

Index

A

Absorbed hydrogen, 129–134
Accelerators, 282
Activated carbon fibers (ACF25), 182–183
Amorphous materials
 bcc phase and nanoparticles, 108
 metal hydride products, 105
 MgCo alloy, 108
 nanocrystalline, 107
 $\text{TbFe}_2\text{D}_{3.0}$, 106
 ZrNiD_x , 105
Amplitude-weighted phonon density,
 259–260
Anderson, C.D., 378
Anharmonic potentials, 251, 254–255
ANTARES, 200, 201, 203, 215
Antiferromagnetic (AFM), 150
ARMCO™, 210
Atomic temperature factor, 55
Avogadro's number, 167

B

Bacon, G.E., 22
Bailey, I.F., 82
Banks, D., 1–5
Barium fluoride, 330
Barium titanate (BTO), 295, 296
Barnes, R.G., 338
Beam geometry, 198–200
Beam lines, 282, 287
Beam transport system, 331–332
Beaucage global scattering model, 186
Becker, H.-W., 315–336

Bee, M., 246, 271
Berger, P., 277–311
BET technique, 178
Billinge, S.J.L., 98
Bithmut Germanate (BGO) detectors, 319, 330
Blomqvist, A., 273
Bochum, 333–334
Bogdanovic, B., 74
Bohrs approximation, 325
Bohr's formula, 324
Borohydrides, 65, 78
Bowden, M., 54
Bowman, A.L., 71
Bragg-edge neutron imaging, 202
 crystal lattices, 202
 high-resolution energy, 202
Bragg equation, 125
Bragg peaks, 2, 123, 129, 137, 139, 164
Bragg scattering/diffraction
 diffuse scattering, 92
 and inelastic scattering, 20
 Rietveld refinement, 92
 specular reflections, 26
Bragg's law, 2, 316
Breit-Wigner curve, 317, 323
Brockhouse, B.N., 8, 252, 261

C

Caglioti, G., 49
Carrier gas hot extraction technique (CGHE),
 204, 205, 208
Catalyst layer, 131–132
Catalytic bulk effect, 3, 130

- Ceramics
- bilayered metal/ceramic hydrogen, 295
 - catalytic H₂ dissociation, 295
 - diffusion and transport models, 298
 - ERDA and RBS, 278–280
 - grain boundaries, 292, 299
 - hydrogen concentration profiles, 298
 - LiTaO₃ wafers, 296, 297
 - STIM mode, 299
- Černý, R., 31–84
- Chudley, C.T., 271
- Chudley–Elliott model
- convolution functions, 272
 - exponential expansion, 272
 - incoherent scattering function, 272
 - Lorentzian expression, 270
 - Poisson function, 271
 - self-correlation function, 270
 - self-diffusion, atoms, 270
 - transparent approach, 271
- Clathrates, 268, 269
- Coherent inelastic neutron scattering
- advantage, 262
 - classical method, 261
 - contour plot, 62, 264
 - DFT, 261
 - energy and momentum conservation, 260–261
 - polycrystals, 261
 - reciprocal lattice vectors, 261
- Coherent neutron scattering, 230–231. *See also*
- Neutron scattering
 - constructive interference, 230
 - nuclei, 230
 - phase-shift, 230
- Coherent scattering
- Bragg scattering, 20
 - double-differential cross section (*see* Differential cross section)
 - length, 48
 - magnetic scattering, 24–25
- Cold liquid hydrogen moderator, 127
- Complex hydrides
- LiAl(ND₂)₄, 109, 110
 - M[Al(NH₂)₄]_n, 108
 - metal aluminium amides, 108
 - tetrahedral Al(NH₂)₄-, 108
- Computed tomography (CT)
- 3D hydrogen distribution, 194, 221
 - 3D sample reconstruction, 201
 - spatial material distribution, 201
- Conduction electrons, 316
- Constant wavelength (CW) techniques, 44–45
- Contrast variation, 176
- Cosmic rays, 332
- Cotts, R.M., 338
- Coulomb interaction, 316
- Cranswick, L.M.D., 15
- Cryogenic techniques, 2, 322
- Crystalline metal hydrides
- amorphous MgCo alloy, 108
 - deuterium on octahedral, 102
 - H-H/D-D separation, 99
 - powder neutron diffraction, 99
 - Reverse Monte Carlo modelling, 96, 100
 - Rietveld refinement, 98–100
 - SRO parameters, 99
 - “Switendick criterion,” 99, 100
 - α-VD_{0.8}, 99, 100
 - α-VD_{0.75}, 100
 - YFe₂D_{4.2}, 104
 - ZrCr₂D₄, 102–104
- Crystallographic Information File (CIF), 63
- Crystallography, 34–36, 42, 58, 62, 63
- Crystal structure
- Bravais lattices, 34, 35
 - crystallographic symmetry, 34
 - definition, 34
 - glide planes and screw axes, 35
 - International tables for crystallography, 35, 58
 - seven crystal systems, 34, 35
- D**
- Dark field imaging, 203
- Dark hydrogen, 220
- de Broglie wavelength, 8
- Debye–Waller factor, 38, 55
- Density functional theory (DFT) simulations, 62, 358
- Denys, R.V., 72–74
- Depth information, 321–322
- Depth profiling, 317–319
- Depth resolution, 322–324
- Deuterium absorption, 122
- DFT simulations. *See* Density functional theory (DFT) simulations
- Differential scattering cross section, 163
- mono-isotopic, 21
 - phase problem, 23
 - protium and deuterium, 24
 - quantum mechanical equation, 22
 - wave vector, 22
- Diffusion measurements, NMR
- application, 350

- hydrogen diffusion coefficients, 351
- PFG technique, 351
- spin-spin interaction, 350
- Digital radiography
 - beamlines, 198
 - CCD cameras, 198
- Dirac, M., 378
- Direct space methods, 66
- DOC. *See* Dynamic occupancy correction (DOC)
- Doppler broadening measurement
 - (coincidence), 322
 - electron momentum, 384
 - histogram, 380, 384
 - quantitative analysis, 396, 397
- Dynamic occupancy correction (DOC), 67
- E**
- Egami, T., 98
- Einstein oscillator model, 257
- EISF. *See* Elastic incoherent structure factor (EISF)
- Elastic incoherent structure factor (EISF), 372
- Elastic Recoil Detection Analysis (ERDA), 4
- Elastic recoil detection analysis (ERDA)
 - CH₄ and C₆H₆ precursors, 303
 - energy loss and depth resolution, 280–281
 - hydrogen concentration determination, 281–282
 - isolated buckle, 286
 - less-conventional detection setups, 283–284
 - mappings and spectra, 300
 - NRA, 285
 - pressure vessel, 301
 - PZT H₂, 296
 - RBS-ERDA measurement, 294
 - titanium sample, 285
 - tungsten sample, 291
- Elastic scattering, 160
 - Bragg diffraction, 25–27
 - Bragg scattering/diffraction, 25
 - Debye–Waller factor, 27
 - Miller indices, 27
 - unit cells, 24
- Electricity and hydrogen, 1
- Electro-impedance spectroscopy (EIS), 145
- Elliott, R.J., 271
- Elsässer, C., 255
- Energy carrier, 1
- Energy straggling, 324
- Epitaxial Nb layers, 136
- Ewald Sphere approach, 261
- Extended X-ray absorption fine structure (EXAFS), 144
- F**
- Fe layers, 117, 137, 140
- Fermi wave vector, 151, 154
- Fernandez, J.F., 258
- Fibre texture, 57
- Flacau, R., 82
- Floppy drive, 199
- Form factor, 164
- Fractals, 169–170
- Frame overlap, 127
- Fresnel's equation, 119
- Fritzsche, H., 1–5, 115–155
- FTIR-ERDA intercalibration curve, 301
- G**
- Giant magnetoresistance (GMR) effect, 150
- Gissler, W., 271
- Glatter, O., 174
- Global energy distribution system, 1
- Global optimization methods, 66
- Graham, T., 83
- Gray, E.M., 71, 84
- Griesche, A., 193–223
- Grosse, M., 193–223
- Guinier approximation, 166–167
- Guinier plot, 166–167
- Guinier regression, 183
- Guzik, M.N., 73
- H**
- Hauback, B.C., 7–29, 31–84
- High-resolution neutron imaging facilities, 203
- Hinczak, I., 63
- Hjörvarsson, B., 115–155
- Ho, K.-M., 255
- Hot-Vacuum Extraction Mass Spectroscopy (HVEMS), 243
- Howard, C.J., 47, 63
- Huot, J., 1–5, 31–84
- Hydrogen
 - algorithm, 66
 - concentration, 320 (*see also* Hydrogen concentration)
 - concentration in metal hydrides, 160
 - DOC, 67
 - embrittlement, 135
 - incoherent scattering, 4
 - intensity extraction (IE), 66
 - interaction with materials, 1
 - isotopes, 116
 - metal atoms, 66
 - metal hydride, 65, 66
 - metal interactions, 2, 5

- Hydrogen (*cont.*)
- metal systems, 2
 - Mg₆Co₂H₁₁, 80
 - NaAlD₄ and LiAlD₄, 76–78
 - nano-confined hydrides, 160
 - nuclear densities, 66
 - from primary energy sources, 1
 - solubility curves, 141
 - storage, 2–3
 - Ti-V-Mn Alloy, 67–69
 - X-ray scatterer, 37, 65
- Hydrogen concentration in metals
- determination, 281–282
 - deuterium, 291, 293
 - generic approach, 290
 - high energy protons, 16, 283, 286, 292
 - hydrided Zircaloy-4, 289
 - in situ measurements, 291
 - molecular deuterium, 291
 - nanostructuring/thin films, 293
 - ODS steels, 290
 - Pd/Mg/Pd trilayers, 294
 - physical and chemical properties, 285
 - PWR, 286, 287
 - steam oxidation, 218, 288
 - steel embrittlement, 284
 - surface oxidation, 293
- Hydrogen depth profiles, 297
- Hydrogen diffusion coefficients
- alloys and intermetallic compounds, 367
 - Laves-phase systems, 370
 - spin-echo technique, 369
- Hydrogen distributions
- concentration profile, 209
 - material damage, 209
 - radiographic projections, 209
- Hydrogen embrittlement (HE)
- atomic hydrogen, 204–206, 209
 - HAC, 204
 - sample-detector distance, 205
 - stress field, 204
 - visualization and measurement, 205
- Hydrogen embrittlement, pure Fe
- annealing temperatures, 387–389
 - cathodic electrolysis, 387–389
 - TDA, 398, 400
 - tensile straining, 398, 400
- Hydrogen-free matrix, 320
- Hydrogen-induced cold cracks, 204
- Hydrogen mobility
- atomic motion, 338, 363
 - borohydrides, 363
 - BPP model, 360
 - clathrate hydrates, 369
 - deuterides, 362, 368
 - diffusion coefficients, 369
 - electric quadrupole interaction, 361
 - intermetallic compounds, 367
 - Lorentzian form, 360
 - motional contribution, 359, 360
 - QENS, 371–372
 - quadrupole relaxation, 363
 - resonance frequency, 363
 - spectral density, 362, 364
 - spin-lattice relaxation, 362, 365
 - static dipole-dipole interactions, 358
- Hydrogen pump effect, 218
- Hydrogen storage materials
- complex hydrides, 108–110
 - metal hydrides (*see* Crystalline metal hydrides)
- I**
- Ikeda, K., 109
- Incoherent inelastic scattering
- analytic model, 252
 - Cartesian directions, 252
 - clathrates, 252
 - Debye-Waller factor, 253
 - Fermi's Golden rule, 253
- Incoherent neutron scattering. *See also*
- Neutron scattering
 - absorption, 232
 - cross sections, 232, 233
 - deuterium, 228
 - diffraction pattern, 232
 - gamma/beta rays, 232
 - hydrogen, 232
 - intensity, 231
 - metallic materials
 - background-corrected diffraction patterns, 235, 241
 - binary H-Zr phase diagram, 238, 239
 - CANDU nuclear power reactors, 227
 - constant temperature, 240
 - Delayed Hydride Cracking, 228
 - 3-dimensional color map and colour contour plot, 241
 - elegant and robust techniques, 244
 - E3 spectrometer, 240
 - excess counts, hydrogen concentration, 236, 243
 - HVEMS, 243
 - initial diffraction pattern, 240
 - least-squares fitting process, 243

- Lever Rule, 239, 243
- matrix/hydride phase, 242
- tail and peak sections, 242, 243
- TSS, 239, 240
- weight fraction hydride, 239
- zirconium, 239
- Zr-2.5Nb pressure-tube, 238, 240
- nuclear fuels
 - acquisition time, 236
 - best fit line, 236
 - cadmium masks, 233
 - 32-channel detector, 235, 240
 - diffraction pattern, 233
 - experimental setup, 233
 - gauge volume, 233, 234
 - germanium mosaic single crystal, 233
 - host material, 238
 - hydrogen concentration, 236
 - instrument configuration, 238
 - L3 diffractometer, 233, 235
 - monitor value (*DBMon*), 236
 - multiple scattering, 236
 - organic lubricants, 233
 - Poisson distribution, 237
 - stochastic process, 236, 237
 - syringe assembly, 234
- phase-shift, 230
- Incoherent scattering length, 48
- Indirect Fourier transform (IFT), 174
- Inelastic incoherent neutron scattering
 - perturbation analysis, 254
- Inelastic scattering, 160
- Iniguez, J., 20, 259
- In situ diffusion measurements
 - ANTARES, 200–203
 - hydrogen effusion, 207, 208
 - neutron radiography, 203, 205–208
- In situ experiment
 - cell design, 82–83
 - metal alloy, 80
 - Mg₆Co₂H₁₁ structure, 81
 - Palladium, 83
 - Zircaloy-4, 84
- Ion beam analysis (IBA), 277
- Itoh, K., 105, 107
- K**
- Kapton[®] film, 278, 281
- Karlsruhe Institute of Technology, 219
- Keen, D.A., 98
- Kemali, M., 255
- Khodja, H., 277–311
- Kiessig fringes, 119, 122, 123, 128
- Kiessig, H., 119
- Kim, H., 108
- Kisi, E.H., 47, 63
- Klose, F., 115–155
- Knudsen, K.D., 159–191
- Koppel, J.A., 246, 264
- L**
- Lanford, W.A., 316
- Langmuir–Blodgett films, 116
- LaNi₅ based alloys, hydrogenation
 - annealing temperature, 387–389
 - dislocation density, 390, 400
 - isochronal annealing, 387, 388, 398
 - positron annihilation experiments, 386, 400
 - trapping model, 390
 - vacancy clusters, 13, 99, 387–388
 - vacancy concentration, 387–390
- LaNi₅Cu, hydrogenation
 - dehydrogenation, 395, 396
 - Doppler broadening spectra, 384–386, 392
 - PAS technique, 377, 379, 391
 - positron lifetimes, 388, 389
 - quantitative analysis, 386, 397
 - ratio curves, 392, 393, 396
- Lattice defects
 - hydrogenation
 - LaNi₅ based alloys, 386–390
 - LaNi₅Cu, 391–397
 - hydrogen embrittlement, pure Fe, 397–400
- Lattice dynamics
 - amplitude-weighted vibrational density, 257
 - binary hydride, 257
 - Born–Mayer potentials, 258
 - coherent scattering, 257
 - inelastic neutron scattering, 18, 82, 260–263
 - metal hydrogen compounds, 257
 - phonon solution, 256, 259
- Lattice gas, 135
- Laves phase
 - amorphous deuteride, 106, 107
 - C15-type, 102, 104
 - hydrides, 367–369
 - ZrTiNiD₂, 105
- Lead zirconate titanate (PZT), 19, 295
- Leich, D.A., 316
- Lelièvre, G., 84
- Less-conventional detection setups, 283–284
- Lever Rule, 239, 243
- Leyer, S., 358

- Liquid hydrogen (LH₂), 171–172
 Loss of Coolant Accident (LOCA), 12, 219
- M**
- Magic-angle spinning (MAS)
 anisotropy, 347
 mechanical rotation, 347
 quadrupole interactions, 347
- Magnesium hydride, 129
- Magnetic and depolarization measurement, 202
- Magnetic neutron scattering, 39
- Magnetism reflectometer (MR), 127
- Magusin, P.C.M.M., 355
- March–Dollase model, 57
- Mark TRIGA reactor, 197
- MAS. *See* Magic angle spinning (MAS)
- Matrix atoms, 320
- Maxwell-Boltzmann distribution
 MeV-energy, 12
 solid line, 12, 27
- McGreevy, R.L., 96, 97
- McLennan, K.G., 83
- Mercury cadmium telluride (MCT), 304
- Metal hydride, 2
- Metal-hydrogen systems, 256–258, 339, 340
- Mg–Al alloy composition, 130–131
- Mg-based alloy layer, 123, 129–134
- Miller indices, 27
- Minerals (hydrogen measurement)
 FTIR calibration, 301
 FTIR-ERDA intercalibration, 301
 H contribution, 301
 rhyolitic melt inclusion, 301
- Mitchell, P.C.H., 259
- Molecular hydrogen
 heterogeneous, 267
 incoherent scattering, 263
 magnetic catalysts, 266
 perturbation theory, 254, 265
 rotational form factors, 265
 scattering function, 264–266
 total scattering function, 266
- Monochromator, 10, 13, 171–172
- Monte Carlo simulation, 324–325
- Multiple scattering, 95, 173, 236, 262, 281
- Muons, 332
- N**
- NaAlH₄, 247, 251, 259, 260
- Nakamura, Y., 67, 69
- Nano-confined hydrides, 160
- Nanoscale, 130
 hydrides, 174
 thin films, 129
- Nano-sized metal hydrides
 FeTiH_x, 108
 LaNi₅, 107
 metallic glasses, 105
 PDFs, 93–95, 98, 104
 RE₄ tetrahedra, 106, 107
 Tb hydride, 106
 titanium and zirconium, 107
- Nanostructures, 3
¹⁵N beam, 323–324
- Nb layer, 143
- Neutron
 beam hitting, 127
 collision between, 4
 imaging, 3
 absorption probability, 195
 calibration, 194
 3D reconstruction, 210
 elastic scattering, 195
 gamma radiation, 197
 hardware limit, 200–201
 high-energy fission neutrons, 195
 horizontal intensity distribution, 213, 214
 hydrogen concentration, 217, 218
 hydrogen-containing systems, 194
 path length, 196, 213
 scattering lengths, 195
 temperature dependence, 218
 X-rays and gamma rays, 196
 powder diffraction, 2
 radiographs, 3
 scattering length, 2
 scattering techniques, 4
 spectrometers, 4
- Neutron powder diffraction (NPD)
 advantage, 37
 coherent neutron scattering, 36
 CsCl structure type, 37
 FeCo alloy, 37, 38
 instrumentation
 CW techniques, 44–45
 CW vs. ToF, 44
 hydride, 32
 materials containing hydrogen, 48–49
 neutron fluxes, 48
 LaNi₅ and LaNi₅D₆, 71
 magnetic neutron scattering, 39
 metal hydrides, 32
 neutron structure factor, 38
 wavelength neutrons, 33, 44

- XPD, 31
- X-rays and electrons, 36
- Neutron reflectometry (NR) technique, 3, 116–117, 145
 - instrumentation, 125–128
 - principles of method
 - determination of hydrogen and deuterium content, 122–124
 - polarized neutrons, 120–121
 - unpolarized neutrons, 117–120
- Neutron scattering. *See also* Coherent neutron scattering, *See also* Incoherent neutron scattering
 - ab initio calculations, 255
 - absorption cross section, 18, 19
 - advantage, 9
 - amplitude-weighted phonon density, 259–260
 - coherent (*see* Neutron scattering:coherent scattering)
 - coherent and incoherent, 250, 251
 - Coulomb interactions, 228, 316
 - de Broglie wavelength, 8
 - detection
 - boron-lined converter, 15
 - fuel cell/hydrogen content, 15
 - gases, 14
 - imaging instruments, 14
 - PSD, 15
 - scintillator, 15
 - ZnS, 15
 - DFT simulations, 258–259
 - elastic scattering, 25–27
 - fragile specimens, 9
 - hydrogen concentration, 228, 233
 - in situ experiment, 228
 - incident and scattered energies, 233, 247
 - incoherent (*see* Incoherent scattering))
 - inelastic (*see* (inelastic neutron scattering))
 - inhomogeneous surface, 247
 - kinetic energy, 10
 - lattice dynamics, 256–258
 - magnetic interactions, 247
 - magnetic scattering, 24–25
 - neelastic neutron scattering, 27–28
 - neutron flux, 10
 - nuclear power-generation industry, 244
 - periodic array of nuclei, 228
 - polycrystals, 260–263
 - production
 - cold/hot moderator, 12
 - Maxwell–Boltzmann distribution, 12
 - monochromator, 13
 - reactors and spallation sources, 12
 - thermal neutron, 12
 - TOF, 13
 - QENS, 28 (*see* (Quasi-elastic neutron scattering (QENS)))
 - reflection, 19
 - refraction, 19
 - scattering length, 16–18
 - spherical wave, 229, 230
 - X-ray and electron scattering, 8
 - zirconium alloy, 238
- Neutron’s magnetic moment, 120
- Nield, V.M., 98
- Nieminen, R.M., 398, 399
- Niobium phase diagram, 135
- NMR. *See* Nuclear magnetic resonance (NMR)
- Nominal anhydrous minerals (NAMs), 328
- NPD. *See* Neutron powder diffraction (NPD)
- NRU research reactor, 125
- Nuclear magnetic resonance (NMR), 4
 - dipole-dipole interaction, 340, 342, 352
 - experimental setup, 343–345
 - external magnetic field, 341, 342
 - gyromagnetic ratios, 338, 340
 - hydrogen mobility (*see* Hydrogen mobility)
 - hyperfine interactions, 341, 356
 - quadrupole interaction, 361, 362
 - spectral measurements, 345–346
 - structural information
 - alane (AlH₃), 355
 - component, 352
 - deuterium and hydrogen site, 352
 - face-centered cubic structure, 352
 - light metal hydrides, 355
 - Mg-Ni hydrides form, 354
 - transition-metal nuclei, 342
- Nuclear reaction analysis (NRA), 4, 134, 315–336
 - principle of method
 - depth information, 321–322
 - depth profiling, 317–319
 - depth resolution, 322–324
 - determining hydrogen concentration, 319–321
 - interaction of ions with matter, 316–317
 - straggling, 324–325
 - special cases and complications, 328
 - example of low concentration detection, 334–335
 - high efficiency γ -ray detection, 330–331
 - hydrogen concentrations strongly varying with depth, 333–334

- Nuclear reaction analysis (NRA) (*cont.*)
 stability of samples under irradiation, 329–330
- Nuclear relaxation time
 application, 348
 diffusive motion, 350
 inhomogeneity, 349
 longitudinal nuclear magnetization, 342
 spin locking experiment, 349
- Nuclear Resonance Reaction Analysis, 316
- O**
- Oak Ridge National Laboratory, 127
- Off-specular scattering, 117
- Olivine, 328
- Optical transfer matrix method, 119
- P**
- Pair distribution function (PDF)
 deuteride, 105–107
 deuterium-free ZrNi glass, 15, 105
 Li_3AlN_2 and AlN, 110
 nano-sized FeTiD_{0.97}, 108
 NOMAD (SNS, US), 94, 110
 NOVA (J-Parc, Japan), 110
 real-space Rietveld refinements, 98
- Palladium hydride, 83
- Parratt, L.G., 119
- Partial pair distribution function, 93
- PAS. *See* Positron annihilation spectroscopy (PAS)
- PDF. *See* Pair distribution function (PDF)
- Pd/H system, 273
- Pd layer, 131
- Peak shift, 123
- Peak width, 41–42
- Percheron-Guegan, A., 71
- Perovskites, 297, 298
- Perturbation analysis, 254
- PFG technique. *See* Pulsed field gradient (PFG) technique
- PG filter, 125
- Phase abundance, 71
- Phase analysis, 40–41
- Phonon/magnon
 coherent processes, 20
 inelastic neutron (*see* Inelastic neutron scattering)
- Photopeak detection efficiency, 326
- Pilling–Bedworth ratio, 147
- Pinhole camera, 198–200
- Planck's constant, 126
- Plasma facing material (PFM), 309
- Polarized neutron reflectometry (PNR), 120–121
- Polycrystalline samples (polyCINS), 252, 261, 263
- Polycrystalline thin Nb layers, 136
- Porod law, 167–168
- Porod plots, 168
- Porous scaffolds, 3, 179
- Position sensitive detectors (PSD), 15
- Positron annihilation spectroscopy (PAS), 5
 annihilation process, 378
 Doppler broadening measurement (coincidence), 384–386
 lattice defects (*see* Lattice defects)
 lifetime measurement, 379–383
 radioisotope, 378
 thermalized positrons diffuse, 378
- Positron lifetime measurement
 digital type system, 380
 discrete multiple components, 383
 electron density, 358, 379, 380
 exponential form, 383
 kapton films, 5, 6, 379, 381, 386
 two-state trapping model, 383
 vacancy clusters, 380, 381, 387
- Powder diffraction pattern
 peak width, 41–42
 qualitative phase analysis, 40
 quantitative phase analysis, 40–41
- Powder neutron diffraction, 99
- Powder pattern
 absorption factor, 53–54
 Bragg peak, 50
 calculation, 51–52
 crystalline material, 60
 CW diffractometer, 50
 displacement factor, 55
 Lorentz factor, 55–56
 preferred orientation, 56–57
 profile function, 58–59
 refined crystal structure, 60–63
 refinement strategy, 63–65
 scale factor, 52
 structural parameters, 50
 structure factor, 57–58
- Powder X-ray diffraction (PXD), 179, 182
- Pressurized water reactors (PWR), 84
- Prisk, T.R., 267
- Profilometric methods, 322
- PSD. *See* Position sensitive detectors (PSD)
- Pulsed field gradient (PFG) technique, 338

- Puska, M.J., 399
Pusztai, L., 96, 97
PWR. *See* Pressurized water reactors (PWR)
Pyrolytic graphite (PG), 125
- Q**
Q-disease, 135
QENS. *See* Quasielastic neutron scattering (QENS); Quasi-elastic neutron scattering (QENS)
Quantum states of Hydrogen, 246
Quasielastic neutron scattering (QENS), 4
 atomic jump motion, 38, 371
 EISF, 372
 incoherent and coherent scattering, 28
 LiBH₄-LiI solid solutions, 38, 371
 spectra and spin relaxation, 371
 tracer diffusion coefficients, 39, 350, 351
Quasi-elastic neutron scattering (QENS)
 atom diffusing, 274–275
 atom/unit cell, 273
 Chemical/Fick's Law, 270
 correlation functions, 270
 inelastic neutron, 250–251
 Pd/H system, 273
 self-correlation function, 274
QUENCH-LOCA, 219
- R**
Radiography experiments, neutron
 installations, 197
 TRIGA reactor, 197
Radius of gyration, 166
Raepsaet, C., 277–311
Reflectivity curve, 131
Reflectometers, 126
Reflectometry, 3, 117
Rehm, C., 115–155
Resonant soft X-ray reflectivity (R-SoXR), 308
Reverse Monte Carlo (RMC)
 amorphous metal hydride, 105, 106
 crystalline solids, 96
 DISCUS software, 105
 real-space Rietveld refinement, 98
 software codes, 97
 α -VD_{0.8}, 99
Rietveld method
 powder pattern, recording and calculation
 (*see* Powder pattern)
 principle, 49–50
Rietveld refinement method, 2
RMC. *See* Reverse Monte Carlo (RMC)
- Roach, D.L., 245–275
Rogalla, D., 315–336
Ropka, J., 104
Ross, D.K., 245–275
Rother, H., 271
Rowe, M.J., 273
Ruderman–Kittel–Kasuya–Yoshida (RKKY), 151
Rudolph, W., 320
Rutherford-Backscattering Spectrometry measurements, 319
Ryan, D.H., 19
Ryan, M., 54
- S**
Sakaki, K., 377–400
Sartori, S., 159–191
Sato, T., 110
Saturated calomel electrode (SCE), 146
Scattering by one/two atom, 161
Scattering geometry, 117, 120
Scattering length
 coherent/incoherent scattering length, 17
 isotopes, 17, 27
 protium (1H) isotope, 17
 SLD, 17
 spherical waves, 16, 28
Scattering length density (SLD), 116, 118, 123–124, 147–150, 178, 181
Scattering vector, 160
Scherrer shape factor, 41
Schillinger, B., 193–223
Schwickardi, M., 74
Search-match program software, 40
Secondary Ion Mass Spectrometry (SIMS), 321
Senadheera, L., 356
Setthan, U., 355
Shelyapina, M.G., 337–372
Silicon wafers, 323
SIMS-FTIR intercalibration, 301
Skripov, A.V., 274, 337–372
SLD. *See* Scattering length density (SLD)
Small angle neutron scattering (SANS), 3, 159–160, 186
 data analysis, 174
 background subtraction, 178
 contrast variation and deuterium labelling, 176–177
 interacting particles, 175–176
 detector, 172
 form factor and particle correlation, 164–166

- Small angle neutron scattering (SANS) (*cont.*)
- fractals, 169–170
 - guinier approximation, 166–167
 - instrumentation, 171–173
 - interaction radiation/sample, 161–164
 - particle shape, 168–169
 - Porod law, 167–168
 - scattering vector, 160
- Sørby, M.H., 91–111
- Spallation neutron source, 127
- Specular reflectivity, 117
- Spin-echo technique, 5
- Spin flipper, 125
- Spin glass systems, 121
- Spin-up/down neutrons, 120–121, 138, 140
- Squires, G.L., 22, 246
- Stewart, A.T., 261
- Stopping power, 316
- Straggling, 324–325
- Strength of resonance, 320
- Stroboscopic neutron imaging, 202
- Subprogram QUENCH-ACM, 219
- Superconducting radio-frequency (SRF) cavities, 135
- Superlattice compounds, 71
- Suzuki, K., 105
- Switendick criterion, 99, 100
- T**
- Tandem accelerator, 323
- Ta/Pd bilayer, 131
- Taylor, J.C., 63
- Terminal Solid Solubility (TSS), 238, 239
- Ternary Mg-based alloys, 133
- Thermal neutrons, 10–12, 43, 44, 84
- Thermal solar, 1
- Thin films
- amorphous carbon films, 302
 - as-deposited layers, 304
 - bubbles and blistering, 306
 - deuterated a-CH films, 280
 - environmental exposure, 304
 - ERDA hydrogen profile, 308
 - FTIR spectroscopy, 307
 - non-diamond phase, 308
 - PECVD to EBE, 306
 - Quantum dots (QDs), 307
 - semiconductors, 304
 - thermal annealing, 296, 306
 - tribological parameters, 303
- Thomas, J.-P., 329
- Ti layer, 132
- Time-of-flight (ToF) techniques, 45–47, 126, 172
- spallation sources, 13
- Titanium-dihydride phase (TiH₂(δ)), 285
- Ti thin films, 148–150
- TOF. *See* Time of flight (TOF)
- ToF techniques. *See* Time-of-flight (ToF) techniques
- Tombrello, T.A., 316
- Tortuosity, 208
- Total cross section, 177
- Total neutron scattering, 2
- data reduction and analysis
 - isotropic scatterer, 95
 - RMC, 96, 97
 - TOF, 95, 97
 - hydrogen storage (*see* Hydrogen storage materials)
 - measurements (*see* Total scattering measurements)
 - spherical shell, 93, 94
 - static approximation, 93
- Total reflectivity, 118–119
- Total scattering measurements
- RMC, 96, 97
 - RMCPow, 98, 100
- Transmission electron microscopy (TEM), 134
- Tritium autoradiography (TARG), 205
- Tun, Z., 115–155
- U**
- Ulivi, L., 268
- Unit cells
- crystalline materials, 25
 - face-centered orthorhombic lattice, 25
- Unpolarized neutrons, 117–120
- V**
- Vanadium deuteride, 95, 99
- Van Hove, L., 22, 247, 270
- Vinyard, G.H., 270
- W**
- Webb, C.J., 61, 82
- Westlake, D.G., 69
- Williamson-Hall plot, 42
- Wolff, M., 115–155

X

XPD. *See* X-ray powder diffraction (XPD)
X-ray diffraction (XRD), 129
X-ray powder diffraction (XPD), 31
X-ray reflectometry (XRR), 3, 116
X-rays, 2

Y

Young, J.A., 246, 264
Yttrium, 326–328

Z

Zabel, 135–136
Zeeman energy, 120
Zircaloy-4, 84
 Arrhenius-plot, 222

 hydrogen concentration, 221, 222
 hydrogen diffusion, 221–222
Zirconium alloys, 3–4
 corrosion, 211
 embrittlement, 212
 ex situ and in situ
 ANTARES, 215
 Ar/O₂ atmosphere, 215
 breakaway effect, 218
 CT value, 216
 horizontal intensity distribution, 215
 hydrided and hydrogen, 212
 oxidation times, 216
 Zry-4 specimen, 218
 Hydrogen uptake, 216
 integral amount, 212
 neutron imaging methods, 212
Zr thin film, 146–148