

5.5. Neutron methods

BY B. T. M. WILLIS

In general, one would not expect to measure lattice parameters as precisely with neutrons as with X-rays. The main reason for this is the need to relax the resolution of the diffraction peaks observed in neutron diffraction, in order to obtain reasonable count rates. However, the high-resolution powder diffractometer D2B (on the reactor source at the Institut Laue-Langevin) and the high-resolution powder instrument HRPD (on the pulsed source at the Rutherford Appleton Laboratory) have resolutions approaching that of X-ray diffractometers. Using Rietveld refinement, lattice parameters can be deter-

mined to a precision of a few parts in 10^4 (Fischer *et al.*, 1986).

Neutron methods are better suited to the indexing of the powder pattern. This requires the accurate measurement of the d spacings of the lowest-index lines in the pattern. Whereas d spacings measured with X-rays at low values of $(\sin \theta)/\lambda$ tend to have systematic errors, this is not such a serious problem with neutrons. It is relatively straightforward, using the time-of-flight pulsed-neutron method, to measure the d spacings of the first 20–30 lines of a powder pattern to better than 0.1%.

References

5.1

- Block, S. & Hubbard, C. R. (1980). Editors. *Accuracy in powder diffraction*. Natl Bur. Stand. US Spec. Publ. No. 567. CSIRO (1988). Papers presented at the International Symposium on X-ray Powder Diffraction, Fremantle, Australia, 20–23 August 1987. *Aust. J. Phys.* **41**(2), iv, 101–335.
- Hubbard, C. R. (1983). *New standard reference materials for X-ray powder diffraction*. *Adv. X-ray Anal.* **26**, 45–51.
- Klug, H. P. & Alexander, L. E. (1974). *X-ray diffraction procedures for polycrystalline and amorphous materials*, 2nd ed. New York: John Wiley.
- Okada, Y. & Tokumaru, Y. (1984). *Precise determination of lattice parameter and thermal expansion coefficient of silicon between 300 and 1500 K*. *J. Appl. Phys.* **56**, 314–320.
- Peiser, H. S., Rooksby, H. P. & Wilson, A. J. C. (1960). Editors. *X-ray diffraction by polycrystalline materials*, 2nd ed. London: Chapman & Hall.
- Prince, E. & Stalick, J. K. (1992). Editors. *Accuracy in powder diffraction. II. NIST Spec. Publ. No. 846*.
- Wilson, A. J. C. (1980). *Accuracy in methods of lattice-parameter measurement*. *Accuracy in powder diffraction*. Natl Bur. Stand. US Spec. Publ. No. 567.

5.2

- Alexander, L. (1948). *Geometrical factors affecting the contours of X-ray spectrometer maxima. I. Factors causing asymmetry*. *J. Appl. Phys.* **19**, 1068–1071.
- Alexander, L. (1950). *Geometrical factors affecting the contours of X-ray spectrometer maxima. II. Factors causing broadening*. *J. Appl. Phys.* **21**, 126–136.
- Alexander, L. (1953). *The effect of vertical divergence on X-ray powder diffraction lines*. *Br. J. Appl. Phys.* **4**, 92–93.
- Alexander, L. (1954). *The synthesis of X-ray spectrometer line profiles with application to crystallite size measurements*. *J. Appl. Phys.* **25**, 155–161.
- Appleman, D. E. & Evans, H. T. (1973). *Indexing and least-squares refinement of powder diffraction data*. US Department of Commerce, National Technical Information Service, 5286 Port Royal Rd, Springfield, VA 22151, USA.
- Barth, H. (1960). *Möglichkeit der Präzisionsgitterkonstantenmessungen mit hochmonochromatischer Röntgenstrahlung*. *Acta Cryst.* **13**, 830–832.

- Bearden, J. A. (1964). *X-ray wavelengths*. US AEC Division of Technical Information Ext., Oak Ridge, Tennessee, USA. [The tables are reprinted more accessibly in *International tables for X-ray crystallography* (1974). Vol. IV, pp. 6–43. Birmingham: Kynoch Press. Present distributor: Kluwer Academic Publishers.]
- Berkum, J. van, Sprong, G. J. M., de Keijser, Th. H., Delhez, R. & Sonneveld, E. J. (1995). *The optimum standard specimen for X-ray diffraction line-profile analysis*. *Powder Diffr.* **10**, 129–139.
- Beu, K. E. (1964). *The evaluation of centroid lattice parameter data for tungsten by the likelihood ratio method*. *Acta Cryst.* **17**, 1149–1164.
- Beu, K. E., Musil, F. J. & Whitney, D. R. (1962). *Precise and accurate lattice parameters by film powder methods. I. The likelihood ratio method*. *Acta Cryst.* **15**, 1292–1301.
- Beu, K. E., Musil, F. J. & Whitney, D. R. (1963). *The likelihood ratio method for the precise and accurate determination of lattice parameters for tetragonal and hexagonal crystals*. *Acta Cryst.* **16**, 1241–1242.
- Beu, K. E. & Whitney, D. R. (1967). *Further developments in a likelihood ratio method for the precise and accurate determination of lattice parameters*. *Acta Cryst.* **22**, 932–933.
- Boom, G. (1966). *Accurate lattice parameters and the LPC method*. Groningen: van Denderen.
- Boom, G. & Smits, D. W. (1965). *Calculation of Debye-Scherrer diffraction line profiles and their applications in precision determination of lattice parameters*. *Proc. K. Ned. Akad. Wet. Ser. B*, **68**, 46–52.
- Bourdillon, A. J., Glazer, A. M., Hidaka, M. & Bordas, J. (1978). *High-resolution energy-dispersive diffraction using synchrotron radiation*. *J. Appl. Cryst.* **11**, 684–687.
- Buras, B., Olsen, J. S., Gerward, L., Will, G. & Hinze, E. (1977). *X-ray energy-dispersive diffractometry using synchrotron radiation*. *J. Appl. Cryst.* **10**, 431–438.
- Cheary, R. W. & Coelho, A. (1992). *A fundamental parameters approach to X-ray line-profile fitting*. *J. Appl. Cryst.* **25**, 109–121.
- Cheary, R. W. & Coelho, A. (1994). *Synthesizing and fitting linear position-sensitive detector step-scanned line profiles*. *J. Appl. Cryst.* **27**, 673–681.
- Chevallier, P., Travennier, M. & Briand, J. P. (1978). *On the natural width of the K_{α} x-ray [sic] line observed at the energy threshold*. *J. Phys. B*, **11**, L171–L179.

5. DETERMINATION OF LATTICE PARAMETERS

5.2 (cont.)

- Cohen, M. U. (1936a). *Elimination of systematic errors in powder photographs*. *Z. Kristallogr.* **94**, 288–298.
- Cohen, M. U. (1936b). *Calculation of precise lattice constants for X-ray powder photographs*. *Z. Kristallogr.* **94**, 306–310.
- Deslattes, R. D. & Henins, A. (1973). *X-ray to visible wavelength ratios*. *Phys. Rev. Lett.* **31**, 972–975.
- Deslattes, R., Henins, A. & Kessler, E. G. (1980). *Accuracy in X-ray wavelengths. Accuracy in powder diffraction*, edited by S. Block & C. R. Hubbard, pp. 55–71. *Natl Bur. Stand. (US) Spec. Publ. No. 567*.
- Dragoo, A. L. (1986). *Standard reference materials for X-ray diffraction. Part I. Overview of current and future standard reference materials*. *Powder Diffr.* **1**, 294–304.
- Edwards, H. J. & Toman, K. (1970). *The additivity of variances in powder diffraction profile analysis*. *J. Appl. Cryst.* **3**, 165–171.
- Fawcett, T. G., Crowder, C. E., Brownell, S. J., Zhang, Y., Hubbard, C., Schreiner, W., Hamill, G. P., Huang, T. C., Sabino, E., Langford, J. I., Hamilton, R. & Louër, D. (1988). *Establishing an instrumental peak profile calibration standard for powder diffraction analyses: international round robin conducted by the JCPDS-ICDD and the US National Bureau of Standards*. *Powder Diffr.* **3**, 209–218.
- Ferguson, I. F., Rogerson, I. F., Wolstenholme, J. F. R., Hughes, T. E. & Huyton, A. (1987). *FIRESTAR-2. A computer program for the evaluation of X-ray powder measurements and the derivation of crystal lattice parameters*. United Kingdom Atomic Energy Authority, Northern Division Report ND-R-909(S). London: HMSO, February 1987.
- Fukamachi, T., Hosoya, S. & Terasaki, D. (1973). *The precision of interplanar distances measured by an energy-dispersive X-ray diffractometer*. *J. Appl. Cryst.* **6**, 117–122.
- Gale, B. (1963). *The positions of Debye diffraction line peaks*. *Br. J. Appl. Phys.* **14**, 357–364.
- Gale, B. (1968). *The aberrations of a focusing X-ray diffraction instrument: second-order theory*. *Br. J. Appl. Phys. (J. Phys. D)*, **1**, 393–408.
- Giessen, B. C. & Gordon, G. E. (1968). *X-ray diffraction: new high-speed technique based on X-ray spectroscopy*. *Science*, **159**, 973–975.
- Gillham, C. J. (1971). *Centroid shifts due to axial divergence and other geometrical factors in Seemann-Bohlin diffractometry*. *J. Appl. Cryst.* **4**, 498–506.
- Gillham, C. J. & King, H. W. (1972). *Measurements of centroid and peak shifts due to dispersion and the Lorentz factor at very high Bragg angles*. *J. Appl. Cryst.* **5**, 23–27.
- Glazer, A. M., Hidaka, M. & Bordas, J. (1978). *Energy-dispersive powder profile refinement using synchrotron radiation*. *J. Appl. Cryst.* **11**, 165–172.
- Greenberg, B. (1989). *Bragg's law with refraction*. *Acta Cryst.* **A45**, 238–241.
- Hart, M. (1981). *Bragg angle measurement and mapping*. *J. Cryst. Growth*, **55**, 409–427.
- Hart, M., Cernik, R., Parrish, W. & Toraya, H. (1990). *Lattice-parameter determination for powders using synchrotron radiation*. *J. Appl. Cryst.* **23**, 286–291.
- Hart, M., Parrish, W., Bellotto, M. & Lim, G. S. (1988). *The refractive-index correction in powder diffraction*. *Acta Cryst.* **A44**, 193–197.
- Huang, T. C. (1988). *Precision peak determination in X-ray powder diffractometry*. *Aust. J. Phys.* **41**, 201–212.
- Huang, T. C., Toraya, H., Blanton, T. N. & Wu, Y. (1993). *X-ray powder diffraction analysis of silver behenate, a possible low-angle diffraction standard*. *J. Appl. Cryst.* **26**, 180–184.
- Hubbard, C. R. (1983). *New standard reference materials for X-ray powder diffraction*. *Adv. X-ray Anal.* **26**, 45–51.
- Hubbard, C. R., Swanson, H. É. & Mauer, F. A. (1975). *A silicon powder diffraction standard reference material*. *J. Appl. Cryst.* **8**, 45–48.
- JCPDS-International Centre for Diffraction Data (1986). *Task group on cell parameter refinement*. *Powder Diffr.* **1**, 66–76.
- Jenkins, R. & Schreiner, W. N. (1986). *Considerations in the design of goniometers for use in X-ray powder diffraction*. *Powder Diffr.* **1**, 305–319.
- Kelly, E. H. (1988). *A summary of a 'round-robin' exercise comparing the output of computer programs for lattice-parameter refinement and calculations*. British Crystallographic Association.
- Kogan, V. A. & Kupriyanov, M. F. (1992). *X-ray powder diffraction line profiles by Fourier synthesis*. *J. Appl. Cryst.* **25**, 16–25.
- Ladell, J., Parrish, W. & Taylor, J. (1959). *Interpretation of diffractometer line profiles*. *Acta Cryst.* **12**, 561–567.
- Laguitton, D. & Parrish, W. (1977). *Experimental spectral distribution versus Kramers' law for quantitative X-ray fluorescence by the fundamental parameters method*. *X-ray Spectrom.* **6**, 201–203.
- Langford, J. I., Louër, D., Sonneveld, E. J. & Visser, J. W. (1986). *Applications of total pattern fitting to a study of crystallite size and strain in powder zinc oxide*. *Powder Diffr.* **1**, 211–221.
- Langford, J. I., Pike, E. R. & Beu, K. E. (1964). *Precise and accurate lattice parameters by film powder methods. IV. Theoretical calculation of axial (vertical) divergence profiles, centroid shifts, and variances for cylindrical powder diffraction cameras*. *Acta Cryst.* **17**, 645–651.
- Langford, J. I. & Wilson, A. J. C. (1962). *Counter diffractometer: the effect of specimen transparency on the intensity, position and breadth of X-ray powder diffraction lines*. *J. Sci. Instrum.* **39**, 581–585.
- Louër, D. & Langford, J. I. (1988). *Peak shape and resolution in conventional diffractometry with monochromatic X-rays*. *J. Appl. Cryst.* **21**, 430–437.
- Mack, M. & Parrish, W. (1967). *Seeman-Bohlin X-ray diffractometry. II. Comparison of aberrations and intensity with conventional diffractometer*. *Acta Cryst.* **23**, 693–700.
- Mack, M. & Spielberg, N. (1958). *Statistical factors in X-ray intensity measurements*. *Spectrochim. Acta*, **12**, 169–178.
- Mantler, M. & Parrish, W. (1977). *Energy dispersive X-ray diffractometry*. *Adv. X-ray Anal.* **20**, 171–186.
- Mighell, A. D., Hubbard, C. R. & Stalick, J. K. (1981). *NBS*EXAIDS83. A Fortran program for crystallographic data evaluation*. *Natl Bur. Stand. (US) Tech. Note*, No. 1141, April 1981.
- Mitra, G. B., Ahmed, A. & Das Gupta, P. (1985). *Precise and accurate estimation of crystallographic parameters by maximum-likelihood and min-max methods. Structure and statistics in crystallography*, edited by A. J. C. Wilson, pp. 151–181. Guilderland, NY: Adenine Press.
- Nakajima, T., Fukamachi, T., Terasaki, O. & Hosoya, S. (1976). *The detection of small differences in lattice constant at low temperature by an energy-dispersive X-ray diffractometer*. *J. Appl. Cryst.* **9**, 286–290.

REFERENCES

5.2 (cont.)

- Nelson, J. B. & Riley, D. P. (1945). *An experimental investigation of extrapolation methods in the derivation of accurate unit-cell dimensions of crystals*. *Proc. Phys. Soc. London*, **57**, 160–177, 477–495.
- Okazaki, A. & Kawaminami, M. (1973). *Accurate measurement of lattice constant in a wide range of temperature: use of white X-rays and double-crystal diffractometry*. *Jpn. J. Appl. Phys.* **12**, 783–789.
- Parrish, W. (1960). *Results of the IUCr precision lattice-parameter project*. *Acta Cryst.* **13**, 838–850.
- Parrish, W. (1988). *Advances in synchrotron X-ray polycrystalline diffraction*. *Aust. J. Phys.* **41**, 101–112.
- Parrish, W. & Hart, M. (1987). *Advantages of synchrotron radiation for polycrystalline diffractometry*. *Z. Kristallogr.* **179**, 161–173.
- Parrish, W., Hart, M., Huang, T. C. & Bellotto, M. (1987). *Lattice-parameter determination using synchrotron powder data*. *Adv. X-ray Anal.* **30**, 373–382.
- Parrish, W. & Huang, T. C. (1980). *Accuracy of the profile fitting method for X-ray polycrystalline diffractometry*. *Natl Bur. Stand. (US) Spec. Publ. No. 457*, pp. 95–110.
- Pawley, G. S. (1981). *Unit-cell refinement from powder diffraction scans*. *J. Appl. Cryst.* **14**, 357–361.
- Pike, E. R. (1957). *Counter diffractometer – the effects of vertical divergence on the displacement and breadth of powder diffraction lines*. *J. Sci. Instrum.* **34**, 355–361.
- Pike, E. R. & Wilson, A. J. C. (1959). *Counter diffractometer – the theory of the use of centroids of diffraction profiles for high accuracy in the measurement of diffraction angles*. *Br. J. Appl. Phys.* **10**, 57–68.
- Popović, S. (1973). *Unit-cell dimension measurements from pairs of X-ray diffraction lines*. *J. Appl. Cryst.* **6**, 122–128.
- Rietveld, H. M. (1967). *Line profiles of neutron powder-diffraction peaks for structure refinement*. *Acta Cryst.* **22**, 151–152.
- Rietveld, H. M. (1969). *A profile refinement method for nuclear and magnetic structures*. *J. Appl. Cryst.* **2**, 65–71.
- Sandström, A. E. (1957). *Experimental methods of X-ray spectroscopy: ordinary wavelengths*. *Handbuch der Physik*, pp. 78–245 (esp. p. 157). Berlin: Springer.
- Scardi, P., Lutterotti, L. & Maistrelli, P. (1994). *Experimental determination of the instrumental broadening in Bragg-Brentano geometry*. *Powder Diffr.* **9**, 180–186.
- Soller, W. (1924). *A new precision X-ray spectrometer*. *Phys. Rev.* **24**, 158–167.
- Sparks, C. J. & Gedcke, D. A. (1972). *Rapid recording of powder diffraction patterns with Si(Li) X-ray energy analysis system: W and Cu targets and error analysis*. *Adv. X-ray Anal.* **15**, 240–253.
- Spencer, R. C. (1931). *Additional theory of the double X-ray spectrometer*. *Phys. Rev.* **38**, 618–629.
- Spencer, R. C. (1935). *The effect of the spectrometer on the width of spectral lines*. *Phys. Rev.* **48**, 473.
- Spencer, R. C. (1937). *A theorem on the effect of vertical divergence*. *Phys. Rev.* **52**, 761.
- Spencer, R. C. (1939). *The correction of experimental curves for the resolving power of the apparatus*. *Phys. Rev.* **55**, 239.
- Spencer, R. C. (1941). *Optimum design of physical apparatus*. *Phys. Rev.* **60**, 172.
- Spencer, R. C. (1949). *Discussion of “Geometrical factors affecting X-ray spectrometer maxima”*. *J. Appl. Phys.* **20**, 413–414.
- Taylor, A. & Sinclair, H. B. (1945a). *The influence of absorption on the shapes and positions of lines in Debye-Scherrer powder photographs*. *Proc. Phys. Soc. London*, **57**, 108–125.
- Taylor, A. & Sinclair, H. B. (1945b). *On the determination of lattice parameters by the Debye-Scherrer method*. *Proc. Phys. Soc. London*, **57**, 126–135.
- Thomsen, J. S. (1974). *High-precision X-ray spectroscopy*. *X-ray spectroscopy*, edited by L. V. Azaroff, pp. 26–132. New York: McGraw-Hill.
- Thomsen, J. S. & Yap, F. Y. (1968a). *Effect of statistical counting errors on wavelength criteria for X-ray spectra*. *J. Res. Natl Bur. Stand. Sect. A*, **72**, 187–205.
- Thomsen, J. S. & Yap, F. Y. (1968b). *Simplified method of computing centroids of X-ray profiles*. *Acta Cryst.* **A24**, 702–703.
- Timmers, J., Delhez, R., Tuinstra, F. & Peerdeman, F. (1992). *X-ray tracing; a tool for improved accuracy in powder diffractometry*. *Accuracy in powder diffraction II*. NIST Spec. Publ. No. 846, edited by E. Prince & J. K. Stalick, p. 217.
- Toraya, H. (1986). *Whole-powder-pattern fitting without reference to a structural model: application to X-ray powder diffractometer data*. *J. Appl. Cryst.* **19**, 440–447.
- Toraya, H. (1988). *The deconvolution of overlapping reflections by the procedure of direct fitting*. *J. Appl. Cryst.* **21**, 192–196.
- Wilkens, M. (1960). *Zur Brechungskorrektur bei Gitterkonstantmessungen an Pulverpräparaten*. *Acta Cryst.* **13**, 826–828.
- Wilson, A. J. C. (1940). *On the correction of lattice spacings for refraction*. *Proc. Cambridge Philos. Soc.* **36**, 485–489.
- Wilson, A. J. C. (1950). *Geiger-counter X-ray spectrometer – influence of the size and absorption coefficient of the specimen on position and shape of powder diffraction maxima*. *J. Sci. Instrum.* **27**, 321–325.
- Wilson, A. J. C. (1958). *Effect of absorption on mean wavelength of X-ray emission lines*. *Proc. Phys. Soc. London*, **72**, 924–925.
- Wilson, A. J. C. (1961). *A note on peak displacements in X-ray diffractometry*. *Proc. Phys. Soc. London*, **78**, 249–255.
- Wilson, A. J. C. (1962). *Refraction broadening in powder diffractometer*. *Proc. Phys. Soc. London*, **80**, 303–305.
- Wilson, A. J. C. (1963). *Mathematical theory of X-ray powder diffractometry*. Eindhoven: Centrex.
- Wilson, A. J. C. (1965a). *On variance as a measure of line broadening in diffractometry. IV. The effect of physical aberrations*. *Proc. Phys. Soc. London*, **85**, 171–176.
- Wilson, A. J. C. (1965b). *The location of peaks*. *Br. J. Appl. Phys.* **16**, 665–674.
- Wilson, A. J. C. (1965c). *Röntgenstrahlpulverdiffractometrie. Mathematische Theorie*. Eindhoven: Centrex.
- Wilson, A. J. C. (1967). *Statistical variance of line-profile parameters. Measures of intensity, location and dispersion*. *Acta Cryst.* **23**, 888–898. *Addenda and Corrigenda, ibid.*, **A24**, 478 and **A25**, 584–585.
- Wilson, A. J. C. (1970a). *Elements of X-ray crystallography*. Reading, MA: Addison-Wesley.
- Wilson, A. J. C. (1970b). *Limitations on the additivity of moments in line-profile analysis*. *J. Appl. Phys.* **3**, 71–73.
- Wilson, A. J. C. (1971). *Some statistical considerations in the location of Mössbauer lines*. *Nucl. Instrum. Methods*, **94**, 225–227.
- Wilson, A. J. C. (1973). *Note on the aberrations of a fixed-angle energy-dispersive diffractometer*. *J. Appl. Cryst.* **6**, 230–237.

5. DETERMINATION OF LATTICE PARAMETERS

5.2 (cont.)

- Wilson, A. J. C. (1974). *Powder diffractometry. X-ray diffraction*, by L. V. Azaroff, R. Kaplow, N. Kato, R. Weiss, A. J. C. Wilson & R. A. Young, Chap. 6. New York: McGraw-Hill.
- Wilson, A. J. C. (1980). *Accuracy in methods of lattice-parameter measurement. Natl Bur. Stand. (US) Spec. Publ.* No. 567, pp. 325–351.
- Wilson, A. J. C. & Delf, B. W. (1961). *Effects of variations in the quantum counting efficiency of detectors on the mean wavelengths of emission lines. Proc. Phys. Soc. London*, **78**, 1256–1258.
- Wilson, A. J. C. & Lipson, H. (1941). *The calibration of Debye-Scherrer X-ray powder cameras. Proc. Phys. Soc. London*, **53**, 245–250.
- Wilson, A. J. C., Thomsen, J. S. & Yap, F. Y. (1965). *Minimization of the variation of parameters derived from X-ray powder diffractometer line profiles. Appl. Phys. Lett.* **7**, 163–165.
- Wong-Ng, W. & Hubbard, C. R. (1987). *Standard reference materials for X-ray diffraction. Part II. Calibration using d-spacing standards. Powder Diffr.* **2**, 242–248.
- Young, R. A. (1988). *Pressing the limits of Rietveld refinement. Aust. J. Phys.* **41**, 294–310.
- Zevin, L. S., Umanskij, M. M., Khejker, D. M. & Pančenko, J. M. (1961). *The question of diffractometer methods of precision measurement of unit-cell parameters. Sov. Phys. Crystallogr.* **6**, 277–283.

5.3

- Abrahams, S. C., Liminga, R., Marsh, P., Schrey, F., Albertsson, J., Svensson, C. & Kvik, A. (1983). *Thermal expansivity of α -LiIO₃ between 20 and 520 K. J. Appl. Cryst.* **16**, 453–457.
- Alcock, N. W. & Sheldrick, G. M. (1967). *The determination of accurate unit-cell dimensions from inclined Weissenberg photographs. Acta Cryst.* **23**, 35–38.
- Alexander, L. (1948). *Geometrical factors affecting the contours of X-ray spectrometer maxima. I. Factors causing asymmetry. J. Appl. Phys.* **19**, 1068–1071.
- Alexander, L. (1950). *Geometrical factors affecting the contours of X-ray spectrometer maxima. II. Factors causing broadening. J. Appl. Phys.* **21**, 126–136.
- Alexander, L. (1954). *The synthesis of X-ray spectrometer line profiles with application to crystallite size measurements. J. Appl. Phys.* **25**, 155–161.
- Alexander, L. E. & Smith, G. (1962). *Single-crystal intensity measurements with the three-circle counter diffractometer. Acta Cryst.* **15**, 983–1004.
- Amorós, J. L., Buerger, M. J. & Amorós, M. C. (1975). *The Laue method*. New York: Academic Press.
- d'Amour, H., Denner, W., Schulz, H. & Cardona, M. (1982). *A uniaxial stress apparatus for single-crystal X-ray diffraction on a four-circle diffractometer: Application to silicon and diamond. J. Appl. Cryst.* **15**, 148–153.
- Ando, M., Bailey, D. & Hart, M. (1978). *A simple Bragg-spacing comparator. Acta Cryst.* **A34**, 484–489.
- Ando, M., Hagashi, Y., Usuda, K., Yasuami, S. & Kawata, H. (1989). *A precision Bond method with SR. Rev. Sci. Instrum.* **60**, 2410–2413.
- Aristov, V. V., Shekhtman, V. Sh. & Shmytko, I. M. (1973). *Precision measurement of crystallographic parameters by the X-ray divergent-beam technique. (In Russian.) Kristallografiya*, **18**, 706–709. (English transl: *Sov. Phys. Crystallogr.* **18**, 445–446.)
- Aristov, V. V. & Shmytko, I. M. (1978). *Precision lattice parameter measurement by the X-ray divergent-beam technique. J. Appl. Cryst.* **11**, 662–668.
- Aristov, V. V., Shmytko, I. M. & Shulakov, E. V. (1974a). *Application of the X-ray divergent-beam technique for the determination of the angles between crystal blocks. I. Reflexion from the planes parallel to the crystal surface. J. Appl. Cryst.* **7**, 409–413.
- Aristov, V. V., Shmytko, I. M. & Shulakov, E. V. (1974b). *Application of the X-ray divergent-beam technique for the determination of the angles between crystal blocks. II. Determination of the total misorientation angle between blocks. J. Appl. Cryst.* **7**, 413–416.
- Arndt, U. W. & Willis, B. T. M. (1966). *Single crystal diffractometry*. Cambridge University Press.
- Åsbrink, S., Wołczyr, M. & Hong, S.-H. (1985). *X-ray Bond-type diffractometric investigations on V₃O₅ in the temperature interval 298 to 480 K including the phase transition temperature T₁ = 428 K. Phys. Status Solidi A*, **87**, 135–140; erratum: **89**, 415.
- Azáróff, L. V. (1974). *X-ray spectroscopy*, Chap. 2. New York: McGraw-Hill.
- Báčkovský, J. (1965). *On the most accurate measurements of the wavelengths of X-ray spectral lines. Czech. J. Phys.* **B15**, 752–759.
- Baker, J. A., Tucker, T. N., Moyer, N. E. & Buschert, R. C. (1968). *Effects of carbon on the lattice parameter of silicon. J. Appl. Phys.* **39**, 4365–4368.
- Baker, J. F. C. & Hart, M. (1975). *An absolute measurement of the lattice parameter of germanium using multiple-beam X-ray diffractometry. Acta Cryst.* **A31**, 364–367.
- Baker, J. F. C., Hart, M., Halliwell, M. A. G. & Heckingbottom, R. (1976). *Precise lattice parameter determination of dislocation-free gallium arsenide. I. X-ray measurements. Solid-State Electron.* **19**, 331–334.
- Baker, T. W., George, J. D., Bellamy, B. A. & Causer, R. (1966). *Very high precision X-ray diffraction. Nature (London)*, **210**, 720–721.
- Baker, T. W., George, J. D., Bellamy, B. A. & Causer, R. (1968). *Fully automated high-precision X-ray diffraction. Adv. X-ray Anal.* **11**, 359–375.
- Barla, K., Herino, R., Bomchil, G. & Pfister, J. C. (1984). *Determination of lattice parameter and elastic properties of porous silicon by X-ray diffraction. J. Cryst. Growth*, **68**, 727–732.
- Barns, R. L. (1972). *A strategy for rapid and accurate (p.p.m.) measurement of lattice parameters of single crystals by Bond's method. Adv. X-ray Anal.* **15**, 330–338.
- Bartels, W. J. (1983). *Characterization of thin layers on perfect crystals with a multipurpose high-resolution X-ray diffractometer. J. Vac. Sci. Technol.* **B1**, 338–345.
- Batchelder, D. N. & Simmons, R. O. (1965). *X-ray lattice constant of crystals by a rotating-camera method: Al, Ar, Au, CaF₂, Cu, Ge, Ne, Si. J. Appl. Phys.* **36**, 2864–2868.
- Bearden, J. A. (1933). *The wavelengths of the silver, molybdenum, copper, iron and chromium K α_1 lines. Phys. Rev.* **43**, 92–97.
- Bearden, J. A. (1965). *Selection of W K α_1 as the X-ray wavelength standard. Phys. Rev.* **137**, BY55–BY61.

REFERENCES

5.3 (cont.)

- Bearden, J. A. (1967). *X-ray wavelengths*. *Rev. Mod. Phys.* **39**, 78–124.
- Bearden, J. A. & Henins, A. (1965). *Precision measurement of lattice imperfections with a photographic two-crystal method*. *Rev. Sci. Instrum.* **36**, 334–338.
- Bearden, J. A., Marzolf, J. G. & Thomsen, J. S. (1968). *Crystal diffraction profiles for monochromatic radiation*. *Acta Cryst.* **A24**, 295–301.
- Bearden, J. A. & Thomsen, J. S. (1971). *The double-crystal X-ray spectrometer: corrections, errors, and alignment procedure*. *J. Appl. Cryst.* **4**, 130–138.
- Becker, P., Dorenwendt, K., Ebeling, G., Lauer, R., Lucas, W., Probst, R., Rademacher, H.-J., Reim, G., Seyfried, P. & Siegert, H. (1981). *Absolute measurement of the (220) lattice plane spacing in silicon crystal*. *Phys. Rev. Lett.* **46**, 1540–1543.
- Becker, P., Seyfried, P. & Siegert, H. (1982). *The lattice parameter of highly pure silicon single crystals*. *Z. Phys. B*, **48**, 17–21.
- Berg, H. M. & Hall, E. L. (1975). *The pseudo-Kossel technique in back reflection as a tool for measuring strains*. *Adv. X-ray Anal.* **18**, 454–465.
- Berger, H. (1984). *A method for precision lattice-parameter measurement of single crystals*. *J. Appl. Cryst.* **17**, 451–455.
- Berger, H. (1986a). *Systematic errors in precision lattice-parameter determination of single crystals caused by asymmetric line profiles*. *J. Appl. Cryst.* **19**, 34–38.
- Berger, H. (1986b). *Study of the $K\alpha$ emission spectrum of copper*. *X-ray Spectrom.* **15**, 241–243.
- Berger, H. (1993). *X-ray diffraction studies on point defects in II–VI compounds*. *Cryst. Res. Technol.* **28**, 795–801.
- Berger, H., Lehmann, A. & Schenk, M. (1985). *Lattice-parameter variations in PbTe single crystals*. *Cryst. Res. Technol.* **20**, 579–581.
- Berger, H., Rosner, B. & Schikora, D. (1989). *Lattice parameter determination of superlattices*. *Cryst. Res. Technol.* **24**, 437–441.
- Beu, K. E. (1967). *The precise and accurate determination of lattice parameters*. *Handbook of X-rays*, edited by E. F. Kaelble, Chap. 10. New York: McGraw-Hill.
- Beu, K. E., Musil, F. J. & Whitney, D. R. (1962). *Precise and accurate lattice parameters by film powder methods. I. The likelihood ratio method*. *Acta Cryst.* **15**, 1292–1301.
- Bevis, M., Fearon, E. O. & Rowlands, P. C. (1970). *The accurate determination of lattice parameters and crystal orientations from Kossel patterns*. *Phys. Status Solidi A*, **1**, 653–659.
- Biggin, S. & Dingley, D. J. (1977). *A general method for locating the X-ray source point in Kossel diffraction*. *J. Appl. Cryst.* **10**, 376–385.
- Bolotina, N. B. (1989). *Refinement of unit-cell parameters and orientation of specimen in diffractometer, taking account of symmetry of single crystal*. *Kristallografiya*, **34**, 598–601. (English transl: *Sov. Phys. Crystallogr.* **34**, 355–357.)
- Bond, W. L. (1960). *Precision lattice constant determination*. *Acta Cryst.* **13**, 814–818.
- Bond, W. L. (1975). *Precision lattice constant determination*. *Erratum*. *Acta Cryst.* **A31**, 698.
- Bonse, U. & te Kaat, E. (1968). *A two-crystal X-ray interferometer*. *Z. Phys.* **214**, 16–21.
- Bowen, D. K. & Tanner, B. K. (1995). *A method for the accurate comparison of lattice parameters*. *J. Appl. Cryst.* **28**, 753–760.
- Bragg, W. H. & Bragg, W. L. (1915). *X-rays and crystal structure*, Chap. 2. London: G. Bell and Sons.
- Brown, B. R., Halliwell, M. A. G. & Isherwood, B. J. (1980). *The characterization of distortions in heteroepitaxial structures by X-ray multiple diffraction*. *J. Microsc.* **118**, 375–381.
- Brühl, H.-G. (1978). *Precision lattice parameter measurements of VPE-GaP-epitaxial layers by the 'Umweganregung' method*. *Krist. Tech.* **13**, 1247–1251.
- Brühl, H.-G. & Rhan, H. (1985). *On the extension of the theory of Umweganregung with respect to the use of divergent white X-ray radiation*. *Phys. Status Solidi A*, **87**, 121–126.
- Buerger, M. J. (1942). *X-ray crystallography*. London: John Wiley.
- Buras, B., Olsen, J. S., Gerward, L., Will, G. & Hinze, E. (1977). *X-ray energy-dispersive diffractometry using synchrotron radiation*. *J. Appl. Cryst.* **10**, 431–438.
- Burke, J. & Tomkeieff, M. V. (1968). *Specimen and beam tilt errors in Bond's method of lattice parameter determination*. *Acta Cryst.* **A24**, 683–685.
- Burke, J. & Tomkeieff, M. V. (1969). *Errors in the Bond method of lattice parameter determinations. Further considerations*. *J. Appl. Cryst.* **2**, 247–248.
- Buschert, R. C. (1965). *X-ray lattice parameter and linewidth studies in silicon*. *Bull. Am. Phys. Soc.* **10**, 125.
- Buschert, R. C., Merlini, A. E., Pace, S., Rodriguez, S. & Grimsditch, M. H. (1988). *Effect of isotope concentration on the lattice parameter of germanium perfect crystals*. *Phys. Rev. B*, **38**, 5219–5221.
- Buschert, R. C., Meyer, A. J., Stuckey Kauffman, D. & Gotwals, J. K. (1983). *A double-source double-crystal X-ray spectrometer for high-sensitivity lattice-parameter difference measurements*. *J. Appl. Cryst.* **16**, 599–605.
- Buschert, R. C., Pace, S., Inzaghi, D. & Merlini, A. E. (1980). *A high-sensitivity double-beam triple-crystal spectrometer for lattice parameter and topographic measurements*. *J. Appl. Cryst.* **13**, 207–210.
- Busing, W. R. & Levy, H. A. (1967). *Angle calculations for 3- and 4-circle X-ray and neutron diffractometers*. *Acta Cryst.* **22**, 457–464.
- Carr, P. D., Cruickshank, D. W. J. & Harding, M. M. (1992). *The determination of unit-cell parameters from Laue diffraction patterns using their gnomonic projections*. *J. Appl. Cryst.* **25**, 294–308.
- Cembali, F., Fabri, R., Servidori, M., Zani, A., Basile, G., Cavagnero, G., Bergamin, A. & Zosi, G. (1992). *Precise X-ray relative measurement of lattice parameters of silicon wafers by multiple-crystal Bragg-case diffractometry. Computer simulation of the experiment*. *J. Appl. Cryst.* **25**, 424–431.
- Černohorský, M. (1960). *The ratio method for absolute measurements of lattice parameters with cylindrical cameras*. *Acta Cryst.* **13**, 823–826.
- Chang, S.-L. (1979). *Direct observation of two-dimensional lattice mismatch parallel to the interfacial boundary between the LPE $Ga_{0.65}Al_{0.35}As$ layer and the GaAs substrate*. *Appl. Phys. Lett.* **34**, 239–240.
- Chang, S.-L. (1984). *Multiple diffraction of X-rays in crystals*, Chap. 7.2 in particular. Berlin: Springer-Verlag.
- Chang, S.-L., Patel, N. B., Nannichi, Y. & de Prince, F. C. (1979). *Determination of lattice mismatch in $Ga_{1-x}Al_xAs$ LPE layer on GaAs substrate by using a divergent X-ray source*. *J. Appl. Phys.* **50**, 2975–2976.
- Clegg, W. (1981). *Least-squares refinement of unit-cell parameters from precession photographs*. *Acta Cryst.* **A37**, 437–438.

5. DETERMINATION OF LATTICE PARAMETERS

5.3 (cont.)

- Clegg, W. (1984). *Orientation matrix refinement during four-circle diffractometer data collection*. *Acta Cryst.* **A40**, 703–704.
- Clegg, W. & Sheldrick, G. M. (1984). *The refinement of unit cell parameters from two-circle diffractometer measurements*. *Z. Kristallogr.* **167**, 23–27.
- Cole, H., Chambers, F. W. & Dunn, H. M. (1962). *Simultaneous diffraction: indexing Umweganregung peaks in simple cases*. *Acta Cryst.* **15**, 138–144.
- Compton, A. H. & Allison, S. K. (1935). *X-rays in theory and experiment*. New York: Van Nostrand.
- Cooper, A. S. (1962). *Precise lattice constants of germanium, aluminium, gallium arsenide, uranium, sulphur, quartz and sapphire*. *Acta Cryst.* **15**, 578–582.
- Cruikshank, D. W. J., Carr, P. D. & Harding, M. M. (1992). *Estimation of d_{\min} , λ_{\min} and λ_{\max} from the gnomonic projections of Laue patterns*. *J. Appl. Cryst.* **25**, 285–293.
- Davis, B. L. & Johnson, L. R. (1984). *The true unit cell of ammonium hydrogen sulfate, $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$* . *J. Appl. Cryst.* **17**, 331–333.
- Deslattes, R. D. (1969). *Optical and X-ray interferometry of a silicon lattice spacing*. *Appl. Phys. Lett.* **15**, 386–388.
- Deslattes, R. D. & Henins, A. (1973). *X-ray to visible wavelength ratios*. *Phys. Rev. Lett.* **31**, 972–975.
- Deslattes, R. D., Henins, A., Bowman, H. A., Schoonover, R. M., Caroll, C. L., Barnes, I. L., Machlan, L. A., Moore, L. J. & Shields, W. R. (1974). *Determination of the Avogadro constant*. *Phys. Rev. Lett.* **33**, 463–466.
- Deslattes, R. D., Henins, A., Schoonover, R. M., Caroll, C. L. & Bowman, H. A. (1976). *Avogadro constant – correction to an earlier report*. *Phys. Rev. Lett.* **36**, 898–900.
- Dressler, L., Griebner, U. & Kittner, R. (1987). *Precision measurement of lattice parameters in LiF monocrystals*. *Cryst. Res. Technol.* **22**, 1431–1435.
- Eastabrook, J. N. (1952). *Effect of vertical divergence on the displacement and breadth of X-ray powder diffraction lines*. *Br. J. Appl. Phys.* **3**, 349–352.
- Ellis, T., Nanni, L. F., Shrier, A., Weissmann, S., Padawer, G. E. & Hosokawa, N. (1964). *Strain and precision lattice parameter measurements by the X-ray divergent beam method*. *I. J. Appl. Phys.* **35**, 3364–3373.
- Evans, H. T. Jr & Lonsdale, K. (1959). *Diffraction geometry*. *International tables for X-ray crystallography*, Vol. II, Chap. 4. Birmingham: Kynoch Press.
- Farquhar, M. C. M. & Lipson, H. (1946). *The accurate determination of cell dimensions from single-crystal X-ray photographs*. *Proc. Phys. Soc. London*, **58**, 200–206.
- Fewster, P. F. (1982). *Absolute lattice-parameter measurements of epitaxial layers*. *J. Appl. Cryst.* **15**, 275–278.
- Fewster, P. F. (1989). *A high-resolution multiple-crystal multiple-reflection diffractometer*. *J. Appl. Cryst.* **22**, 64–69.
- Fewster, P. F. (1993). *Structural characterisation of materials by combining X-ray diffraction space mapping and topography*. *Philips J. Res.* **47**, 235–245.
- Fewster, P. F. & Andrew, N. L. (1995). *Absolute lattice-parameter measurement*. *J. Appl. Cryst.* **28**, 451–458.
- Fewster, P. F. & Willoughby, A. F. W. (1980). *The effect of silicon doping on the lattice parameter of gallium arsenide grown by liquid-phase epitaxy, vapour-phase epitaxy and gradient-freeze techniques*. *J. Cryst. Growth*, **50**, 648–653.
- Filscher, G. & Unangst, D. (1980). *Bond-method for precision lattice constant determination. Dependence of lattice constant error on sample adjustment and collimator tilt*. *Krist. Tech.* **15**, 955–960.
- Fischer, D. G. & Harris, N. (1970). *A computer program for the calculation of lattice spacings from Kossel diffraction patterns*. *J. Appl. Cryst.* **3**, 305–313.
- Fukahara, A. & Takano, Y. (1977). *Determination of strain distributions from X-ray Bragg reflexion by silicon single crystals*. *Acta Cryst.* **A33**, 137–142.
- Fukumori, T. & Futagami, K. (1988). *Measurements of lattice parameters and half-widths of the rocking curve on GaAs crystal by the X-ray double-crystal method using a Cu K α doublet*. *Jpn. J. Appl. Phys.* **27**, 442–443.
- Fukumori, T., Futagami, K. & Matsunaga, K. (1982). *X-ray double-crystal method for crystal lattice parameter measurements using Cu K α doublet*. *Jpn. J. Appl. Phys.* **21**, 1525.
- Fukumori, T., Imai, K., Hasegawa, T. & Akashi, Y. (1997). *Precision lattice spacing measurement using X-ray Cu K α doublet*. *J. Phys. Soc. Jpn*, **66**, 1976–1978.
- Gabe, E. J. (1980). *Diffractometer control with minicomputers*. *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 1.01–1.18. Bangalore: Indian Academy of Sciences.
- Gaáldecka, E. (1985). *The variances and covariances of measured intensities in precise lattice-constant determination by the Bond method*. *Structure & statistics in crystallography*, edited by A. J. C. Wilson, pp. 137–149. New York: Adenine Press.
- Gaáldecka, E. (1993a). *Description and peak-position determination of a single X-ray diffraction profile for high-accuracy lattice-parameter measurements by the Bond method. I. An analysis of descriptions available*. *Acta Cryst.* **A49**, 106–115.
- Gaáldecka, E. (1993b). *Description and peak-position determination of a single X-ray diffraction profile for high-accuracy lattice-parameter measurements by the Bond method. II. Testing and choice of description*. *Acta Cryst.* **A49**, 116–126.
- Gaáldecka, E. (1994). *The extrapolated-peak method for the peak-position determination of an X-ray diffraction profile, and the accuracy of the Bragg-angle measurements*. *Sci. Bull. Tech. Univ. Łódź Branch Bielsko-Biala*, **22**(4), 1–24.
- Gamarnik, M. Ya. (1990). *Size changes of lattice parameters in ultradisperse diamond and silicon*. *Phys. Status Solidi B*, **161**, 457–462.
- Geist, V. & Ascheron, C. (1984). *The proton-induced Kossel effect and its application to crystallographic studies*. *Cryst. Res. Technol.* **19**, 1231–1244.
- Gielen, P., Yakowitz, H., Ganow, D. & Ogilvie, R. E. (1965). *Evaluation of Kossel microdiffraction procedures: the cubic case*. *J. Appl. Phys.* **36**, 773–782.
- Glass, H. L. & Moudy, L. A. (1974). *Measurement of the lattice parameter of gadolinium gallium garnet crystals by the X-ray divergent-beam anomalous-transmission method*. *J. Appl. Cryst.* **7**, 22–24.
- Glass, H. L. & Weissmann, S. (1969). *Synergy of line profile analysis and selected area topography by the X-ray divergent beam method*. *J. Appl. Cryst.* **2**, 200–209.
- Glazer, A. M. (1972). *A technique for the automatic recording of phase transitions in single crystals*. *J. Appl. Cryst.* **5**, 420–423.
- Glazer, A. M. & Megaw, H. D. (1973). *Studies of the lattice parameters and domains in the phase transitions of NaNbO_3* . *Acta Cryst.* **A29**, 489–495.

REFERENCES

5.3 (cont.)

- Godwod, K., Kowalczyk, R. & Szmid, Z. (1974). Application of a precise double X-ray spectrometer for accurate lattice parameter determination. *Phys. Status Solidi A*, **21**, 227–234.
- Golovin, A. L., Imamov, R. M. & Kondrashkina, E. A. (1985). Absolute measurements of lattice spacings in surface layers of crystals. *Phys. Status Solidi A*, **89**, K5–K7.
- Grosswig, S., Härtwig, J., Alter, U. & Christoph, A. (1983). Precision lattice parameter determination of coloured quartz monocrystals. *Cryst. Res. Technol.* **18**, 501–511.
- Grosswig, S., Härtwig, J., Jäckel, K.-H., Kittner, R. & Melle, W. (1986). A novel arrangement for the absolute measurement of geometric lattice parameters of monocrystals with high precision. *Nauch. Appar. Sci. Instrum.* **1**, 29–44.
- Grosswig, S., Jäckel, K.-H. & Kittner, R. (1986). Peak position determination of X-ray diffraction profiles in precision lattice parameter measurements according to the Bond-method with help of the polynomial approximation. *Cryst. Res. Technol.* **21**, 133–139.
- Grosswig, S., Jäckel, K.-H., Kittner, R., Dietrich, B. & Schellenberger, U. (1985). Determination of the coplanar geometric lattice parameters of monocrystals with high precision. *Cryst. Res. Technol.* **20**, 1093–1100.
- Grosswig, S., Melle, W., Schellenberger, U. & Zahorowski, W. (1983). High precision lattice parameter determination of KDP with different crystal perfection. *Cryst. Res. Technol.* **18**, K28–K30.
- Gruber, E. E. & Black, R. E. (1970). Analysis of the axial misalignment error in precision lattice parameter measurement by the Bond technique. *J. Appl. Cryst.* **3**, 354–357.
- Halliwell, M. A. G. (1970). Measurement of specimen tilt and beam tilt in the Bond method. *J. Appl. Cryst.* **3**, 418–419.
- Hamilton, W. C. (1974). Angle settings for four-circle diffractometers. *International tables for X-ray crystallography*, Vol. IV, pp. 274–284. Birmingham: Kynoch Press. (Present distributor: Kluwer Academic Publishers, Dordrecht.)
- Hanneman, R. E., Ogilvie, R. E. & Modrzejewski, A. (1962). Kossel line studies of irradiated nickel crystals. *J. Appl. Phys.* **33**, 1429–1435.
- Harris, N. & Kirkham, A. J. (1971). A single-exposure method for the determination of lattice spacings and crystal orientation from Kossel diffraction patterns. *J. Appl. Cryst.* **4**, 232–240.
- Hart, M. (1969). High precision lattice parameter measurements by multiple Bragg reflexion diffractometry. *Proc. R. Soc. London Ser. A*, **309**, 281–296.
- Hart, M. (1981). Bragg angle measurement and mapping. *J. Cryst. Growth*, **55**, 409–427.
- Hart, M. & Lloyd, K. H. (1975). Measurement of strain and lattice parameter in epitaxial layers. *J. Appl. Cryst.* **8**, 42–44.
- Hart, M., Parrish, W., Bellotto, M. & Lim, G. S. (1988). The refractive-index correction in powder diffraction. *Acta Cryst.* **A44**, 193–197.
- Härtwig, J., Bak-Misiuk, J., Berger, H., Brühl, H.-G., Okada, Y., Grosswig, S., Wokulska, K. & Wolf, J. (1994). Comparison of lattice parameters obtained from an internal monocrystal standard. *Phys. Status Solidi A*, **142**, 19–26.
- Härtwig, J. & Grosswig, S. (1989). Measurement of X-ray diffraction angles of perfect monocrystals with high accuracy using a single crystal diffractometer. *Phys. Status Solidi A*, **115**, 369–382.
- Härtwig, J., Grosswig, S., Becker, P. & Windisch, D. (1991). Remeasurement of the Cu $K\alpha_1$ emission X-ray wavelength in the metrical system (present stage). *Phys. Status Solidi A*, **125**, 79–89.
- Härtwig, J., Hölzer, G., Förster, E., Goetz, K., Wokulska, K. & Wolf, J. (1994). Remeasurement of characteristic X-ray emission lines and their application to line profile analysis and lattice parameter determination. *Phys. Status Solidi A*, **143**, 23–34.
- Härtwig, J., Hölzer, G., Wolf, J. & Förster, E. (1993). Remeasurement of the profile of the characteristic Cu $K\alpha$ emission line with high precision and accuracy. *J. Appl. Cryst.* **26**, 539–548.
- Häusermann, D. & Hart, M. (1990). A fast high-accuracy lattice-parameter comparator. *J. Appl. Cryst.* **23**, 63–69.
- Hebert, H. (1978). A simple method for obtaining triclinic cell parameters from Weissenberg photographs from one crystal setting. *Acta Cryst.* **A34**, 946–949.
- Heise, H. (1962). Precision determination of the lattice constant by the Kossel line technique. *J. Appl. Phys.* **33**, 938–941.
- Henry, N. F. M., Lipson, H. & Wooster, W. A. (1960). *The interpretation of X-ray diffraction photographs*. London: Macmillan.
- Herbstein, F. H. (2000). How precise are measurements of unit-cell dimensions from single crystals? *Acta Cryst.* **B56**, 547–557.
- Holý, V. & Härtwig, J. (1988). The role of diffuse scattering on microdefects in the precise lattice parameter measurement. *Phys. Status Solidi B*, **145**, 363–372.
- Hölzer, G., Fritsch, M., Deutsch, M., Härtwig, J. & Förster, E. (1997). $K\alpha_{1,2}$ and $K\beta_{1,3}$ X-ray emission lines of the 3d transition metals. *Phys. Rev. A*, **56**, 4554–4568.
- Hom, T., Kiszewski, W. & Post, B. (1975). Accurate lattice constants from multiple reflection measurements. II. Lattice constants of germanium, silicon and diamond. *J. Appl. Cryst.* **8**, 457–458.
- Horváth, J. (1983). Lattice-parameter measurements of $PbHPO_4$ single crystals by the ratio method. *J. Appl. Cryst.* **16**, 623–628.
- Horváth, J. & Kucharczyk, D. (1981). Temperature dependence of lattice parameters of $PbHPO_4$ and $PbDPO_4$ single crystals. *Phys. Status Solidi A*, **63**, 687–692.
- Hubbard, C. R. & Mauer, F. A. (1976). Precision and accuracy of the Bond method as applied to small spherical crystals. *J. Appl. Cryst.* **9**, 1–8.
- Hubbard, C. R., Swanson, H. E. & Mauer, F. A. (1975). A silicon powder diffraction standard reference material. *J. Appl. Cryst.* **8**, 45–48.
- Hulme, R. (1966). Triclinic cell parameters from one crystal setting. *Acta Cryst.* **21**, 898–900.
- Imura, T. (1954). The study of deformation of single crystals by the divergent X-ray beams. *Bull. Naniwa. Univ. Ser. A*, **51**.
- Imura, T., Weissmann, S. & Slade, J. J. Jr (1962). A study of age-hardening of Al–3.85%Cu by the divergent X-ray beam method. *Acta Cryst.* **15**, 786–793.
- Irie, K., Koshiji, N. & Okazaki, A. (1989). High-angle double-crystal X-ray diffractometry (HADOX): combination with a sealed-tube X-ray source. *Jpn. J. Appl. Phys.* **28**, 1504–1506.
- Isherwood, B. J. (1968). An X-ray multiple diffraction study of yttrium iron garnet crystals. *J. Appl. Cryst.* **1**, 299–307.
- Isherwood, B. J., Brown, B. R. & Halliwell, M. A. G. (1981). X-ray multiple diffraction as a tool for studying heteroepitaxial layers. I. Coherent, on-axis layers. *J. Cryst. Growth*, **54**, 449–460.

5. DETERMINATION OF LATTICE PARAMETERS

5.3 (cont.)

- Isherwood, B. J., Brown, B. R. & Halliwell, M. A. G. (1982). *X-ray multiple diffraction as a tool for studying heteroepitaxial layers. II. Coherent, off-axis layers.* *J. Cryst. Growth*, **60**, 33–42.
- Isherwood, B. J. & Wallace, C. A. (1966). *Measurement of the lattice parameter of silicon using a double-diffraction effect.* *Nature (London)*, **212**, 173–175.
- Isherwood, B. J. & Wallace, C. A. (1970). *An X-ray multiple diffraction study of crystals of arsenic-doped germanium.* *J. Appl. Cryst.* **3**, 66–71.
- Isherwood, B. J. & Wallace, C. A. (1971). *The geometry of X-ray multiple diffraction in crystals.* *Acta Cryst.* **A27**, 119–130.
- James, R. W. (1967). *The optical principles of the diffraction of X-rays.* London: Bell.
- Keller, H. L., Kucharczyk, D. & Küppers, H. (1982). *The ferroelastic monoclinic low temperature modification of ammonium hydrogen oxalate hemihydrate.* *Z. Kristallogr.* **158**, 221–232.
- Kheiker, D. M. (1973). *Rentgenovskaya diffraktometriya monokristallov*, Chaps. 3, 4, 5. Leningrad: Mashinostroyeniye.
- Kheiker, D. M. & Zevin, L. S. (1963). *Rentgenovskaya diffraktometriya (X-ray diffractometry)*, Chap. 4. Moscow: Fizmatgiz.
- Kirk, D. & Caulfield, P. B. (1977). *Location of diffractometer profiles in X-ray stress analysis.* *Adv. X-ray Anal.* **20**, 283–289.
- Kishino, S. (1973). *Improved techniques of lattice parameter measurements using two X-ray beams.* *Adv. X-ray Anal.* **16**, 367–378.
- Kobayashi, J., Mizutani, I. & Schmidt, H. (1970). *X-ray study on the lattice strains of ferroelectric iron iodine boracite $Fe_3B_7O_{13}$.* *Phys. Rev. B*, **1**, 3801–3808.
- Kobayashi, J., Yamada, N. & Azumi, I. (1968). *An X-ray method for accurate determination of lattice strain of crystals.* *Rev. Sci. Instrum.* **39**, 1647–1650.
- Kobayashi, J., Yamada, N. & Nakamura, T. (1963). *Origin of the visibility of the antiparallel 180° domains in barium titanate.* *Phys. Rev. Lett.* **11**, 410–414.
- Korytár, D. (1984). *Lateral lattice parameter variation measurement by means of a double crystal X-ray method with oscillating slit.* *Czech. J. Phys.* **B34**, 1277–1281.
- Kossel, W. (1936). *Messungen am vollständigen Reflexsystem eines Kristallgitters.* *Ann. Phys. (Leipzig)*, **26**, 533–553.
- Kovalchuk, M. V., Kovev, E. K. & Pinsker, Z. G. (1975). *The X-ray triple-crystal spectrometer and precision determination of Δd_{hkl} .* (In Russian.) *Kristallografiya*, **20**, 142–148.
- Kshevetsky, S. A., Mikhailyuk, I. P., Ostapovich, M. V., Polyak, M. I., Remenyuk, P. I. & Fomin, V. G. (1979). *Application of multiple diffraction to determination of lattice parameters.* (In Russian.) *Ukr. Fiz. Zh.* **24**, 1480–1485.
- Kshevetsky, S. A., Mikhalychenko, V. P., Stetsko, Yu. P. & Shelud'ko, S. A. (1985). *The lattice parameter refinement of single crystals by means of multiple-wave diffractometry.* (In Russian.) *Ukr. Fiz. Zh.* **30**, 1843–1848.
- Kubena, J. & Holý, V. (1988). *Precise relative X-ray measurement of the lattice parameter of silicon crystals with growth striations.* *J. Appl. Cryst.* **21**, 245–251.
- Kucharczyk, D. & Niklewski, T. (1979). *Accurate X-ray determination of the lattice parameters and the thermal expansion coefficients of VO_2 near the transition temperature.* *J. Appl. Cryst.* **12**, 370–373.
- Kucharczyk, D., Pietraszko, A. & Lukaszewicz, K. (1976). *Temperature dependence of lattice parameters of $NaNO_2$ single crystals.* *Phys. Status Solidi A*, **37**, 287–294.
- Kucharczyk, D., Pietraszko, A. & Lukaszewicz, K. (1993). *An automatic four-circle diffractometer designed for precise lattice-parameter determination.* *J. Appl. Cryst.* **26**, 467.
- Kudo, S. (1982). *X-ray determination of incommensurate superlattices in K_2SeO_4 and $(NH_4)_2BeF_4$.* *Jpn. J. Appl. Phys.* **21**, 255–258.
- Kurbatov, B. A., Zubenko, V. V. & Umansky, M. M. (1972). *The use of the monochromator crystal with anomalous transmission of X-rays in precise lattice parameter measurements.* (In Russian.) *Kristallografiya*, **17**, 1058–1060.
- Lang, A. R. & Pang, G. (1995). *A possible new route to precise lattice-parameter measurement of perfect crystals using the divergent-X-ray-beam method.* *J. Appl. Cryst.* **28**, 61–64.
- Larson, B. C. (1974). *High-precision measurements of lattice parameter changes in neutron-irradiated copper.* *J. Appl. Phys.* **45**, 514–518.
- Leszczyński, M., Podlasin, S. & Suski, T. (1993). *A 10^9 Pa high-pressure cell for X-ray and optical measurements.* *J. Appl. Cryst.* **26**, 1–4.
- Lider, V. V. & Rozhansky, V. N. (1967). *A new X-ray method of precision lattice spacing determination by divergent-beam photograph.* *Fiz. Tverd. Tela (Leningrad)*, **9**, 3539–3546.
- Lisoivan, V. I. (1974). *Local determination of all the lattice parameters of single crystals.* (In Russian.) *Appar. Methody Rentgenovskogo Anal.* **14**, 151–157.
- Lisoivan, V. I. (1981). *Experimental refinement of the angles between unit-cell axes.* (In Russian.) *Kristallografiya*, **26**, 458–463.
- Lisoivan, V. I. (1982). *Measurements of unit-cell parameters on one-crystal spectrometer.* (In Russian.) Novosibirsk: Nauka.
- Lisoivan, V. I. & Dikovskaya, R. R. (1969). *Local precision determination of lattice constants of a single crystal.* *Prib. Tech. Eksp.* No. 4, pp. 164–166; English transl: *Instrum. Exp. Tech. (USSR)*, **4**, 992–994.
- Lonsdale, K. (1947). *Divergent-beam X-ray photography of crystals.* *Proc. R. Soc. London Ser. A*, **240**, 219–250.
- Luger, P. (1980). *Modern X-ray analysis of single crystals.* In particular, Chap. 4 and Section 4.2.2. Berlin: de Gruyter.
- Lukaszewicz, K., Kucharczyk, D., Malinowski, M. & Pietraszko, A. (1978). *New model of the Bond diffractometer for precise determination of lattice parameters and thermal expansion of single crystals.* *Krist. Tech.* **13**, 561–567.
- Lukaszewicz, K., Pietraszko, A., Kucharczyk, D., Malinowski, M., Stepień-Damm, J. & Urbanowicz, E. (1976). *Precyzyjne pomiary statycznych sieciowych kryształów metodą Bonda (Precision measurements of lattice constants of crystals by the Bond method).* Wrocław: Instytut Niskich Temperatur i Badań Strukturalnych PAN.
- Lutts, A. (1973). *The geometrical distortion of deficiency conic sections and its influence on lattice-parameter determinations.* *J. Appl. Cryst.* **6**, 428–437.
- Lutts, A. & Gielen, P. (1971). *The precise determination of the lattice parameter of α -iron and some of its alloys.* *J. Appl. Cryst.* **4**, 242–250.
- Lutts, A. H. (1968). *Determination of lattice parameters by the Kossel and divergent X-ray beam techniques.* *Adv. X-ray Anal.* **11**, 345–358.
- Mackay, K. J. H. (1966). *Proceedings of the IVth Congress on X-ray Optics and Microanalysis*, pp. 544–554. Paris: Hermann.

REFERENCES

5.3 (cont.)

- Main, P. & Woolfson, M. M. (1963). *Accurate lattice parameters from Weissenberg photographs*. *Acta Cryst.* **16**, 731–733.
- Mauer, F. A., Hubbard, C. R., Piermarini, G. J. & Block, S. (1975). *Measurement of anisotropic compressibilities by a single crystal diffractometer method*. *Adv. X-ray Anal.* **18**, 437–453.
- Mendelssohn, M. J. & Milledge, H. J. (1999). *Divergent-beam technique used in a SEM to measure the cell parameters of isotopically distinct samples of LiF over the temperature range ~15–375 K*. *Acta Cryst.* **A55**, 204–211.
- Mohr, P. J. & Taylor, B. N. (2000). *CODATA recommended values of the fundamental physical constants*. *Rev. Mod. Phys.* **72**, 351–495.
- Morris, W. G. (1968). *Crystal orientation and lattice parameters from Kossel lines*. *J. Appl. Phys.* **39**, 1813–1823.
- Nemiroff, M. (1982). *Precise lattice-constant determinations using measured beam and crystal tilts*. *J. Appl. Cryst.* **15**, 375–377.
- Newman, B. A. (1970). *The equation of pseudo-Kossel curves*. *J. Appl. Cryst.* **3**, 191–193.
- Newman, B. A. & Shrier, A. (1970). *A new method of determining interplanar spacings with the back-reflection X-ray divergent beam technique*. *J. Appl. Cryst.* **3**, 280–281.
- Newman, B. A. & Weissmann, S. (1968). *Strain inhomogeneities in lightly compressed tungsten crystals*. *J. Appl. Cryst.* **1**, 139–145.
- Obaidur, R. M. (2002). *Energy-selective (+,+) monolithic monochromator and relative lattice-spacing measurement of Si wafers with synchrotron radiation*. *J. Synchrotron Rad.* **9**, 28–35.
- Ohama, N., Sakashita, H. & Okazaki, A. (1979). *Improvement of high-angle double-crystal X-ray diffractometry (HADOX) for measuring temperature dependence of lattice constants. II. Practice*. *J. Appl. Cryst.* **12**, 455–459.
- Okada, Y. (1982). *A high-temperature attachment for precise measurement of lattice parameters by Bond's method between room temperature and 1500 K*. *J. Phys. E*, **15**, 1060–1063.
- Okazaki, A. & Kawaminami, M. (1973a). *Accurate measurement of lattice constants in a wide range of temperature: use of white X-ray and double-crystal diffractometry*. *Jpn. J. Appl. Phys.* **12**, 783–789.
- Okazaki, A. & Kawaminami, M. (1973b). *Lattice constant of strontium titanate at low temperatures*. *Mater. Res. Bull.* **8**, 545–550.
- Okazaki, A. & Ohama, N. (1979). *Improvement of high-angle double-crystal X-ray diffractometry (HADOX) for measuring temperature dependence of lattice constants. I. Theory*. *J. Appl. Cryst.* **12**, 450–454.
- Okazaki, A. & Soejima, Y. (2001). *Ultra-high-angle double-crystal X-ray diffractometry (U-HADOX) for determining a change in the lattice spacing: theory*. *Acta Cryst.* **A57**, 708–712.
- Parrish, W. (1960). *Results of the IUCr precision lattice-parameter project*. *Acta Cryst.* **13**, 838–850.
- Parrish, W. & Wilson, A. J. C. (1959). *Precision measurements of lattice parameters of polycrystalline specimens*. *International tables for X-ray crystallography*, Vol. II, Chap. 4.7, pp. 216–234. Birmingham: Kynoch Press.
- Pick, M. A., Bickmann, K., Pofahl, E., Zwill, K. & Wenzl, H. (1977). *A new automatic triple-crystal X-ray diffractometer for the precision measurement of intensity distribution of Bragg diffraction and Huang scattering*. *J. Appl. Cryst.* **10**, 450–457.
- Pierron, E. D. & McNeely, J. B. (1969). *Precise cell parameters of semiconductor crystals and their applications*. *Adv. X-ray Anal.* **12**, 343–353.
- Pietraszko, A., Tomaszewski, P. E. & Lukaszewicz, K. (1981). *X-ray and optical study of the phase transition in LiCsSO₄*. *Phase Transit.* **2**, 131–150.
- Pietraszko, A., Waškowska, A., Olejnik, S. & Lukaszewicz, K. (1979). *X-ray study of the phase transition in RbHSeO₄*. *Phase Transit.* **1**, 99–106.
- Pihl, C. F., Bieber, R. L. & Schwuttke, G. H. (1973). *Precision lattice parameter studies of ion-implanted silicon*. *Phys. Status Solidi A*, **17**, 359–369.
- Polcarová, M. & Zůra, J. (1977). *A method for the determination of lattice parameters on single crystals*. *Czech. J. Phys.* **B27**, 322–331.
- Popović, S. (1971). *An X-ray diffraction method for lattice parameter measurements from corresponding K α and K β reflexions*. *J. Appl. Cryst.* **4**, 240–241.
- Popović, S. (1974). *Determination of unit-cell parameters of single crystals from rotation patterns*. *J. Appl. Cryst.* **7**, 291–292.
- Popović, S., Šljukić, M. & Hanic, F. (1974). *Precise unit cell parameter and thermal expansion measurements of single crystals by X-ray diffraction*. *Phys. Status Solidi A*, **23**, 265–274.
- Post, B. (1975). *Accurate lattice constants from multiple diffraction measurements. I. Geometry, techniques and systematic errors*. *J. Appl. Cryst.* **8**, 452–456.
- Potts, H. R. & Pearson, G. L. (1966). *Annealing and arsenic over-pressure experiments on defects in gallium arsenide*. *J. Appl. Phys.* **37**, 2098–2103.
- Reeke, G. N. J. (1984). *Eigenvalue filtering in the refinement of crystal and orientation parameters for oscillation photography*. *J. Appl. Cryst.* **17**, 238–243.
- Reichard, T. E. (1969). *A high-precision Kossel camera for research and routine analytical use*. *Adv. X-ray Anal.* **12**, 188–207.
- Renninger, M. (1937). *'Umweganregung', eine bisher unbeachtete Wechselwirkungserscheinung bei Raumgitterinterferenzen*. *Z. Phys.* **106**, 141–176.
- Ridou, C., Rousseau, M. & Freund, A. (1977). *Détermination précise des paramètres cristallins au voisinage de changement de phase cubique quadratique dans RbCaF₃*. *J. Phys. (Paris)*, **38**, L-359–L-363.
- Rossmannith, E. (1985). *UMWEG – a computer program for calculation and graphical representation of Umweganregung patterns*. *Z. Kristallogr.* **171**, 253–254.
- Rossmann, M. G. (1979). *Processing oscillation diffraction data for very large unit cells with an automatic convolution technique and profile fitting*. *J. Appl. Cryst.* **12**, 225–238.
- Rozhansky, V. H., Lider, V. V. & Lyutzaev, V. G. (1966). *An X-ray method for surface topography of crystal structure defects based on Kossel-line scanning*. (In Russian.) *Kristallografiya*, **11**, 701–703.
- Sasvári, J. & Zsoldos, É. (1980). *Accurate lattice parameter measurements of epitaxial layers*. Invited paper at International Symposium on Industrial Applications of X-ray Spectrometry and Diffractometry, Turawa, Poland, 15–18 April 1980.
- Schetelich, Ch. & Geist, V. (1993). *Observation of X-ray Kossel patterns ('Gitterquelleninterferenzen') from quasicrystals*. *Phys. Status Solidi A*, **136**, 283–289.
- Schneider, J. & Weik, H. (1968). *Z. Angew. Phys.* **2**, 75–79.
- Schwartzberger, D. R. (1959). *Philos. Mag.* **4**, 1242–1246.

5. DETERMINATION OF LATTICE PARAMETERS

5.3 (cont.)

- Schwarzenbach, D., Abrahams, S. C., Flack, H. D., Gonschorek, W., Hahn, Th., Huml, K., Marsh, R. E., Prince, E., Robertson, B. E., Rollett, J. S. & Wilson, A. J. C. (1989). *Statistical descriptors in crystallography. Report of the International Union of Crystallography Subcommittee on Statistical Descriptors. Acta Cryst. A* **45**, 63–75.
- Segmüller, A. (1970). *Automated lattice parameter determination on single crystals. Adv. X-ray Anal.* **13**, 455–467.
- Shinoda, G., Isokawa, K. & Umeno, M. (1969). *Kossel line microdiffraction study on precipitation of alpha from beta in copper zinc alloys. Adv. X-ray Anal.* **12**, 174–187.
- Shrier, A., Kalman, Z. H. & Weissmann, S. (1966). US Government Research Report AD 631 179.
- Shvyd'ko, Yu. V., Lerche, M., Jäschke, J., Lucht, M., Gerdau, E., Gerken, M., Rüter, H. D., Wille, H.-C., Becker, P., Alp, E. E., Sturhahn, W., Sutter, J. & Toellner, T. S. (2000). γ -ray wavelength standard for atomic scales. *Phys. Rev. Lett.* **85**, 495–498.
- Shvyd'ko, Yu. V., Lucht, M., Gerdau, E., Lerche, M., Alp, E. E., Sturhahn, W., Sutter, J. & Toellner, T. S. (2002). *Measuring wavelengths and lattice constants with the Mössbauer wavelength standard. J. Synchrotron Rad.* **9**, 17–23.
- Siegert, H., Becker, P. & Seyfried, P. (1984). *Determination of silicon unit-cell parameters by precision measurements of Bragg plane spacings. Z. Phys. B*, **56**, 273–278.
- Singh, K. & Trigunayat, G. C. (1988). *Accurate determination of lattice parameters from XRD oscillation photographs. J. Appl. Cryst.* **21**, 991.
- Skupov, V. D. & Uspeckaya, G. I. (1975). *The combined X-ray spectrometer for deformation measurements in single crystals. (In Russian.) Prib. Tekh. Eksp. No. 2*, pp. 210–213.
- Slade, J. J., Weissmann, S., Nakajima, K. & Hirabayshi, M. (1964). *Stress-strain analysis of single cubic crystals and its application to the ordering of CuAu I. Paper II. J. Appl. Phys.* **35**, 3373–3385.
- Smakula, A. & Kalnajs, J. (1955). *Precision determination of lattice constants with a Geiger-counter X-ray diffractometer. Phys. Rev.* **99**, 1737–1743.
- Soares, D. A. W. & Pimentel, C. A. (1983). *Precision interplanar spacing measurements on boron-doped silicon. J. Appl. Cryst.* **16**, 486–492.
- Soejima, Y., Tomonaga, N., Onitsuka, H. & Okazaki, A. (1991). *Two-dimensional intensity distribution in high-angle double-crystal X-ray diffractometry (HADOX). Z. Kristallogr.* **195**, 161–168.
- Spooner, F. J. & Wilson, C. G. (1973). *The measurement of single-crystal lattice parameters using a double-diffraction technique. J. Appl. Cryst.* **6**, 132–135.
- Stepień, J. A., Auleytner, J. & Lukaszewicz, K. (1972). *X-ray examination of the real structure of γ -irradiated NaClO₃ single crystals. Phys. Status Solidi A*, **10**, 631–638.
- Stepień-Damm, J. A., Kucharczyk, D., Urbanowicz, E. & Lukaszewicz, K. (1975). *Effect of γ -irradiation on the thermal expansion of sodium chlorate NaClO₃. Bull. Acad. Pol. Sci. Ser. Sci. Chim. Geol. Geogr.* **23**, 985–988.
- Stepień-Damm, J. A., Suski, T., Meysner, L., Hilczer, B. & Lukaszewicz, K. (1974). *Effect of X-ray irradiation on the lattice constant of TGS crystal in the vicinity of phase transition. Bull. Acad. Pol. Sci. Ser. Sci. Chim. Geol. Geogr.* **22**, 685–688.
- Stout, G. H. & Jensen, L. H. (1968). *X-ray structure determination. London: Macmillan.*
- Straumanis, M. E., Borgeaud, P. & James, W. J. (1961). *Perfection of the lattice of dislocation-free silicon, studied by the lattice-constant and density method. J. Appl. Phys.* **32**, 1382–1384.
- Straumanis, M. & Ieviņš, A. (1940). *Die Präzisionsbestimmung von Gitterkonstanten nach der asymmetrischen Methode. Berlin: Springer. [Reprinted by Edwards Brothers Inc., Ann Arbor, Michigan (1948).]*
- Takano, Y. & Maki, M. (1972). *X-ray measurement of lattice strain of oxygen diffused silicon. Acta Cryst. A* **28**, S171.
- Terminasov, Yu. S. & Tuzov, L. V. (1964). *The double-diffraction of X-rays in crystals. (In Russian.) Usp. Phys. Nauk*, **83**, 223–258. (English transl: *Sov. Phys. Usp.* **7**, 734.)
- Thomsen, J. S. (1974). *High-precision X-ray spectroscopy. X-ray spectroscopy*, edited by L. V. Azároff, pp. 26–132. New York: McGraw-Hill.
- Thomsen, J. S. & Yap, Y. (1968). *Effect of statistical counting errors on wavelengths criteria for X-ray spectra. J. Res. Natl Bur. Stand. Sect. A*, **72**, 187–205.
- Tixier, R. & Waché, C. (1970). *Kossel patterns. J. Appl. Cryst.* **3**, 466–485.
- Ullrich, H.-J. (1967). *Precision lattice parameter measurements by interferences from lattice sources (Kossel lines) and divergent beam X-ray diffraction (pseudo-Kossel-lines) in back reflection. Phys. Status Solidi*, **20**, K113–K117.
- Ullrich, H.-J. & Schulze, G. E. R. (1972). *Röntgenographische Mikrobeugungsuntersuchungen an kristallinen Festkörpern mittels Gitterquelleninterferenzen (Kossel-Linien) und Weitwinkelinterferenzen (Pseudo-Kossel-Linien). Krist. Tech.* **7**, 207–220.
- Umansky, M. M. (1960). *Apparatura rentgenostrukturnykh issledovanij. Moscow: Fizmatgiz.*
- Urbanowicz, E. (1981a). *The influence of in-plane collimation on the precision and accuracy of lattice-constant determination by the Bond method. I. A mathematical model. Statistical errors. Acta Cryst. A* **37**, 364–368.
- Urbanowicz, E. (1981b). *The influence of in-plane collimation on the precision and accuracy of lattice-constant determination by the Bond method. II. Verification of the mathematical model. Systematic errors. Acta Cryst. A* **37**, 369–373.
- Walder, V. & Burke, J. (1971). *The elimination of specimen and beam tilt errors in the Bond method of precision lattice parameter determinations. J. Appl. Cryst.* **4**, 337–339.
- Weisz, O., Cochran, W. & Cole, W. F. (1948). *The accurate determination of cell dimensions from single-crystal X-ray photographs. Acta Cryst.* **1**, 83–88.
- Wilson, A. J. C. (1950). *Geiger-counter X-ray spectrometer – influence of size and absorption coefficient of specimen on position and shape of powder diffraction maxima. J. Sci. Instrum.* **27**, 321–325.
- Wilson, A. J. C. (1963). *Mathematical theory of X-ray powder diffractometry. Philips Technical Library. Eindhoven: Centrex Publishing Company.*
- Wilson, A. J. C. (1965). *The location of peaks. Br. J. Appl. Phys.* **16**, 665–674.
- Wilson, A. J. C. (1967). *Statistical variance of line-profile parameters. Measures of intensity, location and dispersion. Acta Cryst.* **23**, 888–898. Corrigenda: **A24** (1968), 478, Addendum: **A25** (1969), 584–585.
- Wilson, A. J. C. (1980). *Accuracy in methods of lattice-parameter measurement. Natl Bur. Stand. (US) Spec. Publ. No. 567. Proceedings of Symposium on Accuracy in Powder Diffraction, NBS, Gaithersburg, MD, USA, 11–15 June 1979.*

REFERENCES

5.3 (cont.)

- Windisch, D. & Becker, P. (1990). *Silicon lattice parameters as an absolute scale of length for high precision measurements of fundamental constants*. *Phys. Status Solidi A*, **118**, 379–388.
- Wołczyrz, M. & Łukaszewicz, K. (1982). *The evaluation of crystal perfection by means of the asymmetric Bragg reflections*. *J. Appl. Cryst.* **15**, 406–411.
- Wołczyrz, M., Pietraszko, A. & Łukaszewicz, K. (1980). *The application of asymmetric Bragg reflections in the Bond method of measuring lattice parameters*. *J. Appl. Cryst.* **13**, 12–16.
- Wölfel, E. R. (1971). *A new film instrument for the exploration of reciprocal space*. *J. Appl. Cryst.* **4**, 297–302.
- Woolfson, M. M. (1970). *An introduction to X-ray crystallography*. Cambridge University Press.
- Yakowitz, H. (1966a). *Effect of sample thickness and operating voltage on the contrast of Kossel transmission photographs*. *J. Appl. Phys.* **37**, 4455–4458.
- Yakowitz, H. (1966b). *Precision of cubic lattice parameter measurement by the Kossel technique*. *The electron microprobe*, edited by T. D. McKinley, K. F. J. Heinrich & D. B. Wittry, pp. 417–438. New York: John Wiley.
- Yakowitz, H. (1969). *The divergent beam X-ray technique*. *Advances in electronics and electron physics*, edited by A. J. Tousimis & L. Marton, Suppl. 6, pp. 361–431. New York: Academic Press.
- Yakowitz, H. (1972). *Use of divergent-beam X-ray diffraction to measure lattice expansion in LiF as a function of thermal-neutron dose up to 6×10^{16} nvt*. *J. Appl. Phys.* **43**, 4793–4794.
- Zolotoyabko, E., Sander, B., Komem, Y. & Kantor, B. (1993). *Improved strain analysis in semiconductor crystals by X-ray diffractometry enhanced with ultrasound*. *Appl. Phys. Lett.* **63**, 1540–1542.

5.4.1

- Edington, J. W. (1975). *Electron diffraction in the electron microscope*. *Monographs in practical electron microscopy in materials science*, No. 2. Eindhoven: N. V. Philips Gloeilampenfabrieken.
- Gard, J. A. (1976). *Electron microscopy in mineralogy*, p. 52. Berlin: Springer.
- Hirsch, P. B., Howie, A., Nicholson, R. B., Pashley, D. W. & Whelan, M. J. (1965). *Electron microscopy of thin crystals*. London: Butterworth.
- International Tables for Crystallography* (1983). Vol. A. Dordrecht: Kluwer Academic Publishers.
- LePage, Y. (1992). *Ab initio primitive cell parameters from single convergent beam patterns: a converse route to the identification of microcrystals with electrons*. *Miscrosc. Res. Tech.* **21**, 158–165.

- Zuo, J. M. (1993). *New method of Bravais lattice determination*. *Ultramicroscopy*, **52**, 459–464.

5.4.2

- FitzGerald, J. D. & Johnson, A. W. S. (1984). *A simplified method of electron microscope voltage measurement*. *Ultramicroscopy*, **12**, 231–236.
- Gjønnnes, J. & Olsen, A. (1984). *Analytical electron microscopy*. *JEOL News*, **22E**, 13–18.
- Høier, R. (1969). *A method to determine the ratio between lattice parameter and electron wavelength from Kikuchi line intersections*. *Acta Cryst.* **A25**, 516–518.
- Jones, P. M., Rackham, G. M. & Steeds, J. W. (1977). *Higher order Laue zone effects in electron diffraction and their use in lattice parameter determination*. *Proc. R. Soc. London Ser. A*, **354**, 197–222.
- Olsen, A. (1976a). *Lattice parameter determination using Kikuchi-line intersections: application to olivine and feldspar*. *J. Appl. Cryst.* **9**, 9–13.
- Olsen, A. (1976b). *Determination of lattice constants using Kikuchi line intersections*. Solid State Group Report Series. Institute of Physics, University of Oslo, Norway.
- Rackham, G. M., Jones, P. M. & Steeds, J. W. (1974). *Upper layer diffraction effects in zone axis patterns*. Proceedings of the Eighth International Congress on Electron Microscopy, Canberra, Australia, pp. 336–337.
- Steeds, J. W. (1979). *Convergent beam electron diffraction*. *Introduction to analytical electron microscopy*, edited by J. J. Hren, J. I. Goldstein & D. C. Joy, pp. 387–422. New York: Plenum.
- Thomas, G. (1970). *Kikuchi electron diffraction and applications*. *Modern diffraction and imaging techniques in material science*, edited by S. Amelinckx, S. Gevers, G. Remaut & J. Van Landuyt, pp. 131–185. Amsterdam: North-Holland.
- Uyeda, R., Nonoyama, M. & Kogiso, M. (1965). *Determination of the wavelength of electrons from a Kikuchi pattern*. *J. Electron Microsc.* **14**, 296–300.
- Walker, A. R. & Booker, G. R. (1982). *A selected-area channelling pattern (SACP) method for measuring small local changes in lattice parameter with bulk specimens*. *Electron microscopy 1982*, Vol. 1, pp. 651–652. Hamburg: Elsevier.

5.5

- Fischer, P., Zolliker, P., Meier, B. H., Ernst, R. R., Hewat, A. W., Jorgensen, J. D. & Rotella, F. J. (1986). *Structure and dynamics of terephthalic acid from 2 to 300 K*. *J. Solid State Chem.* **61**, 109–125.