietveld programs 210
- Rietveld refinement 131, 132
- rock salt structure 242
- rocking curve and reflectivity simulations (RRefSim) 166, 322
- rocking curves 184, 210, 297
  - corrected 214
  - high-resolution 306
  - measurement 211
- rotating anode 35
- rotational symmetry
  - biaxial residual stress state 275, 284
  - thin films 204
- roughness, surface 168, 171
- RTMS *see* real-time multiple strip
- Rutherford backscattering 65
- rutile films 154
- rutile structure 149–150
  
- s**
- sample
  - adjustment 146
  - chemical composition 290
  - depth 153
  - length 45
  - reference frame 11, 69, 221
  - rotation 69, 151, 279, 284, 286, 306
  - tilt 196
  - transparency 77
  - XRR 165
- satellite peaks 110
  - parallelepipeds 113
- SAW *see* surface acoustic wave
- SAXS *see* small-angle x-ray scattering
- SBT *see* SrBi<sub>2</sub>(Ta<sub>1-x</sub>Nb<sub>x</sub>)O<sub>1</sub> (SBT)
- scaling factor 36
- scan
  - azimuthal 218–220
  - radial 334
  - $\theta/2\theta$  1, 11–13, 211
  - $\omega$  211

- scattering 55
  - coherent 1
  - diffuse 337–338
  - from atomic nuclei 3
  - inelastic 1
  - Rutherford backscattering 65
  - Thomson 2
- scattering angle 2
- scattering factors, anomalous 18
- scattering plane 2
- scattering vector 6, 102, 151, 284, 332
  - construction 7
  - GIXRD 150
- Scherrer constants 115
- Scherrer equation 108–110
- scintillation counter 253, 255, 256
- screw dislocation 90
- secondary extinction 317
- selective perception, subsets of crystallites 13
- semiconducting layers, texture 232
- semiconductors 48, 76
  - doping 328
  - high dielectric constants 176
- shadowing optics 44
- shape parameter 89
- sharpness, texture 224
- signal-to-noise ratio, improvement 69
- silane (SiH<sub>4</sub>) 70
- silicon 75
  - amorphous 70
- simple cubic lattice 9, 19
- single-crystal heteroepitaxy 271
- single-crystalline film 217
- single crystals 36, 325
  - microstructure 315
- single layer, reflectivity 168–171
- single-line analysis 129–130
- size broadening 101, 120–134
- size distribution function 107
- size parameter 110
  - average 119
- slip system 91, 125
  - fcc lattices 92
- slits 44, 144
  - detector 45
  - divergence 45, 97
  - receiving 78, 97, 132
  - Soller 46, 78, 97
- small-angle grain boundaries, mosaic block 315
- small-angle x-ray scattering (SAXS) 135
- Snell's law 161–162
- solar cells 70, 80
- Soller slits 46, 78, 97
- sphalerite structure 50–52, 299–300
- spherical harmonic functions 204
- splitting
  - Bragg peaks 13, 33, 45, 98–99
  - tetragonal 185–187
- square root intensity plot 13
- SrBi<sub>2</sub>Nb<sub>2</sub>O<sub>9</sub> (SBNO) 135
- SrBi<sub>2</sub>(Ta<sub>1-x</sub>Nb<sub>x</sub>)O<sub>1</sub> (SBT) 198
- stacking faults 92, 107, 121, 135
- standard data 106
- standard profile 128
- standard sample 75
  - LPA 100
- steep residual strain, detection 284
- stereographic projection 192
- stick pattern 47
- stoichiometry determination 74–75
- stoichiometry deviation 81
- Stoney's formula 253
- strain 121, 244, 303–306
  - root mean square 122
- strain broadening 101, 120–134
- strain distribution, thin films 265
- strain field 85, 90
- strain tensor 246
- strain-free direction, determination 250
- strain-free tilt angle 248
- stress
  - classification of 268–277
  - extrinsic 271
  - first kind 240
  - intrinsic 75, 271
- stress components 260, 274
- stress model, biaxial 244
- stress states, formation 289
- stress-free tilt angle 260
- stress-strain relation 261
- structure
  - body-centered cubic (bcc) 20–21, 91
  - chalcopyrite 82
  - close-packed 21
  - columnar honeycomb 316
  - crystallographic 43
  - diamond 48–49, 299
  - face-centered cubic (fcc) 20–21, 91
  - fine 57
  - hexagonal 22
  - hexagonal close-packed (hcp) 20
  - micro- *see* microstructure
  - perovskite *see* perovskite structure
  - polonium 4
  - profiles 324–332
  - rock salt 242

## 354 | Index

- rutile 149–150
  - simple cubic 4, 5
  - sphalerite *see* sphalerite structure
  - wurtzite *see* wurtzite structure
  - zinc blende-type 242
  - structure factor 19–24
    - diamond lattice 48
    - perovskite structure 185
    - rock salt structure 242
    - rutile structure 149
    - zinc blende structure 50
  - substrate, reflectivity 166–168
  - substrate normal 204
  - substrate peak 61
  - substrate temperatures 53
  - superlattices 173
    - layer structures 332
    - reflectivity 171–175
  - surface, ideally smooth 168
  - surface acoustic wave (SAW) 189
  - surface layers, thin 176
  - surface oxidation, analysis 178
  - surface roughness 168, 171
  - surface sensitivity 171
    - GID 176
  - surface-induced disorder phase transitions 178
  - symmetry
    - crystals 193
    - perovskite 185
    - rotational *see* rotational symmetry
    - *see also* asymmetry
  - symmetry constraints, ODF 223
  - symmetry-adapted functions, cubic crystal class 223
  - synchrotron GID study 177
  - synchrotron radiation sources 229
- t**
- Takagi–Taupin equations 323–324, 328
  - take-off angle, anode focus 34
  - tensor transformation 246
  - tetragonal crystals 149
  - tetragonal distortion, heteroepitaxy 303
  - tetragonal splitting 185–187
  - tetrahedral coordination 48
  - tetrahedrons 113
  - texture analysis 201, 211
    - Ca-doped PbTiO<sub>3</sub> film 209
    - computer programs 206
  - texture factors 25, 63, 184, 188–190, 208
    - derivation 204
  - texture influence, minimization 266
  - texture profile, normalized 214
  - texture states, formation 289
  - textures 25, 134, 183–238
    - axisymmetric 204
    - biaxial 184, 216–228
      - effect 265–268
    - fiber *see* fiber textures
    - fully general 225–228
    - general 216–228
    - high-temperature superconducting composite ribbons 231
    - layer 204–215
    - metals 227
    - optoelectronic thin-film applications 231
    - polycrystals 325
    - residual stress analysis (RSA) 265
    - semiconducting layers 232
    - sharpness 224
      - thin-film 228–230
  - thermal barrier coatings 172, 173
  - thermal expansion coefficients 299
  - thermal stresses 271
  - thermal vibrations 23
  - thickness 60, 80
    - film 27
    - geometrical 64
    - mass 65
  - thickness factor, metals 28
  - thickness homogeneity 46
  - thickness inhomogenities 65
  - thin films 52
    - absorption effect 27
    - aluminum 13, 178
    - amorphous 70–74
    - analysis 143, 162, 333
    - CrN 266
    - defect incorporation 272, 275
    - depth dependency 80, 228–230
    - diamond 233
    - diffraction pattern 189
    - elasticity 289
    - epitaxial 315
    - ferroelectric 203
    - GID measurement 178
    - growth 55, 124, 129, 155, 230
    - macroresidual stress 273
    - magnetic 177
    - material parameters 305
    - mechanical stress 239
    - metal 37
    - microstructure 134, 136
    - nanocrystalline 102
    - piezoelectric 188
    - pole figure measurement 198

- polycrystalline 36, 54
- polycrystalline 183
- powder pattern 250
- Pr<sub>2</sub>O<sub>3</sub> 177
- property profiles 159
- refractive index 161
- residual stress analysis (RSA) 159
- residual stress gradients 276
- rotational symmetry 204
- silicon 61
- strain distribution 265
- strains 244
- stress gradient analysis 281
- structural properties 313
- thickness 156
- TiN 247
- TiO<sub>2</sub> 154
- titanium 38
- W-C:H 135
- *see also* layers
- Thomson scattering 2
- three-bounce configuration, CCC 328
- tilt angle 191
  - strain-free 248
- total absorption 163
- total external reflection 161–165
- triaxial residual stress 276
- triple-crystal diffractometer 337
- tube window 44
- twin planes 92, 107
- twist and tilt, minimized 217
- two-dimensional wire detector 257
  
- u**
- ultrahigh density recordings 107
- unit cell 48
  - columns 111
  - crystallographic 9
  - edge 74
  - perovskite 186
  - *see also* structure
- unit vectors 200
- unmeasured reflections, computation 206
  
- v**
- VCSEL *see* vertical-cavity surface-emitting laser
- Vegard's rule 75, 80, 306
- vertical-cavity surface-emitting laser (VCSEL) 301
- voids
  - mosaic blocks 315–316
  - thin-film growth 64
- Voigt approach 261–262
  
- Voigt function 95, 129
- volume
  - sample 35
  - unit cell 35
  
- w**
- Warren-Averbach analysis 126, 134
- wave field 319
- wave vector 2, 161, 172
  - GID 175
- whole pattern fitting (WPF) 207–210, 289, 130–133
- Williamson-Hall analysis 122–126
- Williamson-Hall plot 123, 134
  - modified 126
- WPF *see* whole pattern fitting
- wurtzite compounds 188
- wurtzite structure 50–52, 242, 299, 301
  - ZnO 231
  
- x**
- XANES *see* x-ray absorption near-edge spectroscopy
- XAS *see* x-ray absorption spectroscopy
- x-ray absorption near-edge spectroscopy (XANES) 57
- x-ray absorption spectroscopy (XAS) 57
- x-ray attenuation coefficient 143
- x-ray beam conditioners 325
- x-ray beam divergence 213
- x-ray diffraction 1–41
  - high-resolution 297–342
  - perovskites 186
- x-ray emission 31–35
- x-ray fluorescence 30
- x-ray mirrors 175
- x-ray penetration depth 278
- x-ray reflectivity (XRR) 143, 165–175
- x-ray reflectometry (XRR) 143, 257
  - curve 166–167
  - fringing 171
  - patterns 173
  - Ta<sub>2</sub>O<sub>5</sub> 169
- x-ray refractive index 44
- x-ray residual stress analysis (XSA) 240, 247
  - fundamental equations 246
- x-ray stress analysis 243
- x-ray stress gradient analysis 281–282
- x-ray topography 338
- x-ray tubes 30–35, 249
  - ceramic 31
  - copper 13
  - focus modes 34

356 | *Index*

- laboratory 31
- mode 146
- XRR *see* x-ray reflectometry
- XSA *see* x-ray residual stress analysis

**y**

- YBCO film 216
  - critical current density 217
- Young's modulus 260

**z**

- zero shift 76
- zinc blende-type structures 242
  - structure factor 50
- zinc sulfide (ZnS) 50
- ZnO:Al layers, resistivity 232
- ZnSe films 53
  - diffraction pattern 54