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7.3 (cont.)

- Allemand, R., Bourdel, J., Roudaut, E., Convert, P., Ibel, K., Jacobé, J., Cotton, J. P. & Farnoux, B. (1975). *Position-sensitive detectors (P.S.D.) for neutron diffraction*. *Nucl. Instrum. Methods*, **126**, 29–42.
- Baruchel, J., Malgrange, C. & Schlenker, M. (1983). *Neutron diffraction topography: using position-sensitive photographic detection to investigate defects and domains in single crystals*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 400–406. London: Academic Press.
- Berliner, R., Mildner, D. F. R., Sudol, J. & Taub, H. (1983). *Position-sensitive detectors and data collection systems at the University of Missouri Research Reactor Facility*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 120–128. London: Academic Press.
- Boie, R. A., Fischer, J., Inagaki, Y., Merritt, F. C., Okuno, H. & Radeka, V. (1982). *Two-dimensional high precision thermal neutron detector*. *Nucl. Instrum. Methods*, **200**, 533–545.
- Borkowski, C. J. & Kopp, M. K. (1975). *Design and properties of position-sensitive proportional counters using resistance-capacitance position encoding*. *Rev. Sci. Instrum.* **46**, 951–962.
- Convert, P. & Chieux, P. (1986). *From BF₃ counter to PSD. An impressive and continuous increase of the data acquisition rate*. *Fifty years of neutron diffraction*, edited by G. E. Bacon, pp. 218–227. Bristol: Adam Hilger.
- Convert, P. & Forsyth, J. B. (1983). *Position-sensitive detection of thermal neutrons: Part 1, Introduction*. *Position-sensitive detection of thermal neutrons*, pp. 1–90. London: Academic Press.
- Fischer, J., Radeka, V. & Boie, R. A. (1983). *High position resolution and accuracy in ³He two-dimensional thermal neutron PSDs*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 129–140. London: Academic Press.
- Hohlwein, D. (1983). *Photographic methods in neutron scattering*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 379–390. London: Academic Press.
- Ibel, K. (1976). *The neutron small-angle camera D11 at the high-flux reactor, Grenoble*. *J. Appl. Cryst.* **9**, 296–309.
- Institut Laue–Langevin (1988). *Guide to neutron research facilities at the ILL*. Grenoble: Institut Laue–Langevin.
- Isis (1992). *User Guide*. Didcot: Rutherford Appleton Laboratory.
- Kurz, R. & Schelten, J. (1983). *Properties of various scintillators for thermal neutron detection*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 192–196. London: Academic Press.
- Naday, I. & Schaefer, W. (1983). *A new processing method and gain stabilisation for scintillation position-sensitive detectors*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 197–202. London: Academic Press.
- Roudaut, E. (1983). *Evolution of position-sensitive detectors for neutron diffraction experiments from 1966 to 1982 in the Nuclear Centre of Grenoble*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 294–301. London: Academic Press.
- Schaefer, W., Naday, I. & Will, G. (1983). *Neutron powder diffractometry with the linear position-sensitive scintillation detector*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 209–214. London: Academic Press.
- Strauss, M. G., Brenner, R., Chou, H. P., Schultz, A. J. & Roche, C. T. (1983). *Spatial resolution of neutron position scintillation detectors*. *Position-sensitive detection of thermal neutrons*, edited by P. Convert & J. B. Forsyth, pp. 175–187. London: Academic Press.
- Strauss, M. G., Brenner, R., Lynch, F. J. & Morgan, C. B. (1981). *2-D position-sensitive scintillation detector for neutrons*. *IEEE Trans. Nucl. Sci.* **28**(1), 800–806.
- Thomas, P. (1972). *Production of sensitive converter screens for thermal neutron diffraction patterns*. *J. Appl. Cryst.* **5**, 373–374.
- Whaling, W. (1958). *The energy loss of charged particles in matter*. *Handbuch der Physik*, Vol. 34. *Corpuscles and radiation in matter II*, edited by S. Flugge, pp. 193–217. Berlin: Springer-Verlag.
- Windsor, C. G. (1981). *Pulsed neutron scattering*. London: Taylor and Francis.
- Wolf, R. S. (1974). *Measurement of the gas constants for various proportional counter gas mixtures*. *Nucl. Instrum. Methods*, **115**, 461–463.

7.4.2

- Bachmann, R., Kohler, H., Schulz, H. & Weber, H. (1985). *Structure investigation of a CaF₂-crystal with synchrotron radiation*. *Acta Cryst.* **A41**, 35–40.
- Cooper, M. J. (1971). *The evaluation of thermal diffuse scattering of neutrons for a one velocity model*. *Acta Cryst.* **A27**, 148–157.
- Dorner, B., Burkel, E., Illini, Th. & Peisl, J. (1987). *First measurement of a phonon dispersion curve by inelastic X-ray scattering*. *Z. Phys. B*, **69**, 179–183.
- Helmholdt, R. B., Braam, A. W. M. & Vos, A. (1983). *Improved corrections for thermal diffuse scattering*. *Acta Cryst.* **A39**, 90–94.
- Helmholdt, R. B. & Vos, A. (1977). *Errors in atomic parameters and electron density distributions due to thermal diffuse scattering of X-rays*. *Acta Cryst.* **A33**, 38–45.
- International Tables for Crystallography* (1992). Vol. B. *Reciprocal space*, edited by U. Shmueli. Dordrecht: Kluwer.
- Jahn, H. A. (1942). *Diffuse scattering of X-rays by crystals. The Faxen–Waller theory and the surfaces of isodiffusion for cubic crystals*. *Proc R. Soc. London Ser. A*, **179**, 320–340; **180**, 476–483.
- James, R. W. (1962). *The optical principles of the diffraction of X-rays*. London: Bell.
- Krec, K. & Steiner, W. (1984). *Investigation of a silicon single crystal by means of the diffraction of Mössbauer radiation*. *Acta Cryst.* **A40**, 459–465.
- Krec, K., Steiner, W., Pongratz, P. & Skalicky, P. (1984). *Separation of elastically and inelastically scattered γ -radiation by Mössbauer diffraction*. *Acta Cryst.* **A40**, 465–468.
- Merisalo, M. & Kurittu, J. (1978). *Correction of integrated Bragg intensities for anisotropic thermal scattering*. *J. Appl. Cryst.* **11**, 179–183.
- Popa, N. C. & Willis, B. T. M. (1994). *Thermal diffuse scattering in time-of-flight diffractometry*. *Acta Cryst.* **A50**, 57–63.

REFERENCES

7.4.2 (cont.)

- Rouse, K. D. & Cooper, M. J. (1969). *The correction of measured integrated Bragg intensities for anisotropic thermal diffuse scattering*. *Acta Cryst.* **A25**, 615–621.
- Sakata, M., Stevenson, A. W. & Harada, J. (1983). *G-TDSCOR: one-phonon TDS corrections for measured integrated Bragg intensities*. *J. Appl. Cryst.* **16**, 154–156.
- Stevens, E. D. (1974). *Thermal diffuse scattering corrections for single-crystal integrated intensity measurements*. *Acta Cryst.* **A30**, 184–189.
- Stevenson, A. W. & Harada, J. (1983). *The consequences of the neglect of TDS correction for temperature parameters*. *Acta Cryst.* **A39**, 202–207.
- Suortti, P. (1980). *Powder TDS and multiple scattering. Accuracy in powder diffraction*, edited by S. Block & C. R. Hubbard. *Natl Bur. Stand. (US) Spec. Publ. No. 567*, pp. 8–12.
- Voigt, W. (1910). *Lehrbuch der Kristallphysik*. Leipzig: Teubner.
- Willis, B. T. M. (1970). *The correction of measured neutron structure factors for thermal diffuse scattering*. *Acta Cryst.* **A26**, 396–401.
- Willis, B. T. M., Carlile, C. J. & Ward, R. C. (1986). *Neutron diffraction from single-crystal silicon: the dependence of the thermal diffuse scattering on the velocity of sound*. *Acta Cryst.* **A42**, 188–191.
- Wooster, W. A. (1962). *Diffuse X-ray reflections from crystals*. Oxford: Clarendon Press.
- 7.4.3**
- Åberg, T. & Tulkki, J. (1985). *Inelastic X-ray scattering including resonance phenomena. Atomic inner shell physics*, edited by B. Crasemann, Chap. 10. New York: Plenum.
- Bannett, Y. B. & Freund, I. (1975). *Resonant X-ray Raman scattering*. *Phys. Rev. Lett.* **34**, 372–376.
- Bewilogua, L. (1931). *Incoherent scattering of X-rays*. *Phys. Z.* **32**, 740–744.
- Biggs, F., Mendelsohn, L. B. & Mann, J. B. (1975). *Hartree Fock Compton profiles for the elements*. *At. Data Nucl. Data Tables*, **16**, 201–309.
- Bloch, B. J. & Mendelsohn, L. B. (1974). *Atomic L-shell Compton profiles and incoherent scattering factors: theory*. *Phys. Rev. A*, **9**, 129–155.
- Bloch, F. (1934). *Contribution to the theory of the Compton line shift*. *Phys. Rev.* **46**, 674–687.
- Blume, M. & Gibbs, D. (1988). *Polarisation dependence of magnetic X-ray scattering*. *Phys. Rev. B*, **37**, 1779–1789.
- Brown, W. D. (1966). *Cross-sections for coherent/incoherent X-ray scattering*. Reports D2-125136-1 and 125137-1. Boeing Co.
- Bushuev, V. A. & Kuz'min, R. N. (1977). *Inelastic scattering of X-ray and synchrotron radiation in crystals, coherent effects in inelastic scattering*. *Sov. Phys. Usp.* **20**, 406–431.
- Cooper, M. J. (1985). *Compton scattering and electron momentum determination*. *Rep. Prog. Phys.* **48**, 415–481.
- Cromer, D. T. (1969). *Compton scattering factors for aspherical free atoms*. *J. Chem. Phys.* **50**, 4857–4859.
- Cromer, D. T. & Mann, J. B. (1967). *Compton scattering factors for spherically symmetric free atoms*. *J. Chem. Phys.* **47**, 1892–1893.
- Currat, R., DeCicco, P. D. & Weiss, R. J. (1971). *Impulse approximation in Compton scattering*. *Phys. Rev. B*, **4**, 4256–4261.
- Eisenberger, P. & Platzman, P. M. (1970). *Compton scattering of X-rays from bound electrons*. *Phys. Rev. A*, **2**, 415–423.
- Eisenberger, P., Platzman, P. M. & Winick, M. (1976). *Resonant X-ray Raman scattering studies using synchrotron radiation*. *Phys. Rev. B*, **13**, 2377–2380.
- Fermi, E. (1928). *Statistical methods of investigating electrons in atoms*. *Z. Phys.* **48**, 73–79.
- Gavrila, M. & Tugulea, M. N. (1975). *Compton scattering by L shell electrons*. *Rev. Roum. Phys.* **20**, 209–230.
- Hubbell, J. H., Veigele, W. J., Briggs, E. A., Brown, R. T., Cromer, D. T. & Howerton, R. J. (1975). *Atomic form factors, incoherent scattering functions and photon scattering cross-sections*. *J. Phys. Chem. Ref. Data*, **4**, 471–538.
- Jauch, J. M. & Rohrlich, F. (1976). *The theory of photons and electrons*. Berlin: Springer-Verlag.
- Klein, O. & Nishina, Y. (1929). *Über die Streuung von Strahlung durch freie Elektronen nach der neuen relativistischen Quantendynamik von Dirac*. *Z. Phys.* **52**, 853–868.
- Lipps, F. W. & Tolhoek, H. A. (1954). *Polarisation phenomena of electrons and photons I and II*. *Physica (Utrecht)*, **20**, 85–98, 395–405.
- Lovesey, S. W. (1993). *Photon scattering by magnetic solids*. *Rep. Prog. Phys.* **56**, 257–326.
- Manninen, S., Paakkari, T. & Kajantie, K. (1976). *Gamma ray Compton profile of aluminium*. *Philos. Mag.* **29**, 167–178.
- Pattison, P. & Schneider, J. R. (1979). *Test of the relativistic Is wavefunction in Au and Pb using experimental Compton profiles*. *J. Phys. B*, **12**, 4013–4019.
- Pratt, R. H. & Tseng, H. K. (1972). *Behaviour of electron wavefunctions near the atomic nucleus and normalisation screening theory in the atomic photoeffect*. *Phys. Rev. A*, **5**, 1063–1072.
- Ribberfors, R. (1975). *Relationship of the relativistic Compton cross-section to the momentum distribution of bound electron states. II. Effects of anisotropy and polarisation*. *Phys. Rev. B*, **12**, 2067–2074, 3136–3141.
- Ribberfors, R. (1983). *X-ray incoherent scattering total cross-sections and energy absorption cross-sections by means of simple calculation routines*. *Phys. Rev. A*, **27**, 3061–3070.
- Ribberfors, R. & Berggren, K.-F. (1982). *Incoherent X-ray scattering functions and cross sections by means of a pocket calculator*. *Phys. Rev. A*, **26**, 3325–3333.
- Schaupp, D., Czerwinski, H., Smend, F., Wenskus, R., Schumacher, M., Millhouse, A. H. & Strauss, S. (1984). *Resonant Raman scattering of synchrotron X-rays by neodymium: observation of fine structure in K-L-RRS and of K-N-RRS*. *Z. Phys. A*, **319**, 1–7.
- Slater, J. C. (1937). *Wavefunctions in a periodic crystal*. *Phys. Rev.* **51**, 846–851.
- Sparks, C. J. (1974). *Inelastic resonance emission of X-rays: anomalous scattering associated with anomalous dispersion*. *Phys. Rev. Lett.* **33**, 262–265.
- Thomas, L. H. (1927). *Calculation of atomic fields*. *Proc. Cambridge Philos. Soc.* **33**, 542–548.
- Veigele, W. J. (1967). *Research of X-ray scattering cross sections: final report*. Report KN-379-67-3(R). Kaman Sciences Corp.
- Waller, I. & Hartree, D. R. (1929). *Intensity of total scattering of X-rays*. *Proc. R. Soc. London Ser. A*, **124**, 119–142.
- Williams, B. G. (1977). *Compton scattering*. New York: McGraw-Hill.

7. MEASUREMENT OF INTENSITIES

7.4.4

- Brown, G. S. & Lindau, I. (1986). Editors, *Synchrotron radiation instrumentation*. Proceedings of the International Conference on X-ray and VUV Synchrotron Radiation Instrumentation. *Nucl. Instrum. Methods*, **A246**, 511–595.
- Mathieson, A. McL. (1985). *Small-crystal X-ray diffractometry with a crystal ante-monochromator*. *Acta Cryst.* **A41**, 309–316.
- Matsushita, T. & Hashizume, H. (1983). *Handbook of synchrotron radiation*, Vol. I, edited by E. E. Koch, pp. 261–314. Amsterdam: North-Holland.
- Matsushita, T. & Kaminaga, U. (1980). *A systematic method of estimating the performance of X-ray optical systems for synchrotron radiation. I. Description of various optical elements in position-angle space for ideally monochromatic X-rays*. *J. Appl. Cryst.* **13**, 465–471; *II. Treatment in position-angle-wavelength space*. *J. Appl. Cryst.* **13**, 472–478.
- Suortti, P. (1980). *Components of the total X-ray scattering. Accuracy in powder diffraction*, edited by S. Block & C. R. Hubbard, pp. 1–20. *Natl. Bur. Stand. (US) Spec. Publ.* No. 567.
- Suortti, P. (1985). *Parallel beam geometry for single-crystal diffraction*. *J. Appl. Cryst.* **18**, 272–274.
- Suortti, P., Hastings, J. B. & Cox, D. E. (1985). *Powder diffraction with synchrotron radiation. I. Absolute measurements*. *Acta Cryst.* **A41**, 413–416.
- Suortti, P. & Jennings, L. D. (1977). *Accuracy of structure factors from X-ray powder intensity measurements*. *Acta Cryst.* **A33**, 1012–1027.
- Thomlinson, W. & Williams, G. P. (1984). Editors. *Synchrotron radiation instrumentation 3*. Proceedings of the Third National Conference on Synchrotron Radiation Instrumentation. *Nucl. Instrum. Methods*, **222**, 215–278.
- Killean, R. C. G. (1973). *Optimization of scan procedure for single-crystal X-ray diffraction intensities*. *Acta Cryst.* **A29**, 216–217.
- Mack, M. & Spielberg, N. (1958). *Statistical factors in X-ray intensity measurements*. *Spectrochim. Acta*, **12**, 169–178.
- Mackenzie, J. K. & Williams, E. J. (1973). *The optimum distribution of counting times for determining integrated intensities with a diffractometer*. *Acta Cryst.* **A29**, 201–204.
- Olkha, G. S. & Rathie, P. N. (1971). *On a generalized Bessel function and an integral transform*. *Math. Nachr.* **51**, 231–240.
- Paciorek, W. A. & Chapuis, G. (1994). *Generalized Bessel functions in incommensurate structure analysis*. *Acta Cryst.* **A50**, 194–203.
- Parrish, W. (1956). *X-ray intensity measurements with counter tubes*. *Philips Tech. Rev.* **17**, 206–221.
- Prince, E. & Nicholson, W. L. (1985). *The influence of individual reflections on the precision of parameter estimates in least squares refinement*. *Structure & statistics in crystallography*, edited by A. J. C. Wilson, pp. 183–195. Guilderland, NY: Adenine Press.
- Shmueli, U. (1993). Editor. *International tables for crystallography*. Vol. B. *Reciprocal space*. Dordrecht: Kluwer.
- Shoemaker, D. P. (1968). *Optimization of counting times in computer-controlled X-ray and neutron single-crystal diffraction*. *Acta Cryst.* **A24**, 136–142.
- Shoemaker, D. P. & Hamilton, W. C. (1972). *Further remarks concerning optimization of counting times in single-crystal diffraction: rebuttal to Killean; consideration of background counting and slewing times*. *Acta Cryst.* **A28**, 408–411.
- Skellam, J. G. (1946). *The frequency distribution of the difference between two Poisson values belonging to different populations*. *J. R. Stat. Soc.* **109**, 296.
- Szabó, P. (1978). *Optimization of the measuring time in diffraction intensity measurements*. *Acta Cryst.* **A34**, 551–553.
- Thomsen, J. S. & Yap, F. Y. (1968). *Simplified method of computing centroids of X-ray profiles*. *Acta Cryst.* **A24**, 702–703.
- Werner, S. A. (1972a). *Choice of scans in X-ray diffraction*. *Acta Cryst.* **A28**, 143–151.
- Werner, S. A. (1972b). *Choice of scans in neutron diffraction*. *Acta Cryst.* **A28**, 665–669.
- Wilson, A. J. C. (1967). *Statistical variance of line-profile parameters. Measures of intensity, location and dispersion*. *Acta Cryst.* **23**, 888–898.
- Wilson, A. J. C. (1978). *On the probability of measuring the intensity of a reflection as negative*. *Acta Cryst.* **A34**, 474–475.
- Wilson, A. J. C. (1980). *Relationship between 'observed' and 'true' intensity: effect of various counting modes*. *Acta Cryst.* **A36**, 929–936.
- Wilson, A. J. C., Thomsen, J. S. & Yap, F. Y. (1965). *Minimization of the variance of parameters derived from X-ray powder diffractometer line profiles*. *Appl. Phys. Lett.* **7**, 163–165.
- Wright, E. M. (1933). *On the coefficients of power series having exponential singularities*. *J. London Math. Soc.* **8**, 71–79.
- Zevin, L. S., Umanskii, M. M., Kheiker, D. M. & Panchenko, Yu. M. (1961). *K voprosu o difraktometricheskikh priemah pretsizionnykh izmerenii elementarnykh yacheek*. *Kristallografiya*, **6**, 348–356.

7.5

- Abramowitz, M. & Stegun, I. A. (1964). *Handbook of mathematical functions*. National Bureau of Standards Publication AMS 55.
- Boer, J. L. de (1982). *Statistics of recorded counts*. *Crystallographic statistics*, edited by S. Ramaseshan, M. F. Richardson & A. J. C. Wilson, pp. 179–186. Bangalore: Indian Academy of Sciences.
- Eastabrook, J. N. & Hughes, J. W. (1953). *Elimination of dead-time corrections in monitored Geiger-counter X-ray measurements*. *J. Sci. Instrum.* **30**, 317–320.
- French, S. & Wilson, K. (1978). *On the treatment of negative intensity observations*. *Acta Cryst.* **A34**, 517–525.
- Grant, D. F. (1973). *Single-crystal diffractometer data: the on-line control of the precision of intensity measurement*. *Acta Cryst.* **A29**, 217.
- Hirshfeld, F. L. & Rabinovich, D. (1973). *Treating weak reflexions in least-squares calculations*. *Acta Cryst.* **A29**, 510–513.
- Killean, R. C. G. (1967). *A note on the a priori estimation of R factors for constant-count-per-reflection diffractometer experiments*. *Acta Cryst.* **23**, 1109–1110.
- Killean, R. C. G. (1972). *The a priori optimization of diffractometer data to achieve the minimum average variance in the electron density*. *Acta Cryst.* **A28**, 657–658.