

## REFERENCES

## 2.4 (cont.)

- Robertson, J. M. (1936). *An X-ray study of the phthalocyanines. Part II. Quantitative structure determination of the metal-free compound.* *J. Chem. Soc.* pp. 1195–1209.
- Robertson, J. M. & Woodward, I. (1937). *An X-ray study of the phthalocyanines. Part III. Quantitative structure determination of nickel phthalocyanine.* *J. Chem. Soc.* pp. 219–230.
- Rossmann, M. G. (1960). *The accurate determination of the position and shape of heavy-atom replacement groups in proteins.* *Acta Cryst.* **13**, 221–226.
- Rossmann, M. G. (1961). *The position of anomalous scatterers in protein crystals.* *Acta Cryst.* **14**, 383–388.
- Rossmann, M. G. & Blow, D. M. (1961). *The refinement of structures partially determined by the isomorphous replacement method.* *Acta Cryst.* **14**, 641–647.
- Sayre, D. (1952). *The squaring method: a new method for phase determination.* *Acta Cryst.* **5**, 60–65.
- Sayre, D. (1974). *Least-squares phase refinement. II. High-resolution phasing of a small protein.* *Acta Cryst.* **A30**, 180–184.
- Schevitz, R. W., Podjarny, A. D., Zwick, M., Hughes, J. J. & Sigler, P. B. (1981). *Improving and extending the phases of medium- and low-resolution macromolecular structure factors by density modification.* *Acta Cryst.* **A37**, 669–677.
- Schoenborn, B. P. (1975). *Phasing of neutron protein data by anomalous dispersion.* In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abrahams, pp. 407–416, Copenhagen: Munksgaard.
- Sheriff, S. & Hendrickson, W. A. (1987). *Location of iron and sulfur atoms in myohemerythrin from anomalous-scattering measurements.* *Acta Cryst.* **B43**, 209–212.
- Sikka, S. K. (1969). *On the application of the symbolic addition procedure in neutron diffraction structure determination.* *Acta Cryst.* **A25**, 539–543.
- Sikka, S. K. & Rajagopal, H. (1975). *Application of neutron anomalous dispersion in the structure determination of cadmium tartrate pentahydrate.* In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abrahams, pp. 503–514, Copenhagen: Munksgaard.
- Singh, A. K. & Ramaseshan, S. (1966). *The determination of heavy atom positions in protein derivatives.* *Acta Cryst.* **21**, 279–280.
- Singh, A. K. & Ramaseshan, S. (1968). *The use of neutron anomalous scattering in crystal structure analysis. I. Non-centrosymmetric structures.* *Acta Cryst.* **B24**, 35–39.
- Srinivasan, R. (1972). *Applications of X-ray anomalous scattering in structural studies.* In *Advances in structure research by diffraction methods*, Vol. 4, edited by W. Hoppe & R. Mason, pp. 105–197, Braunschweig: Vieweg & Sohn; and Oxford: Pergamon Press.
- Srinivasan, R. & Chacko, K. K. (1970). *On the determination of phases of a noncentrosymmetric crystal by the anomalous dispersion method.* *Z. Kristallogr.* **131**, 29–39.
- Sussman, J. L., Holbrook, S. R., Church, G. M. & Kim, S.-H. (1977). *A structure-factor least-squares refinement procedure for macromolecular structures using constrained and restrained parameters.* *Acta Cryst.* **A33**, 800–804.
- Templeton, D. H., Templeton, L. K., Phillips, J. C. & Hodgson, K. O. (1980). *Anomalous scattering of X-rays by cesium and cobalt measured with synchrotron radiation.* *Acta Cryst.* **A36**, 436–442.
- Templeton, L. K., Templeton, D. H. & Phizackerley, R. P. (1980). *L<sub>3</sub>-edge anomalous scattering of X-rays by praseodymium and samarium.* *J. Am. Chem. Soc.* **102**, 1185–1186.
- Templeton, L. K., Templeton, D. H., Phizackerley, R. P. & Hodgson, K. O. (1982). *L<sub>3</sub>-edge anomalous scattering by gadolinium and samarium measured at high resolution with synchrotron radiation.* *Acta Cryst.* **A38**, 74–78.
- Terwilliger, T. C. & Eisenberg, D. (1983). *Unbiased three-dimensional refinement of heavy-atom parameters by correlation of origin-removed Patterson functions.* *Acta Cryst.* **A39**, 813–817.
- Ueki, T., Zalkin, A. & Templeton, D. H. (1966). *Crystal structure of thorium nitrate pentahydrate by X-ray diffraction.* *Acta Cryst.* **20**, 836–841.
- Vijayan, M. (1980a). *On the Fourier refinement of protein structures.* *Acta Cryst.* **A36**, 295–298.
- Vijayan, M. (1980b). *Phase evaluation and some aspects of the Fourier refinement of macromolecules.* In *Computing in crystallography*, edited by R. Diamond, S. Ramaseshan & K. Venkatesan, pp. 19.01–19.25, Bangalore: Indian Academy of Sciences.
- Vijayan, M. (1981). *X-ray analysis of 2Zn insulin: some crystallographic problems.* In *Structural studies on molecules of biological interest*, edited by G. Dodson, J. P. Glusker & D. Sayre, pp. 260–273, Oxford: Clarendon Press.
- Vijayan, M. (1987). *Anomalous scattering methods.* In *Direct methods, macromolecular crystallography and crystallographic statistics*, edited by H. Schenk, A. J. C. Wilson & S. Parthasarathy, pp. 121–139, Singapore: World Scientific Publishing Co. Pte. Ltd.
- Vos, A. (1975). *Anomalous scattering and chemical crystallography.* In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abrahams, pp. 307–317, Copenhagen: Munksgaard.
- Wang, B. C. (1985). *Resolution of phase ambiguity in macromolecular crystallography.* *Methods Enzymol.* **115**, 90–112.
- Watenpaugh, K. D., Sieker, L. C., Herriot, J. R. & Jensen, L. H. (1973). *Refinement of the model of a protein: rubredoxin at 1.5 Å resolution.* *Acta Cryst.* **B29**, 943–956.
- Watenpaugh, K. D., Sieker, L. C. & Jensen, L. H. (1975). *Anomalous scattering in protein structure analysis.* In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abrahams, pp. 393–405, Copenhagen: Munksgaard.
- Wilson, A. J. C. (1942). *Determination of absolute from relative X-ray intensity data.* *Nature (London)*, **150**, 151–152.
- Wilson, A. J. C. (1975). *Effect of neglect of dispersion on apparent scale and temperature parameters.* In *Anomalous scattering*, edited by S. Ramaseshan & S. C. Abrahams, pp. 325–332, Copenhagen: Munksgaard.
- Zachariasen, W. H. (1965). *Dispersion in quartz.* *Acta Cryst.* **18**, 714–716.

## 2.5

- Avilov, A. S. (1979). *Electrical measurement of reflection intensities on electron diffraction from mosaic single crystals.* *Sov. Phys. Crystallogr.* **24**, 103–104.
- Avilov, A. S., Kuligin, A. K., Pietsch, U., Spence, J. C. H., Tsirelson, V. G. & Zuo, J. M. (1999). *Scanning system for high-energy electron diffractometry.* *J. Appl. Cryst.* **32**, 1033–1038.
- Avilov, A. S., Parmon, V. S., Semiletov, S. A. & Sirota, M. I. (1984). *Calculation of reflected intensities in multiple-beam diffraction of fast electrons by polycrystalline specimens.* *Sov. Phys. Crystallogr.* **29**, 5–7.
- Bando, Y. (1981). *Weak asymmetry in  $\beta$ -Si<sub>3</sub>N<sub>4</sub> as revealed by convergent beam electron diffraction.* *Acta Cryst.* **B39**, 185–189.
- Bethe, H. A. (1928). *Theorie der Beugung von Elektronen an Kristallen.* *Ann. Phys. (Leipzig)*, **87**, 55–129.
- Bilhorn, D. E., Foldy, L. L., Thaler, R. M. & Tobacman, W. (1964). *Remarks concerning reciprocity in quantum mechanics.* *J. Math. Phys.* **5**, 435–441.
- Blackman, M. (1939). *On the intensities of electron diffraction rings.* *Proc. R. Soc. London Ser. A*, **173**, 68–82.
- Bracewell, B. N. (1956). *Strip integration in radio astronomy.* *Austr. J. Phys.* **9**, 198–217.
- Bricogne, G. & Gilmore, C. J. (1990). *A multisolution method of phase determination by combined maximization of entropy and likelihood. I. Theory, algorithms and strategy.* *Acta Cryst.* **A46**, 284–297.
- Brisse, F. (1989). *Electron diffraction of synthetic polymers: the model compound approach to polymer structure.* *J. Electron Microsc. Tech.* **11**, 272–279.
- Buxton, B., Eades, J. A., Steeds, J. W. & Rackham, G. M. (1976). *The symmetry of electron diffraction zone axis patterns.* *Philos. Trans. R. Soc. London Ser. A*, **181**, 171–193.

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

### 2.5 (cont.)

- Carpenter, R. W. & Spence, J. C. H. (1982). *Three-dimensional strain-field information in convergent-beam electron diffraction patterns*. *Acta Cryst.* **A38**, 55–61.
- Chou, C. T., Anderson, S. C., Cockayne, D. J. H., Sikorski, A. Z. & Vaughan, M. R. (1994). *Ultramicroscopy*, **55**, 334–347.
- Cochran, W., Crick, F. H. C. & Vand, V. (1952). *The structure of synthetic polypeptides. I. The transform of atoms on a helix*. *Acta Cryst.* **5**, 581–586.
- Cowley, J. M. (1953). *Structure analysis of single crystals by electron diffraction. II. Disordered boric acid structure*. *Acta Cryst.* **6**, 522–529.
- Cowley, J. M. (1956). *A modified Patterson function*. *Acta Cryst.* **9**, 397–398.
- Cowley, J. M. (1961). *Diffraction intensities from bent crystals*. *Acta Cryst.* **14**, 920–927.
- Cowley, J. M. (1969). *Image contrast in transmission scanning electron microscopy*. *Appl. Phys. Lett.* **15**, 58–59.
- Cowley, J. M. (1981). *Diffraction physics*, 2nd ed. Amsterdam: North-Holland.
- Cowley, J. M. (1995). *Diffraction physics*, 3rd ed. Amsterdam: North-Holland.
- Cowley, J. M. & Au, A. Y. (1978). *Image signals and detector configurations for STEM*. In *Scanning electron microscopy*, Vol. 1, pp. 53–60. AMF O'Hare, Illinois: SEM Inc.
- Cowley, J. M. & Moodie, A. F. (1957). *The scattering of electrons by atoms and crystals. I. A new theoretical approach*. *Acta Cryst.* **10**, 609–619.
- Cowley, J. M. & Moodie, A. F. (1959). *The scattering of electrons by atoms and crystals. III. Single-crystal diffraction patterns*. *Acta Cryst.* **12**, 360–367.
- Cowley, J. M. & Moodie, A. F. (1960). *Fourier images. IV. The phase grating*. *Proc. Phys. Soc. London*, **76**, 378–384.
- Cowley, J. M., Moodie, A. F., Miyake, S., Takagi, S. & Fujimoto, F. (1961). *The extinction rules for reflections in symmetrical electron diffraction spot patterns*. *Acta Cryst.* **14**, 87–88.
- Cowley, J. M., Rees, A. L. G. & Spink, J. A. (1951). *Secondary elastic scattering in electron diffraction*. *Proc. Phys. Soc. London Sect. A*, **64**, 609–619.
- Cramér, H. (1954). *Mathematical methods of statistics*. University of Princeton.
- Creek, R. C. & Spargo, A. E. C. (1985). *Electron optical study of rutile*. *J. Appl. Cryst.* **18**, 197–204.
- Crowther, R. A. & Amos, L. A. (1971). *Harmonic analysis of electron microscope images with rotational symmetry*. *J. Mol. Biol.* **60**, 123–130.
- Crowther, R. A., Amos, L. A., Finch, J. T., DeRosier, D. J. & Klug, A. (1970). *Three dimensional reconstruction of spherical viruses by Fourier synthesis from electron micrographs*. *Nature (London)*, **226**, 421–425.
- Crowther, R. A., DeRosier, D. J. & Klug, A. (1970). *The reconstruction of a three-dimensional structure from projections and its application to electron microscopy*. *Proc. R. Soc. London Ser. A*, **317**, 319–340.
- Crowther, R. A. & Klug, A. (1974). *Three dimensional image reconstruction on an extended field – a fast, stable algorithm*. *Nature (London)*, **251**, 490–492.
- Dawson, B., Goodman, P., Johnson, A. W. S., Lynch, D. F. & Moodie, A. F. (1974). *Some definitions and units in electron diffraction*. *Acta Cryst.* **A30**, 297–298.
- Deans, S. R. (1983). *The Radon transform and some of its applications*. New York: John Wiley.
- DeRosier, D. J. & Klug, A. (1968). *Reconstruction of three dimensional structures from electron micrographs*. *Nature (London)*, **217**, 130–134.
- DeRosier, D. J. & Moore, P. B. (1970). *Reconstruction of three-dimensional images from electron micrographs of structure with helical symmetry*. *J. Mol. Biol.* **52**, 355–369.
- De Titta, G. T., Edmonds, J. W., Langs, D. A. & Hauptman, H. (1975). *Use of negative quartet cosine invariants as a phasing figure of merit: NQUEST*. *Acta Cryst.* **A31**, 472–479.
- Dong, W., Baird, T., Fryer, J. R., Gilmore, C. J., MacNicol, D. D., Bricogne, G., Smith, D. J., O'Keefe, M. A. & Hovmöller, S. (1992). *Electron microscopy at 1 Å resolution by entropy maximization and likelihood ranking*. *Nature (London)*, **355**, 605–609.
- Dorset, D. L. (1976). *The interpretation of quasi-kinematical single-crystal electron diffraction intensity data from paraffins*. *Acta Cryst.* **A32**, 207–215.
- Dorset, D. L. (1987). *Electron diffraction structure analysis of phospholipids*. *J. Electron Microsc. Tech.* **7**, 35–46.
- Dorset, D. L. (1990a). *Direct structure analysis of a paraffin solid solution*. *Proc. Natl Acad. Sci. USA*, **87**, 8541–8544.
- Dorset, D. L. (1990b). *Direct determination of crystallographic phases for diffraction data from phospholipid multilamellar arrays*. *Biophys. J.* **58**, 1077–1087.
- Dorset, D. L. (1991a). *Electron diffraction structure analysis of diketopiperazine – a direct phase determination*. *Acta Cryst.* **A47**, 510–515.
- Dorset, D. L. (1991b). *Is electron crystallography possible? The direct determination of organic crystal structures*. *Ultramicroscopy*, **38**, 23–40.
- Dorset, D. L. (1991c). *Electron diffraction structure analysis of polyethylene. A direct phase determination*. *Macromolecules*, **24**, 1175–1178.
- Dorset, D. L. (1991d). *Electron crystallography of linear polymers: direct structure analysis of poly( $\epsilon$ -caprolactone)*. *Proc. Natl Acad. Sci. USA*, **88**, 5499–5502.
- Dorset, D. L. (1991e). *Direct determination of crystallographic phases for diffraction data from lipid bilayers. I. Reliability and phase refinement*. *Biophys. J.* **60**, 1356–1365.
- Dorset, D. L. (1991f). *Direct determination of crystallographic phases for diffraction data from lipid bilayers. II. Refinement of phospholipid structures*. *Biophys. J.* **60**, 1366–1373.
- Dorset, D. L. (1992a). *Direct phasing in electron crystallography: determination of layer silicate structures*. *Ultramicroscopy*, **45**, 5–14.
- Dorset, D. L. (1992b). *Direct methods in electron crystallography – structure analysis of boric acid*. *Acta Cryst.* **A48**, 568–574.
- Dorset, D. L. (1992c). *Electron crystallography of linear polymers: direct phase determination for zonal data sets*. *Macromolecules*, **25**, 4425–4430.
- Dorset, D. L. (1992d). *Automated phase determination in electron crystallography: thermotropic phases of thiourea*. *Ultramicroscopy*, **45**, 357–364.
- Dorset, D. L. (1994a). *Electron crystallography of organic molecules*. *Adv. Electron. Electron Phys.* **88**, 111–197.
- Dorset, D. L. (1994b). *Electron crystallography of linear polymers*. In *Characterization of solid polymers. New techniques and developments*, edited by S. J. Spells, pp. 1–16. London: Chapman and Hall.
- Dorset, D. L. (1994c). *Electron crystallography of inorganic compounds. Direct determination of the basic copper chloride structure  $\text{CuCl}_2 \cdot 3\text{Cu}(\text{OH})_2$* . *J. Chem. Crystallogr.* **24**, 219–224.
- Dorset, D. L. (1994d). *Direct determination of layer packing for a phospholipid solid solution at 0.32 nm resolution*. *Proc. Natl Acad. Sci. USA*, **91**, 4920–4924.
- Dorset, D. L., Beckmann, E. & Zemlin, F. (1990). *Direct determination of a phospholipid lamellar structure at 0.34 nm resolution*. *Proc. Natl Acad. Sci. USA*, **87**, 7570–7573.
- Dorset, D. L. & Hauptman, H. A. (1976). *Direct phase determination for quasi-kinematical electron diffraction intensity data from organic microcrystals*. *Ultramicroscopy*, **1**, 195–201.
- Dorset, D. L., Jap, B. K., Ho, M.-H. & Glaeser, R. M. (1979). *Direct phasing of electron diffraction data from organic crystals: the effect of  $n$ -beam dynamical scattering*. *Acta Cryst.* **A35**, 1001–1009.
- Dorset, D. L., Kopp, S., Fryer, J. R. & Tivol, W. F. (1995). *The Sayre equation in electron crystallography*. *Ultramicroscopy*, **57**, 59–89.
- Dorset, D. L. & McCourt, M. P. (1992). *Effect of dynamical scattering on successful direct phase determination in electron crystallography – a model study*. *Trans. Am. Crystallogr. Assoc.* **28**, 105–113.

## REFERENCES

## 2.5 (cont.)

- Dorset, D. L. & McCourt, M. P. (1993). *Electron crystallographic analysis of a polysaccharide structure – direct phase determination and model refinement for mannan I*. *J. Struct. Biol.* **111**, 118–124.
- Dorset, D. L. & McCourt, M. P. (1994a). *Automated structure analysis in electron crystallography: phase determination with the tangent formula and least-squares refinement*. *Acta Cryst.* **A50**, 287–292.
- Dorset, D. L. & McCourt, M. P. (1994b). *Disorder and molecular packing of C<sub>60</sub> buckminsterfullerene: a direct electron-crystallographic analysis*. *Acta Cryst.* **A50**, 344–351.
- Dorset, D. L., McCourt, M. P., Fryer, J. R., Tivol, W. F. & Turner, J. N. (1994). *The tangent formula in electron crystallography: phase determination of copper perchlorophthalocyanine*. *Microsc. Soc. Am. Bull.* **24**, 398–404.
- Dorset, D. L., McCourt, M. P., Kopp, S., Wittmann, J.-C. & Lotz, B. (1994). *Direct determination of polymer crystal structures by electron crystallography – isotactic poly(1-butene), form III*. *Acta Cryst.* **B50**, 201–208.
- Dorset, D. L., McCourt, M. P., Tivol, W. F. & Turner, J. N. (1993). *Electron diffraction from phospholipids – an approximate correction for dynamical scattering and tests for a correct phase determination*. *J. Appl. Cryst.* **26**, 778–786.
- Dorset, D. L., Tivol, W. F. & Turner, J. N. (1991). *Electron crystallography at atomic resolution: ab initio structure analysis of copper perchlorophthalocyanine*. *Ultramicroscopy*, **38**, 41–45.
- Dorset, D. L., Tivol, W. F. & Turner, J. N. (1992). *Dynamical scattering and electron crystallography – ab initio structure analysis of copper perbromophthalocyanine*. *Acta Cryst.* **A48**, 562–568.
- Dorset, D. L. & Zemlin, F. (1990). *Direct phase determination in electron crystallography: the crystal structure of an n-paraffin*. *Ultramicroscopy*, **33**, 227–236.
- Dorset, D. L. & Zhang, W. P. (1991). *Electron crystallography at atomic resolution: the structure of the odd-chain paraffin n-tritriacontane*. *J. Electron Microsc. Tech.* **18**, 142–147.
- Dvoryankin, V. F. & Vainshtein, B. K. (1960). *An electron diffraction study of thiourea*. *Sov. Phys. Crystallogr.* **5**, 564–574.
- Dvoryankin, V. F. & Vainshtein, B. K. (1962). *An electron diffraction study of the low-temperature ferroelectric form of thiourea*. *Sov. Phys. Crystallogr.* **6**, 765–772.
- Eades, J. A. (1980). *Another way to form zone axis patterns*. *Inst. Phys. Conf. Ser.* **52**, 9–12.
- Eades, J. A., Shannon, M. D. & Buxton, B. F. (1983). *Crystal symmetry from electron diffraction*. In *Scanning electron microscopy, 1983/III*, pp. 1051–1060. Chicago: SEM Inc.
- Erickson, H. P. & Klug, A. (1971). *Measurements and compensation of defocusing and aberrations by Fourier processing of electron micrographs*. *Philos. Trans. R. Soc. London Ser. B*, **261**, 105–118.
- Fan, H. F., Xiang, S. B., Li, F. H., Pan, Q., Uyeda, N. & Fujiyoshi, Y. (1991). *Image resolution enhancement by combining information from electron diffraction pattern and micrograph*. *Ultramicroscopy*, **36**, 361–365.
- Fan, H.-F., Zhong, Z.-Y., Zheng, C.-D. & Li, F.-H. (1985). *Image processing in high-resolution electron microscopy using the direct method. I. Phase extension*. *Acta Cryst.* **A41**, 163–165.
- Frank, J. (1975). *Averaging of low exposure electron micrographs of non-periodic objects*. *Ultramicroscopy*, **1**, 159–162.
- Frank, J. (1980). *The role of correlation techniques in computer image processing*. In *Computer processing of electron microscopy images*, edited by P. W. Hawkes, pp. 187–222. Berlin: Springer-Verlag.
- Fraser, H. L., Maher, D. M., Humphreys, C. J., Hetherington, C. J. D., Knoell, R. V. & Bean, J. C. (1985). *The detection of local strains in strained superlattices*. In *Microscopy of semiconducting materials*, pp. 1–5. London: Institute of Physics.
- Fryer, J. R. (1993). *Electron crystallography of small organic molecules*. *Microsc. Soc. Am. Bull.* **23**, 44–56.
- Fujimoto, F. (1959). *Dynamical theory of electron diffraction in Laue-case. I. General theory*. *J. Phys. Soc. Jpn*, **14**(11), 1158–1168.
- Fujiwara, K. (1961). *Relativistic dynamical theory of electron diffraction*. *J. Phys. Soc. Jpn*, **16**, 2226–2238.
- Fukuhara, A. (1966). *Many-ray approximations in the dynamical theory of electron diffraction*. *J. Phys. Soc. Jpn*, **21**, 2645–2662.
- Gabor, D. (1949). *Microscopy by reconstructed wavefronts*. *Proc. R. Soc. London Ser. A*, **197**, 454–487.
- Gassmann, J. (1976). *Improvement and extension of approximate phase sets in structure determination*. In *Crystallographic computing techniques*, edited by F. R. Ahmed, pp. 144–154. Copenhagen: Munksgaard.
- Gassmann, J. & Zechmeister, K. (1972). *Limits of phase expansion in direct methods*. *Acta Cryst.* **A28**, 270–280.
- Germain, G., Main, P. & Woolfson, M. M. (1971). *The application of phase relationships to complex structures. III. The optimum use of phase relationships*. *Acta Cryst.* **A27**, 368–376.
- Gilbert, P. F. C. (1972a). *The reconstruction of a three-dimensional structure from projections and its application to electron microscopy. II. Direct methods*. *Proc. R. Soc. London Ser. B*, **182**, 89–102.
- Gilbert, P. F. C. (1972b). *Iterative methods for the three-dimensional reconstruction of an object from projections*. *J. Theor. Biol.* **36**, 105–117.
- Gilmore, C. J., Bricogne, G. & Bannister, C. (1990). *A multiresolution method of phase determination by combined maximization of entropy and likelihood. II. Application to small molecules*. *Acta Cryst.* **A46**, 297–308.
- Gilmore, C. J., Shankland, K. & Bricogne, G. (1993). *Applications of the maximum entropy method to powder diffraction and electron crystallography*. *Proc. R. Soc. London Ser. A*, **442**, 97–111.
- Gilmore, C. J., Shankland, K. & Fryer, J. R. (1992). *The application of the maximum entropy method to electron microscopy data for purple membrane*. *Trans. Am. Crystallogr. Assoc.* **28**, 129–139.
- Gilmore, C. J., Shankland, K. & Fryer, J. R. (1993). *Phase extension in electron crystallography using the maximum entropy method and its application to two-dimensional purple membrane data from Halobacterium halobium*. *Ultramicroscopy*, **49**, 132–146.
- Gjønnnes, J. & Høier, R. (1971). *The application of non-systematic many-beam dynamic effects to structure-factor determination*. *Acta Cryst.* **A27**, 313–316.
- Gjønnnes, J. & Moodie, A. F. (1965). *Extinction conditions in dynamic theory of electron diffraction patterns*. *Acta Cryst.* **19**, 65–67.
- Glauber, R. & Schomaker, V. (1953). *The theory of electron diffraction*. *Phys. Rev.* **89**, 667–670.
- Goncharov, A. B. (1987). *Integral geometry and 3D-reconstruction of arbitrarily oriented identical particles from their electron micrographs*. *Sov. Phys. Crystallogr.* **32**, 663–666.
- Goncharov, A. B., Vainshtein, B. K., Ryskin, A. I. & Vagin, A. A. (1987). *Three-dimensional reconstruction of arbitrarily oriented identical particles from their electron photomicrographs*. *Sov. Phys. Crystallogr.* **32**, 504–509.
- Goodman, P. (1974). *The role of upper layer interactions in electron diffraction*. *Nature (London)*, **251**, 698–701.
- Goodman, P. (1976). *Examination of the graphite structure by CBED*. *Acta Cryst.* **A32**, 793–798.
- Goodman, P. (1984a). *A matrix basis for CBED pattern analysis*. *Acta Cryst.* **A40**, 522–526.
- Goodman, P. (1984b). *A retabulation of the 80 layer groups for electron diffraction usage*. *Acta Cryst.* **A40**, 633–642.
- Goodman, P., McLean, J. D., Wilson, I. J. & Olsen, A. (1984). *Optical microdiffraction and image analysis of subsymmetries in Nb<sub>2</sub>O<sub>5</sub> tunnel structures*. In *Analytical electron microscopy–1984*, pp. 130–134. San Francisco Press.
- Goodman, P. & Miller, P. (1993). *Reassessment of the symmetry of the 221 PbBiSrCaCuO structure using LACBED and high-resolution SAD: the relevance of Cowley's theory of disorder scattering to a real-space structural analysis*. *Ultramicroscopy*, **52**, 549–556.

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

### 2.5 (cont.)

- Goodman, P., Miller, P., White, T. J. & Withers, R. L. (1992). *Symmetry determination and Pb-site ordering analysis for the  $n = 1, 2 \text{ Pb}_x\text{Bi}_{2-x}\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{4+2n+\delta}$  compounds by convergent-beam and selected-area electron diffraction.* *Acta Cryst.* **B48**, 376–387.
- Goodman, P. & Whitfield, H. J. (1980). *The space group determination of GaS and  $\text{Cu}_3\text{As}_2\text{S}_3\text{I}$  by convergent beam electron diffraction.* *Acta Cryst.* **A36**, 219–228.
- Gordon, R. (1974). *A tutorial on ART (algebraic reconstruction techniques).* *IEEE Trans. Nucl. Sci.* **NS-21**, 78–93.
- Gordon, R., Bender, R. & Herman, G. T. (1970). *Algebraic reconstruction techniques (ART) for three-dimensional electron microscopy and X-ray photography.* *J. Theor. Biol.* **29**, 471–481.
- Gordon, R. & Herman, G. T. (1971). *Reconstruction of pictures from their projections.* *Commun. ACM*, **14**, 759–768.
- Grzanic, G. (1985). *Calculation of incommensurate diffraction intensities from disordered crystals.* *Philos. Mag. A*, **52**, 161–187.
- Gunning, J. & Goodman, P. (1992). *Reciprocity in electron diffraction.* *Acta Cryst.* **A48**, 591–595.
- Gurskaya, G. V., Lobanova, G. M. & Vainshtein, B. K. (1971). *X-ray diffraction and electron-microscope study of hexagonal catalase crystal.* *Sov. Phys. Crystallogr.* **16**, 662–669.
- Hashimoto, H., Endoh, H., Tanji, T., Ono, A. & Watanabe, E. (1977). *Direct observation of fine structure within images of atoms in crystals by transmission electron microscopy.* *J. Phys. Soc. Jpn*, **42**, 1073–1074.
- Hashimoto, H., Mannami, M. & Naiki, T. (1961). *Dynamical theory of electron diffraction for the electron microscope image of crystal lattices. I. Image of single crystals. II. Image of superposed crystals (moiré pattern).* *Philos. Trans. R. Soc. London*, **253**, 459–516.
- Hauptman, H. (1972). *Crystal structure determination. The role of the cosine seminvariants.* NY: Plenum Press.
- Hauptman, H. (1993). *A minimal principle in X-ray crystallography: starting in a small way.* *Proc. R. Soc. London Ser. A*, **442**, 3–12.
- Hauptman, H. & Karle, J. (1953). *Solution of the phase problem. I. The centrosymmetric crystal.* American Crystallographic Association Monograph No. 3. Ann Arbor, MI: Edwards Brothers.
- Havelka, W., Henderson, R., Heymann, J. A. W. & Oesterhelt, D. (1993). *Projection structure of halorhodopsin from Halobacterium halobium at 6 Å resolution obtained by electron cryomicroscopy.* *J. Mol. Biol.* **234**, 837–846.
- Henderson, R., Baldwin, J. M., Ceska, T. A., Zemlin, F., Beckmann, E. & Downing, K. H. (1990). *Model for the structure of bacteriorhodopsin based on high-resolution electron cryomicroscopy.* *J. Mol. Biol.* **213**, 899–929.
- Henderson, R., Baldwin, J. M., Downing, K. H., Lepault, J. & Zemlin, F. (1986). *Structure of purple membrane from Halobacterium halobium: recording, measurement and evaluation of electron micrographs at 3.5 Å resolution.* *Ultramicroscopy*, **19**, 147–178.
- Henderson, R. & Unwin, P. N. T. (1975). *Three-dimensional model of purple membrane obtained by electron microscopy.* *Nature (London)*, **257**, 28–32.
- Herman, G. T. (1980). *Image reconstruction from projection: the fundamentals of computerized tomography.* New York: Academic Press.
- Herrmann, K. H., Krahl, D. & Rust, H.-P. (1980). *Low-dose image recording by TV techniques.* In *Electron microscopy at molecular dimensions*, edited by W. Baumeister & W. Vogell, pp. 186–193. Berlin: Springer-Verlag.
- Hirsch, P. B., Howie, A., Nicholson, R. B., Pashley, D. W. & Whelan, M. J. (1965). *Electron microscopy of thin crystals.* London: Butterworths.
- Hoppe, W. (1971). *Use of zone correction plate and other techniques for structure determination of aperiodic objects at atomic resolution using a conventional electron microscope.* *Philos. Trans. R. Soc. London Ser. B*, **261**, 71–94.
- Hoppe, W., Bussler, P., Feltynowski, A., Hunsmann, N. & Hirt, A. (1973). *Some experience with computerized image reconstruction methods.* In *Image processing and computer-aided design in electron optics*, edited by R. W. Hawkes, pp. 92–126. London: Academic Press.
- Hoppe, W. & Gassmann, J. (1968). *Phase correction, a new method to solve partially known structures.* *Acta Cryst.* **B24**, 97–107.
- Hoppe, W. & Typke, D. (1979). *Three-dimensional reconstruction of aperiodic objects in electron microscopy.* In *Advances in structure research by diffraction method.* Oxford: Pergamon Press.
- Horstmann, M. & Meyer, G. (1965). *Messung der Elektronenbeugungsintensitäten polykristalliner Aluminiumschichten bei tiefer Temperatur und Vergleich mit der dynamischen Theorie.* *Z. Phys.* **182**, 380–397.
- Hovmöller, S., Sjögren, A., Farrants, G., Sundberg, M. & Marinder, B. O. (1984). *Accurate atomic positions from electron microscopy.* *Nature (London)*, **311**, 238–241.
- Hu, H. H., Li, F. H. & Fan, H. F. (1992). *Crystal structure determination of  $\text{K}_2\text{O} \cdot 7\text{Nb}_2\text{O}_5$  by combining high resolution electron microscopy and electron diffraction.* *Ultramicroscopy*, **41**, 387–397.
- Hurley, A. C. & Moodie, A. F. (1980). *The inversion of three-beam intensities for scalar scattering by a general centrosymmetric crystal.* *Acta Cryst.* **A36**, 737–738.
- International Tables for Crystallography* (1995). Vol. A. *Space-group symmetry*, edited by Th. Hahn, 4th ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (1999). Vol. C. *Mathematical, physical and chemical tables*, edited by A. J. C. Wilson and E. Prince, 2nd ed. Dordrecht: Kluwer Academic Publishers.
- International Tables for X-ray Crystallography* (1952). Vol. I. *Symmetry groups*. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- Ishizuka, K., Miyazaki, M. & Uyeda, N. (1982). *Improvement of electron microscope images by the direct phasing method.* *Acta Cryst.* **A38**, 408–413.
- Ishizuka, K. & Taftø, J. (1982). *Kinematically allowed reflections caused by scattering via HOLZ.* *Proc. Electron Microsc. Soc. Am.* pp. 688–689.
- Jap, B. K. & Glaeser, R. M. (1980). *The scattering of high-energy electrons. II. Quantitative validity domains of the single-scattering approximations for organic crystals.* *Acta Cryst.* **A36**, 57–67.
- Jap, B. K., Walian, P. J. & Gehring, K. (1991). *Structural architecture of an outer membrane channel as determined by electron crystallography.* *Nature (London)*, **350**, 167–170.
- Johnson, A. W. S. (1972). *Stacking faults in graphite.* *Acta Cryst.* **A28**, 89–93.
- Johnson, A. W. S. & Preston, A. R. (1994). *Some notes on the selection of structural chirality by CBED.* *Ultramicroscopy*, **55**, 348–355.
- 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.
- Kam, Z. (1980). *Three-dimensional reconstruction of aperiodic objects.* *J. Theor. Biol.* **82**, 15–32.
- Kambe, K. (1982). *Visualization of Bloch waves of high energy electrons in high resolution electron microscopy.* *Ultramicroscopy*, **10**, 223–228.
- Karle, J. & Hauptman, H. (1956). *A theory of phase determination for the four types of non-centrosymmetric space groups  $1P22$ ,  $2P22$ ,  $3P12$ ,  $3P22$ .* *Acta Cryst.* **9**, 635–651.
- Kirkland, E. J., Siegel, B. M., Uyeda, N. & Fujiyoshi, Y. (1980). *Digital reconstruction of bright field phase contrast images from high resolution electron micrographs.* *Ultramicroscopy*, **5**, 479–503.
- Kiselev, N. A., Lerner, F. Ya. & Livanova, N. B. (1971). *Electron microscopy of muscle phosphorylase B.* *J. Mol. Biol.* **62**, 537–549.
- Klug, A. & Berger, J. E. (1964). *An optical method for the analysis of periodicities in electron micrographs and some observations on the mechanism of negative staining.* *J. Mol. Biol.* **10**, 565–569.



## REFERENCES

## 2.5 (cont.)

- Klug, A. & DeRosier, D. J. (1966). *Optical filtering of electron micrographs: reconstruction of one-sided images*. *Nature (London)*, **212**, 29–32.
- Kossel, W. & Möllenstedt, G. (1938). *Electron interference in a convergent beam*. *Nature (London)*, **26**, 660.
- Kosykh, V. P., Pustovskikh, A. I., Kirichuk, V. S., Kühne, T., Orlova, E. V., Tsuprun, V. L. & Kiselev, N. A. (1983). *Use of digital storage methods to recover images of monocrystalline layers of virus particles*. *Sov. Phys. Crystallogr.* **28**, 637–643.
- Kühlbrandt, W., Wang, D. N. & Fujiyoshi, Y. (1994). *Atomic model of plant light-harvesting complex by electron crystallography*. *Nature (London)*, **367**, 614–621.
- Kuwabara, S. (1978). *Nearly aberration-free crystal images in high voltage electron microscopy*. *J. Electron Microsc.* **27**, 161–169.
- Langer, R., Frank, J., Feltynowski, A. & Hoppe, W. (1970). *Anwendung des Bilddifferenzverfahrens auf die Untersuchung von Strukturänderungen dünner Kohlefolien bei Elektronenbestrahlung*. *Ber. Bunsenges Phys. Chem.* **74**(11), 1120–1126.
- Langs, D. A. & DeTitta, G. T. (1975). *A flexible and rapid phase determination and refinement procedure*. *Acta Cryst.* **A31**, S16.
- Laue, M. von (1935). *Die Fluoreszenzrontgenstrahlung von Einkristallen*. *Ann. Phys. (Leipzig)*, **23**, 703–726.
- Li, D. X. & Hovmöller, S. (1988). *The crystal structure of  $\text{Na}_3\text{Nb}_{12}\text{O}_{31}\text{F}$  determined by HREM and image processing*. *J. Solid State Chem.* **73**, 5–10.
- Li, F. H. (1991). *Crystal structures from high-resolution electron microscopy*. In *Electron crystallography of organic molecules*, edited by J. R. Fryer & D. L. Dorset, pp. 153–167. Dordrecht: Kluwer Academic Publishers.
- Liebman, G. (1955). *A unified representation of magnetic electron lens properties*. *Proc. Phys. Soc. London Sect. B*, **68**, 737–745.
- Liu, Y.-W., Fan, H.-F. & Zheng, C.-D. (1988). *Image processing in high-resolution electron microscopy using the direct method. III. Structure-factor extrapolation*. *Acta Cryst.* **A44**, 61–63.
- Lobachev, A. N. & Vainshtein, B. K. (1961). *An electron diffraction study of urea*. *Sov. Phys. Crystallogr.* **6**, 313–317.
- Lynch, D. F. & Moodie, A. F. (1972). *Numerical evaluation of low energy electron diffraction intensity. I. The perfect crystal with no upper layer lines and no absorption*. *Surf. Sci.* **32**, 422–438.
- Lynch, D. F., Moodie, A. F. & O'Keefe, M. A. (1975). *n-Beam lattice images. V. The use of the charge-density approximation in the interpretation of lattice images*. *Acta Cryst.* **A31**, 300–307.
- McLachlan, D. (1958). *Crystal structure and information theory*. *Proc. Natl Acad. Sci. USA*, **44**, 948–956.
- Mansfield, J. (1984). *Convergent beam electron diffraction of alloy phases by the Bristol Group under the direction of John Steeds*. Bristol: Adam Hilger.
- Markham, R., Frey, S. & Hills, G. J. (1963). *Methods for the enhancement of image detail and accentuation of structure in electron microscopy*. *Virology*, **20**, 88–102.
- Matsuda, T., Tomomura, A. & Komada, T. (1978). *Observation of lattice images with a field emission electron microscope*. *Jpn. J. Appl. Phys.* **17**, 2073–2074.
- Mermin, N. D. (1992). *The space groups of icosahedral quasicrystals and cubic, orthorhombic, monoclinic and triclinic crystals*. *Rev. Mod. Phys.* **64**, 3–49.
- Mersereau, R. M. & Oppenheim, A. V. (1974). *Digital reconstruction of multi-dimensional signals from their projections*. *Proc. IEEE*, **62**(10), 1319–1338.
- Miyake, S. & Uyeda, R. (1950). *An exception to Friedel's law in electron diffraction*. *Acta Cryst.* **3**, 314.
- Mo, Y. D., Cheng, T. Z., Fan, H. F., Li, J. Q., Sha, B. D., Zheng, C. D., Li, F. H. & Zhao, Z. X. (1992). *Structural features of the incommensurate modulation in the Pb-doped Bi-2223 high- $T_c$  phase by defect method electron diffraction analysis*. *Supercond. Sci. Technol.* **5**, 69–72.
- Moodie, A. F. (1965). *Some structural implications of n-beam interactions*. International Conference on Electron Diffraction and Crystal Defects, Melbourne, Australia, paper ID-1.
- Moodie, A. F. (1972). *Reciprocity and shape function in multiple scattering diagrams*. *Z. Naturforsch. Teil A*, **27**, 437–440.
- Moodie, A. F. & Whitfield, H. J. (1984). *CBED and HREM in the electron microscope*. *Ultramicroscopy*, **13**, 265–278.
- Moss, B. & Dorset, D. L. (1982). *Effect of crystal bending on direct phasing of electron diffraction data from cytosine*. *Acta Cryst.* **A38**, 207–211.
- Ogawa, T., Moriguchi, S., Isoda, S. & Kobayashi, T. (1994). *Application of an imaging plate to electron crystallography at atomic resolution*. *Polymer*, **35**, 1132–1136.
- Orlov, S. S. (1975). *Theory of three-dimensional reconstruction. II. The recovery operator*. *Sov. Phys. Crystallogr.* **20**, 429–433.
- Ottensmeyer, F. P., Andrews, J. W., Basett-Jones, D. P., Chan, A. S. & Hewitt, J. (1977). *Signal to noise enhancement in dark field electron micrographs of vasopressin: filtering of arrays of images in reciprocal space*. *J. Microsc.* **109**, 256–268.
- Pan, M. & Crozier, P. A. (1993). *Quantitative imaging and diffraction of zeolites using a slow-scan CCD camera*. *Ultramicroscopy*, **52**, 487–498.
- Pérez, S. & Chanzy, H. (1989). *Electron crystallography of linear polysaccharides*. *J. Electron Microsc. Tech.* **11**, 280–285.
- Picture Processing and Digital Filtering* (1975). Edited by T. S. Huang. Berlin: Springer-Verlag.
- Pinsker, Z. G. (1953). *Electron diffraction*. London: Butterworth.
- Pinsker, Z. G., Zvyagin, B. B. & Imamov, R. M. (1981). *Principal results of electron-diffraction structural investigations*. *Sov. Phys. Crystallogr.* **26**, 669–674.
- Pogany, A. P. & Turner, P. S. (1968). *Reciprocity in electron diffraction and microscopy*. *Acta Cryst.* **A24**, 103–109.
- Pond, R. C. & Vlachavas, D. S. (1983). *Bicrystallography*. *Proc. R. Soc. London Ser. A*, **386**, 95–143.
- Portier, R. & Gratias, D. (1981). *Diffraction symmetries for elastic scattering*. In *Electron microscopy and analysis*. *Inst. Phys. Conf. Ser. No. 61*, pp. 275–278. Bristol, London: Institute of Physics.
- Radermacher, M., McEwen, B. & Frank, J. (1987). *Three-dimensional reconstruction of asymmetrical object in standard and high voltage electron microscopy*. *Proc. Microscop. Soc. Canada, XII Annual Meet.*, pp. 4–5.
- Radi, G. (1970). *Complex lattice potentials in electron diffraction calculated for a number of crystals*. *Acta Cryst.* **A26**, 41–56.
- Radon, J. (1917). *Über die Bestimmung von Funktionen durch ihre Integralwerte längs gewisser Mannigfaltigkeiten. (On the determination of functions from their integrals along certain manifolds)*. *Ber. Verh. Saechs. Akad. Wiss. Leipzig Math. Phys. Kl.* **69**, 262–277.
- Ramachandran, G. N. & Lakshminarayanan, A. V. (1971). *Three-dimensional reconstruction from radiographs and electron micrographs: application of convolutions instead of Fourier transforms*. *Proc. Natl Acad. Sci. USA*, **68**(9), 2236–2240.
- Revol, J. F. (1991). *Electron crystallography of radiation-sensitive polymer crystals*. In *Electron crystallography of organic molecules*, edited by J. R. Fryer & D. L. Dorset, pp. 169–187. Dordrecht: Kluwer Academic Publishers.
- Revol, J. F. & Manley, R. St. J. (1986). *Lattice imaging in polyethylene single crystals*. *J. Mater. Sci. Lett.* **5**, 249–251.
- Rez, P. (1978). In *Electron diffraction 1927–1977*, edited by P. J. Dobson, J. B. Pendry & C. J. Humphreys, pp. 61–67. *Inst. Phys. Conf. Ser. No. 41*. Bristol, London: Institute of Physics.
- Rozenfeld, A. (1969). *Picture processing by computer*. New York: Academic Press.
- Sayre, D. (1952). *The squaring method: a new method for phase determination*. *Acta Cryst.* **5**, 60–65.
- Sayre, D. (1980). *Phase extension and refinement using convolutional and related equation systems*. In *Theory and practice of direct methods in crystallography*, edited by M. F. C. Ladd & R. A. Palmer, pp. 271–286. NY: Plenum Press.
- Scaringe, R. P. (1992). *Crystallography in two dimensions: comparison of theory and experiment for molecular layers*. *Trans. Am. Crystallogr. Assoc.* **28**, 11–23.
- Schapink, F. W., Forgany, S. K. E. & Buxton, B. F. (1983). *The symmetry of convergent-beam electron diffraction patterns from bicrystals*. *Acta Cryst.* **A39**, 805–813.

## 2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

### 2.5 (cont.)

- Scherzer, O. (1949). *The theoretical resolution limit of the electron microscope*. *J. Appl. Phys.* **20**, 20–29.
- Schiske, P. (1968). *Zur Frage der Bildrekonstruktion durch Fokusreihen*. 1 *Y Eur. Reg. Conf. Electron Microsc. Rome*, **1**, 145–146.
- Schwartzman, A., Goodman, P. & Johnson, A. W. S. (1996). IUCr XVII Congress and General Assembly, Seattle, Washington, USA, August 8–16, Collected Abstracts, p. C-54, Abstract PS02.03.18.
- Sha, B.-D., Fan, H.-F. & Li, F.-H. (1993). *Correction for the dynamical electron diffraction effect in crystal structure analysis*. *Acta Cryst.* **A49**, 877–880.
- Shechtman, D., Blech, I., Gratias, D. & Cahn, J. W. (1984). *Metallic phase with long-range orientational order and no translational symmetry*. *Phys. Rev. Lett.* **53**, 1951–1953.
- Shoemaker, V. & Glauber, R. (1952). *The Born approximation in electron diffraction*. *Nature (London)*, **170**, 290–291.
- Spence, J. C. H., O'Keefe, M. A. & Kolar, H. (1977). *Image interpretation in crystalline germanium*. *Optik (Stuttgart)*, **49**, 307–323.
- Spence, J. C. H. & Zuo, J. M. (1992). *Electron microdiffraction*. New York: Plenum Press.
- Steeds, J. W. (1979). *Convergent beam electron diffraction*. In *Introduction to analytical electron microscopy*, edited by J. J. Hren, J. I. Goldstein & D. C. Joy, pp. 387–422. New York: Plenum.
- Steeds, J. W. (1983). *Developments in convergent beam electron diffraction*. Report to the Commission on Electron Diffraction of the International Union of Crystallography.
- Steeds, J. W. & Evans, N. S. (1980). *Practical examples of point and space group determination in convergent beam diffraction*. *Proc. Electron Microsc. Soc. Am.* pp. 188–191.
- Steeds, J. W., Rackham, G. M. & Shannon, M. D. (1978). *On the observation of dynamically forbidden lines in two and three dimensional electron diffraction*. In *Electron diffraction 1927–1977. Inst. Phys. Conf. Ser. No. 41*, pp. 135–139.
- Steeds, J. W. & Vincent, R. (1983). *Use of high symmetry zone axes in electron diffraction in determining crystal point and space groups*. *J. Appl. Cryst.* **16**, 317–324.
- Steinkilberg, M. & Schramm, H. J. (1980). *Eine verbesserte Drehkorrelations Methode für die Strukturbestimmung biologischer Macromoleküle durch Mittelung elektronenmikroskopischer Bilder*. *Hoppe-Seyler's Z. Physiol. Chem.* **361**, 1363–1369.
- Stereochemical Applications of Gas-Phase Electron Diffraction* (1988). Part A, edited by I. Hargittai & M. Hargittai. New York: VCH.
- Tanaka, M. (1994). *Convergent-beam electron diffraction*. *Acta Cryst.* **A50**, 261–286.
- Tanaka, M., Saito, P., Ueno, K. & Harada, Y. (1980). *Large angle convergent-beam electron diffraction*. *J. Electron. Microsc.* **29**, 408–412.
- Tanaka, M., Sekii, H. & Nagasawa, T. (1983). *Space group determination by dynamic extinction in convergent beam electron diffraction*. *Acta Cryst.* **A39**, 825–837.
- Tanaka, M. & Terauchi, M. (1985). *Convergent-beam electron diffraction*. Tokyo: JEOL Ltd.
- Tanaka, M., Terauchi, M. & Tsuda, K. (1994). *Convergent-beam electron diffraction III*. Tokyo: JEOL–Maruzen.
- Thon, F. (1966). *On the defocusing dependence of phase contrast in electron microscopical images*. *Z. Naturforsch. Teil A*, **21**, 476–478.
- Tivol, W. F., Dorset, D. L., McCourt, M. P. & Turner, J. N. (1993). *Voltage-dependent effect on dynamical scattering and the electron diffraction structure analysis of organic crystals: copper perchlorophthalocyanine*. *Microsc. Soc. Am. Bull.* **23**, 91–98.
- Tournaire, M. (1962). *Recent developments of the matrical and semi-reciprocal formulation in the field of dynamical theory*. *J. Phys. Soc. Jpn*, **17**, Suppl. B11, 98–100.
- Tsipursky, S. I. & Drits, V. A. (1977). *Efficiency of electronometric intensity registration at electron diffraction structural studies*. *Izv. Akad. Nauk SSSR Ser. Fiz.* **41**, 2263–2271. (In Russian.)
- Tsuji, M. (1989). *Electron microscopy*. In *Comprehensive polymer science*, Vol. 1. *Polymer characterization*, edited by C. Booth & C. Price, pp. 785–840. Oxford: Pergamon Press.
- Turner, P. S. & Cowley, J. M. (1969). *The effects of n-beam dynamical diffraction on electron diffraction intensities from polycrystalline materials*. *Acta Cryst.* **A25**, 475–481.
- Unwin, P. N. T. & Henderson, R. (1975). *Molecular structure determination by electron microscopy of unstained crystalline specimens*. *J. Mol. Biol.* **94**, 425–440.
- Uyeda, N., Kobayashi, T., Ishizuka, K. & Fujiyoshi, Y. (1978–1979). *High voltage electron microscopy for image discrimination of constituent atoms in crystals and molecules*. *Chem. Scr.* **14**, 47–61.
- Vainshtein, B. K. (1952). *Dependence of electron scattering on the atomic number*. *Dokl. Akad. Nauk SSSR*, **85**, 1239–1242. (In Russian.)
- Vainshtein, B. K. (1954). *On the studies of crystal lattice potential by electron diffraction*. *Tr. Inst. Krist. Akad. Nauk SSSR*, **9**, 259–276. (In Russian.)
- Vainshtein, B. K. (1955). *Elektronograficheskoe issledovanie diketopiperazina*. *Zh. Fiz. Khim.* **29**, 327–344.
- Vainshtein, B. K. (1956). *Structure analysis by electron diffraction*. Moscow: Akad. Sci. USSR. [English edition (1964): Oxford: Pergamon Press.]
- Vainshtein, B. K. (1964). *Structure analysis by electron diffraction*. Oxford: Pergamon Press.
- Vainshtein, B. K. (1971a). *The synthesis of projecting functions*. *Sov. Phys. Dokl.* **16**, 66–69.
- Vainshtein, B. K. (1971b). *Finding the structure of objects from projections*. *Sov. Phys. Crystallogr.* **15**, 781–787.
- Vainshtein, B. K. (1978). *Electron microscopical analysis of the three-dimensional structure of biological macromolecules*. In *Advances in optical and electron microscopy*, Vol. 7, edited by V. E. Cosslett & R. Barer, pp. 281–377. London: Academic Press.
- Vainshtein, B. K., Barynin, V. V. & Gurskaya, G. V. (1968). *The hexagonal crystalline structure of catalase and its molecular structure*. *Sov. Phys. Dokl.* **13**, 838–841.
- Vainshtein, B. K., D'yakon, I. A. & Ablov, A. V. (1971). *Electron diffraction determination of the structure of copper DL-alaninate*. *Sov. Phys. Dokl.* **15**, 645–647.
- Vainshtein, B. K. & Goncharov, A. B. (1986a). *Determination of the spatial orientation of arbitrarily arranged identical particles of unknown structure from their projections*. *Sov. Phys. Dokl.* **287**, 278–283; (1986b). Proceedings of the 11th International Congress on Electron Microscopy, Kyoto, Vol. 1, pp. 459–460.
- Vainshtein, B. K. & Klechkovskaya, V. V. (1993). *Electron diffraction by Langmuir–Blodgett films*. *Proc. R. Soc. London Ser. A*, **442**, 73–84.
- Vainshtein, B. K. & Orlov, S. S. (1972). *Theory of the recovery of functions from their projections*. *Sov. Phys. Crystallogr.* **17**, 213–216.
- Vainshtein, B. K. & Orlov, S. S. (1974). *General theory of direct 3D reconstruction*. Proceedings of International Workshop, Brookhaven National Laboratory, pp. 158–164.
- Van Heel, M. (1984). *Multivariate statistical classification of noisy images (randomly oriented biological macromolecules)*. *Ultra-microscopy*, **13**, 165–184.
- Vilkov, L. V., Mastryukov, V. S. & Sadova, N. I. (1978). *Determination of geometrical structure of free molecules*. Leningrad: Khimiya. (In Russian.)
- Vincent, R. & Exelby, D. R. (1991). *Structure of metastable Al–Ge phases determined from HOLZ Patterson transforms*. *Philos. Mag. Lett.* **63**, 31–38.
- Vincent, R. & Exelby, D. R. (1993). *Structure of a metastable Al–Ge phase determined from large angle CBED patterns*. *Philos. Mag. B*, **68**, 513–528.
- Vincent, R. & Midgley, P. A. (1994). *Double conical beam rocking system for measurement of integrated electron diffraction intensities*. *Ultramicroscopy*, **53**, 271–282.

## REFERENCES

## 2.5 (cont.)

- Voronova, A. A. & Vainshtein, B. K. (1958). *An electron diffraction study of  $\text{CuCl}_2 \cdot 3\text{Cu}(\text{OH})_2$* . *Sov. Phys. Crystallogr.* **3**, 445–451.
- Watanabe, D., Uyeda, R. & Kogiso, M. (1968). *An apparent variation of structure factors for electrons with accelerating voltage. An observation through Kikuchi patterns*. *Acta Cryst.* **A24**, 249–250.
- Wenk, H.-R., Downing, K. H., Ho, M.-S. & O'Keefe, M. A. (1992). *3D structure determination from electron-microscope images: electron crystallography of staurolite*. *Acta Cryst.* **A48**, 700–716.
- Wilson, A. J. C. (1949). *The probability distribution of X-ray intensities*. *Acta Cryst.* **2**, 318–321.
- Withers, R. L., Schmid, S. & Thompson, J. G. (1993). *A composite modulated structure approach to the lanthanide oxide fluoride, uranium nitride fluoride and zirconium nitride fluoride solid-solution fields*. *Acta Cryst.* **B49**, 941–951.
- Wolff, P. M. de, Janssen, T. & Janner, A. (1981). *The superspace groups for incommensurate crystal structures with a one-dimensional modulation*. *Acta Cryst.* **A37**, 625–636.
- Xiang, S.-B., Fan, H.-F., Wu, X.-J., Li, F.-H. & Pan, Q. (1990). *Direct methods in superspace. II. The first application to an unknown incommensurate modulated structure*. *Acta Cryst.* **A46**, 929–934.
- Yao, J.-X. (1981). *On the application of phase relationships to complex structures. XVIII. RANTAN – random MULTAN*. *Acta Cryst.* **A37**, 642–644.
- Zemlin, F., Reuber, E., Beckmann, E., Zeitler, E. & Dorset, D. L. (1985). *Molecular resolution electron micrographs of monolamellar paraffin crystal*. *Science*, **229**, 461–462.
- Zhukhlistov, A. P., Avilov, A. S., Ferraris, G., Zvyagin, B. B. & Plotnikov, V. P. (1997). *Statistical distribution of hydrogen over three positions in the brucite  $\text{Mg}(\text{OH})_2$  structure from electron diffractometry data*. *Crystallogr. Rep.* **42**, 774–777.
- Zhukhlistov, A. P. & Zvyagin, B. B. (1998). *Crystal structure of lizardite 1T from electron diffractometry data*. *Crystallogr. Rep.* **43**, 950–955.
- Zuo, J. M., Gjønnes, K. & Spence, J. C. H. (1989). *A FORTRAN source listing for simulating three-dimensional CBED patterns with absorption by the Bloch wave method*. *J. Electron Microsc. Tech.* **12**, 29–55.
- Zvyagin, B. B. (1967). *Electron-diffraction analysis of clay mineral structures*. New York: Plenum.
- Zvyagin, B. B., Vrublevskaya, Z. V., Zhukhlistov, A. P., Sidorenko, S. V., Soboleva, A. F. & Fedotov, A. F. (1979). *High-voltage electron diffraction investigations of layered minerals*. Moscow: Nauka. (In Russian).
- Zvyagin, B. B., Zhukhlistov, A. P. & Plotnikov, A. P. (1996). *Development of the electron diffractometry of minerals. Structural studies of crystals*. (Coll. Works 75th Anniversary Acad. B. K. Vainshtein.) *Nauka-Physmathlit*, pp. 225–234. (In Russian.)