

4. DIFFUSE SCATTERING AND RELATED TOPICS

4.5

- Alexeev, D. G., Lipanov, A. A. & Skuratovskii, I. Y. (1992). *Patterson methods in fibre diffraction*. *Int. J. Biol. Macromol.* **14**, 139–144.
- Arnott, S. (1980). *Twenty years hard labor as a fibre diffractionist*. In *Fibre diffraction methods*, ACS Symposium Series, Vol. 141, edited by A. D. French & K. H. Gardner, pp. 1–30. Washington DC: American Chemical Society.
- Arnott, S., Chandrasekaran, R., Millane, R. P. & Park, H. (1986). *DNA–RNA hybrid secondary structures*. *J. Mol. Biol.* **188**, 631–640.
- Arnott, S. & Mitra, A. K. (1984). *X-ray diffraction analyses of glycosaminoglycans*. In *Molecular biophysics of the extracellular matrix*, edited by S. Arnott, D. A. Rees & E. R. Morris, pp. 41–67. Clifton: Humana Press.
- Arnott, S., Wilkins, M. H. F., Fuller, W. & Langridge, R. (1967). *Molecular and crystal structures of double-helical RNA III. An 11-fold molecular model and comparison of the agreement between the observed and calculated three-dimensional diffraction data for 10- and 11-fold models*. *J. Mol. Biol.* **27**, 535–548.
- Arnott, S. & Wonacott, A. J. (1966). *The refinement of the crystal and molecular structures of polymers using X-ray data and stereochemical constraints*. *Polymer*, **7**, 157–166.
- Atkins, E. D. T. (1989). *Crystal structure by X-ray diffraction*. In *Comprehensive polymer science*, Vol. 1. *Polymer characterization*, edited by G. A. Allen, pp. 613–650. Oxford: Pergamon Press.
- Barham, P. J. (1993). *Crystallization and morphology of semicrystalline polymers*. In *Materials science and technology. A comprehensive treatment*, Vol. 12. *Structure and properties of polymers*, edited by E. L. Thomas, pp. 153–212. Weinheim: VCH.
- Baskaran, S. & Millane, R. P. (1999a). *Bayesian image reconstruction from partial image and aliased spectral intensity data*. *IEEE Trans. Image Process.* **8**, 1420–1434.
- Baskaran, S. & Millane, R. P. (1999b). *Model bias in Bayesian image reconstruction from X-ray fiber diffraction data*. *J. Opt. Soc. Am. A*, **16**, 236–245.
- Biswas, A. & Blackwell, J. (1988a). *Three-dimensional structure of main-chain liquid-crystalline copolymers. 1. Cylindrically averaged intensity transforms of single chains*. *Macromolecules*, **21**, 3146–3151.
- Biswas, A. & Blackwell, J. (1988b). *Three-dimensional structure of main-chain liquid-crystalline copolymers. 2. Interchain interference effects*. *Macromolecules*, **21**, 3152–3158.
- Biswas, A. & Blackwell, J. (1988c). *Three-dimensional structure of main-chain liquid-crystalline copolymers. 3. Chain packing in the solid state*. *Macromolecules*, **21**, 3158–3164.
- Blackwell, J., Gutierrez, G. A. & Chivers, R. A. (1984). *Diffraction by aperiodic polymer chains: the structure of liquid crystalline copolyesters*. *Macromolecules*, **17**, 1219–1224.
- Blundell, D. J., Keller, A. & Kovacs, A. J. (1966). *A new self-nucleation phenomenon and its application to the growing of polymer crystals from solution*. *J. Polym. Sci. Polym. Lett. Ed.* **4**, 481–486.
- Brisse, F. (1989). *Electron diffraction of synthetic polymers: the model compound approach to polymer structure*. *J. Electron Microsc. Tech.* **11**, 272–279.
- Brisse, F., Remillard, B. & Chanzy, H. (1984). *Poly(1,4-trans-cyclohexanediyldimethylene succinate). A structural determination using X-ray and electron diffraction*. *Macromolecules*, **17**, 1980–1987.
- Brünger, A. T. (1992). *X-PLOR*. Version 3.1. New Haven: Yale University Press.
- Brünger, A. T. (1997). *Free R value: cross-validation in crystallography*. *Methods Enzymol.* **277**, 366–396.
- Cael, J. J., Winter, W. T. & Arnott, S. (1978). *Calcium chondroitin 4-sulfate: molecular conformation and organization of polysaccharide chains in a proteoglycan*. *J. Mol. Biol.* **125**, 21–42.
- Campbell Smith, P. J. & Arnott, S. (1978). *LALS: a linked-atom least-squares reciprocal-space refinement system incorporating stereochemical constraints to supplement sparse diffraction data*. *Acta Cryst. A* **34**, 3–11.
- Chandrasekaran, R. & Arnott, S. (1989). *The structures of DNA and RNA helices in oriented fibres*. In *Landolt–Bornstein numerical data and functional relationships in science and technology*, Vol. VII/1b, edited by W. Saenger, pp. 31–170. Berlin, Heidelberg: Springer-Verlag.
- Chandrasekaran, R., Radha, A. & Lee, E. J. (1994). *Structural roles of calcium ions and side chains in welan: an X-ray study*. *Carbohydr. Res.* **252**, 183–207.
- Chanzy, H., Perez, S., Miller, D. P., Paradossi, G. & Winter, W. T. (1987). *An electron diffraction study of mannan I. Crystal and molecular structure*. *Macromolecules*, **20**, 2407–2413.
- Chivers, R. A. & Blackwell, J. (1985). *Three-dimensional structure of copolymers of p-hydroxybenzoic acid and 2-hydroxy-6-naphthoic acid: a model for diffraction from a nematic structure*. *Polymer*, **26**, 997–1002.
- Clark, E. S. & Muus, I. T. (1962). *The relationship between Bragg reflections and disorder in crystalline polymers*. *Z. Kristallogr.* **117**, 108–118.
- 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. (1961). *Diffraction intensities from bent crystals*. *Acta Cryst.* **14**, 920–927.
- Cowley, J. M. (1981). *Diffraction physics. Second revised edition*. Amsterdam: North-Holland.
- Cowley, J. M. (1988). *Imaging [and] imaging theory*. In *High-resolution transmission electron microscopy and associated techniques*, edited by P. Busek, J. M. Cowley & L. Eyring, pp. 3–57. New York: Oxford University Press.
- 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**, 319–344.
- Daubeny, R. de P., Bunn, C. W. & Brown, C. J. (1954). *The crystal structure of polyethylene terephthalate*. *Proc. R. Soc. London Ser. A*, **226**, 531–542.
- Day, D. & Lando, J. B. (1980). *Structure determination of a poly(diacetylene) monolayer*. *Macromolecules*, **13**, 1483–1487.
- 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.
- Dorset, D. L. (1989). *Electron diffraction from crystalline polymers*. In *Comprehensive polymer science*, Vol. 1. *Polymer characterization*, edited by G. A. Allen, pp. 651–668. Oxford: Pergamon Press.
- Dorset, D. L. (1991a). *Is electron crystallography possible? The direct determination of organic crystal structures*. *Ultramicroscopy*, **38**, 23–40.
- Dorset, D. L. (1991b). *Electron diffraction structure analysis of polyethylene. A direct phase determination*. *Macromolecules*, **24**, 1175–1178.
- Dorset, D. L. (1991c). *Electron crystallography of linear polymers: direct structure analysis of poly(ϵ -caprolactone)*. *Proc. Natl Acad. Sci. USA*, **88**, 5499–5502.
- Dorset, D. L. (1992). *Electron crystallography of linear polymers: direct phase determination for zonal data sets*. *Macromolecules*, **25**, 4425–4430.
- Dorset, D. L. (1995a). *Comments on the validity of the direct phasing and Fourier methods in electron crystallography*. *Acta Cryst.* **A51**, 869–879.
- Dorset, D. L. (1995b). *Structural electron crystallography*. New York: Plenum.
- Dorset, D. L. (1995c). *Filling the cone – overcoming the goniometric tilt limit in electron crystallography by direct methods*. *Am. Cryst. Assoc. Abstr. Series 2*, **23**, p. 89.
- Dorset, D. L., Kopp, S., Fryer, J. R. & Tivol, W. T. (1995). *The Sayre equation in electron crystallography*. *Ultramicroscopy*, **57**, 59–89.
- 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.

REFERENCES

4.5 (cont.)

- 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.
- Doyle, P. A. & Turner, P. S. (1968). Relativistic Hartree–Fock X-ray and electron scattering factors. *Acta Cryst.* **A24**, 390–397.
- Drenth, J. (1994). *Principles of protein X-ray crystallography*. New York: Springer-Verlag.
- Finkenstadt, V. L. & Millane, R. P. (1998). Fiber diffraction patterns for general unit cells: the cylindrically projected reciprocal lattice. *Acta Cryst.* **A54**, 240–248.
- Forsyth, V. T., Mahendrasingam, A., Pigram, W. J., Greenall, R. J., Bellamy, K., Fuller, W. & Mason, S. A. (1989). Neutron fibre diffraction study of DNA hydration. *Int. J. Biol. Macromol.* **11**, 236–240.
- Franklin, R. E. (1955). Structure of tobacco mosaic virus. *Nature (London)*, **175**, 379–381.
- Franklin, R. E. & Gosling, R. G. (1953). The structure of sodium thymonucleate fibres. II. The cylindrically symmetrical Patterson function. *Acta Cryst.* **6**, 678–685.
- Franklin, R. E. & Holmes, K. C. (1958). Tobacco mosaic virus: application of the method of isomorphous replacement to the determination of the helical parameters and radial density distribution. *Acta Cryst.* **11**, 213–220.
- Franklin, R. E. & Klug, A. (1955). The splitting of layer lines in X-ray fibre diagrams of helical structures: application to tobacco mosaic virus. *Acta Cryst.* **8**, 777–780.
- Fraser, R. D. B. & MacRae, T. P. (1973). *Conformations in fibrous proteins*. New York: Academic Press.
- Fraser, R. D. B., MacRae, T. P., Miller, A. & Rowlands, R. J. (1976). Digital processing of fibre diffraction patterns. *J. Appl. Cryst.* **9**, 81–94.
- Fraser, R. D. B., Suzuki, E. & MacRae, T. P. (1984). Computer analysis of X-ray diffraction patterns. In *Structure of crystalline polymers*, edited by I. H. Hall, pp. 1–37. New York: Elsevier.
- French, A. D. & Gardner, K. H. (1980). Editors. *Fibre diffraction methods*. ACS Symposium Series, Vol. 141. Washington DC: American Chemical Society.
- Geil, P. H. (1963). *Polymer single crystals*. New York: John Wiley & Sons.
- Gilmore, C. J., Shankland, K. & Bricogne, G. (1993). Application of the maximum entropy method to powder diffraction and electron crystallography. *Proc. R. Soc. London Ser. A*, **442**, 97–111.
- Gonzalez, A., Nave, C. & Marvin, D. A. (1995). Pfl filamentous bacteriophage: refinement of a molecular model by simulated annealing using 3.3 Å resolution X-ray fiber diffraction data. *Acta Cryst.* **D51**, 792–804.
- Graaf, H. de (1989). On the calculation of small-angle diffraction patterns from distorted lattices. *Acta Cryst.* **A45**, 861–870.
- Grubb, D. T. (1993). Elastic properties of crystalline polymers. In *Materials science and technology. A comprehensive treatment*, Vol. 12. *Structure and properties of polymers*, edited by E. L. Thomas, pp. 301–356. Weinheim: VCH.
- Hall, I. H. (1984). Editor. *Structure of crystalline polymers*. New York: Elsevier.
- Hall, I. H., Neisser, J. Z. & Elder, M. (1987). A computer-based method of measuring the integrated intensities of the reflections on the X-ray diffraction photograph of an oriented crystalline polymer. *J. Appl. Cryst.* **20**, 246–255.
- Hamilton, W. C. (1965). Significance tests on the crystallographic R factor. *Acta Cryst.* **18**, 502–510.
- Hauptman, H. A. (1993). A minimal principle in X-ray crystallography: starting in a small way. *Proc. R. Soc. London Ser. A*, **442**, 3–12.
- Hendricks, S. & Teller, E. (1942). X-ray interference in partially ordered layer lattices. *J. Chem. Phys.* **10**, 147–167.
- Hirsch, P. B., Howie, A., Nicholson, P. B., Pashley, D. W. & Whelan, M. J. (1965). *Electron microscopy of thin crystals*. London: Butterworths.
- Hofmann, D., Schneider, A. I. & Blackwell, J. (1994). Molecular modelling of the structure of a wholly aromatic thermotropic copolyester. *Polymer*, **35**, 5603–5610.
- Holmes, K. C. & Barrington Leigh, J. (1974). The effect of disorientation on the intensity distribution of non-crystalline fibres. I. Theory. *Acta Cryst.* **A30**, 635–638.
- Holmes, K. C., Popp, D., Gebhard, W. & Kabsch, W. (1990). Atomic model of the actin filament. *Nature (London)*, **347**, 44–49.
- Holmes, K. C., Stubbs, G. J., Mandelkow, E. & Gallwitz, U. (1975). Structure of tobacco mosaic virus at 6.7 Å resolution. *Nature (London)*, **254**, 192–196.
- Hosemann, R. & Bagchi, S. N. (1962). *Direct analysis of diffraction by matter*. Amsterdam: North-Holland.
- Hu, H. & Dorset, D. L. (1989). Three-dimensional electron diffraction structure analysis of polyethylene. *Acta Cryst.* **B45**, 283–290.
- Hu, H. & Dorset, D. L. (1990). Crystal structure of poly(ϵ -caprolactone). *Macromolecules*, **23**, 4604–4607.
- Hudson, L., Harford, J. J., Denny, R. C. & Squire, J. M. (1997). Myosin head configuration in relaxed fish muscle: resting state myosin heads must swing axially by up to 150 Å or turn upside down to reach rigor. *J. Mol. Biol.* **273**, 440–455.
- Iannelli, P. (1994). FWR: a computer program for refining the molecular structure in the crystalline phase of polymers based on the analysis of the whole X-ray fibre diffraction patterns. *J. Appl. Cryst.* **27**, 1055–1060.
- Isoda, S., Tsuji, M., Ohara, M., Kawaguchi, A. & Katayama, K. (1983a). Structural analysis of β -form poly(p-xylene) starting from a high-resolution image. *Polymer*, **24**, 1155–1161.
- Isoda, S., Tsuji, M., Ohara, M., Kawaguchi, A. & Katayama, K. (1983b). Direct observation of dislocations in polymer single crystals. *Makromol. Chem. Rapid Commun.* **4**, 141–144.
- Ivanova, M. I. & Makowski, L. (1998). Iterative low-pass filtering for estimation of the background in fiber diffraction patterns. *Acta Cryst.* **A54**, 626–631.
- Klug, A., Crick, F. H. C. & Wyckoff, H. W. (1958). Diffraction from helical structures. *Acta Cryst.* **11**, 199–213.
- Kopp, S., Wittmann, J. C. & Lotz, B. (1994). Epitaxial crystallization and crystalline polymorphism of poly(1-butene): form (III) and (II). *Polymer*, **35**, 908–915.
- Lipson, H. & Cochran, W. (1966). *The determination of crystal structures*, p. 381. Ithaca: Cornell University Press.
- Liu, J. & Geil, P. H. (1993). Morphological observations of nascent poly(p-oxabenzate). *Polymer*, **34**, 1366–1374.
- Liu, J., Yuan, B.-L., Geil, P. H. & Dorset, D. L. (1997). Chain conformation and molecular packing in poly(p-oxbenzoate) single crystals at ambient temperature. *Polymer*, **38**, 6031–6047.
- Lobert, S., Heil, P. D., Namba, K. & Stubbs, G. (1987). Preliminary X-ray fibre diffraction studies of cucumber green mottle mosaic virus, watermelon strain. *J. Mol. Biol.* **196**, 935–938.
- Lobert, S. & Stubbs, G. (1990). Fibre diffraction analysis of cucumber green mottle mosaic virus using limited numbers of heavy-atom derivatives. *Acta Cryst.* **A46**, 993–997.
- Lorenz, M. & Holmes, K. C. (1993). Computer processing and analysis of X-ray fibre diffraction data. *J. Appl. Cryst.* **26**, 82–91.
- Lorenz, M., Popp, D. & Holmes, K. C. (1993). Refinement of the F-actin model against X-ray fibre diffraction data by the use of a directed mutation algorithm. *J. Mol. Biol.* **234**, 826–836.
- Lotz, B. & Wittmann, J. C. (1993). Structure of polymer single crystals. In *Materials science and technology. A comprehensive treatment*, Vol. 12. *Structure and properties of polymers*, edited by E. L. Thomas, pp. 79–154. Weinheim: VCH.
- MacGillivray, C. H. & Bruins, E. M. (1948). On the Patterson transforms of fibre diagrams. *Acta Cryst.* **1**, 156–158.
- Makowski, L. (1978). Processing of X-ray diffraction data from partially oriented specimens. *J. Appl. Cryst.* **11**, 273–283.
- Makowski, L. (1982). The use of continuous diffraction data as a phase constraint. II. Application to fibre diffraction data. *J. Appl. Cryst.* **15**, 546–557.

4. DIFFUSE SCATTERING AND RELATED TOPICS

4.5 (cont.)

- Makowski, L., Caspar, D. L. D. & Marvin, D. A. (1980). *Filamentous bacteriophage Pfl structure determined at 7 Å resolution by refinement of models for the α -helical subunit*. *J. Mol. Biol.* **140**, 149–181.
- Mandelkern, L. (1989). *Crystallization and melting*. In *Comprehensive polymer science*, Vol. 2. *Polymer properties*, edited by C. Booth & C. Price, pp. 363–414. Oxford: Pergamon Press.
- Mandelkowitz, E. & Holmes, K. C. (1974). *The positions of the N-terminus and residue 68 in tobacco mosaic virus*. *J. Mol. Biol.* **87**, 265–273.
- Mandelkowitz, E., Stubbs, G. & Warren, S. (1981). *Structures of the helical aggregates of tobacco mosaic virus protein*. *J. Mol. Biol.* **152**, 375–386.
- Marvin, D. A., Bryan, R. K. & Nave, C. (1987). *Pfl ino virus. Electron density distribution calculated by a maximum entropy algorithm from native fiber diffraction data to 3 Å resolution and single isomorphous replacement data to 5 Å resolution*. *J. Mol. Biol.* **193**, 315–343.
- Mauritz, K. A., Baer, E. & Hopfinger, A. J. (1978). *The epitaxial crystallization of macromolecules*. *J. Polym. Sci. Macromol. Rev.* **13**, 1–61.
- Mazeau, K., Winter, W. T. & Chanzy, H. (1994). *Molecular and crystal structure of a high-temperature polymorph of chitosan from electron diffraction data*. *Macromolecules*, **27**, 7606–7612.
- Millane, R. P. (1988). *X-ray fibre diffraction*. In *Crystallographic computing 4. Techniques and new technologies*, edited by N. W. Isaacs & M. R. Taylor, pp. 169–186. Oxford University Press.
- Millane, R. P. (1989a). *R factors in X-ray fibre diffraction. I. Largest likely R factors for N overlapping terms*. *Acta Cryst. A* **45**, 258–260.
- Millane, R. P. (1989b). *R factors in X-ray fibre diffraction. II. Largest likely R factors*. *Acta Cryst. A* **45**, 573–576.
- Millane, R. P. (1989c). *Relating reflection boundaries in X-ray fibre diffraction patterns to specimen morphology and their use for intensity measurement*. *J. Macromol. Sci. Phys.* **B28**, 149–166.
- Millane, R. P. (1990a). *Intensity distributions in fibre diffraction*. *Acta Cryst. A* **46**, 552–559.
- Millane, R. P. (1990b). *Phase retrieval in crystallography and optics*. *J. Opt. Soc. Am. A*, **7**, 394–411.
- Millane, R. P. (1990c). *Polysaccharide structures: X-ray fibre diffraction studies*. In *Computer modeling of carbohydrate molecules*. ACS Symposium Series No. 430, edited by A. D. French & J. W. Brady, pp. 315–331. Washington DC: American Chemical Society.
- Millane, R. P. (1990d). *R factors in X-ray fibre diffraction. III. Asymptotic approximations to largest likely R factors*. *Acta Cryst. A* **46**, 68–72.
- Millane, R. P. (1991). *An alternative approach to helical diffraction*. *Acta Cryst. A* **47**, 449–451.
- Millane, R. P. (1992a). *Largest likely R factors for normal distributions*. *Acta Cryst. A* **48**, 649–650.
- Millane, R. P. (1992b). *R factors in X-ray fibre diffraction. IV. Analytic expressions for largest likely R factors*. *Acta Cryst. A* **48**, 209–215.
- Millane, R. P. (1993). *Image reconstruction from cylindrically averaged diffraction intensities*. In *Digital image recovery and synthesis II*, Proc. SPIE, Vol. 2029, edited by P. S. Idell, pp. 137–143. Bellingham, WA: SPIE.
- Millane, R. P. & Arnott, S. (1985). *Background removal in X-ray fibre diffraction patterns*. *J. Appl. Cryst.* **18**, 419–423.
- Millane, R. P. & Arnott, S. (1986). *Digital processing of X-ray diffraction patterns from oriented fibres*. *J. Macromol. Sci. Phys.* **B24**, 193–227.
- Millane, R. P. & Baskaran, S. (1997). *Optimal difference Fourier synthesis in fibre diffraction*. *Fiber Diffr. Rev.* **6**, 14–18.
- Millane, R. P., Byler, M. A. & Arnott, S. (1985). *Implementing constrained least squares refinement of helical polymers on a vector pipeline machine*. In *Supercomputer applications*, edited by R. W. Numrich, pp. 137–143, New York: Plenum.
- Millane, R. P., Chandrasekaran, R., Arnott, S. & Dea, I. C. M. (1988). *The molecular structure of kappa-carrageenan and comparison with iota-carrageenan*. *Carbohydr. Res.* **182**, 1–17.
- Millane, R. P. & Stroud, W. J. (1991). *Effects of disorder on fibre diffraction patterns*. *Int. J. Biol. Macromol.* **13**, 202–208.
- Millane, R. P. & Stubbs, G. (1992). *The significance of R factors in fibre diffraction*. *Polym. Prepr.* **33**(1), 321–322.
- Miller, R., DeTitta, G. T., Jones, R., Langs, D. A., Weeks, C. M. & Hauptman, H. A. (1993). *On the application of the minimal principle to solve unknown structures*. *Science*, **259**, 1430–1433.
- Namba, K., Pattanayek, R. & Stubbs, G. J. (1989). *Visualization of protein–nucleic acid interactions in a virus. Refined structure of intact tobacco mosaic virus at 2.9 Å resolution by X-ray fibre diffraction*. *J. Mol. Biol.* **208**, 307–325.
- Namba, K. & Stubbs, G. (1985). *Solving the phase problem in fibre diffraction. Application to tobacco mosaic virus at 3.6 Å resolution*. *Acta Cryst. A* **41**, 252–262.
- Namba, K. & Stubbs, G. (1987a). *Difference Fourier syntheses in fibre diffraction*. *Acta Cryst. A* **43**, 533–539.
- Namba, K. & Stubbs, G. (1987b). *Isomorphous replacement in fibre diffraction using limited numbers of heavy-atom derivatives*. *Acta Cryst. A* **43**, 64–69.
- Namba, K., Wakabayashi, K. & Mitsui, T. (1980). *X-ray structure analysis of the thin filament of crab striated muscle in the rigor state*. *J. Mol. Biol.* **138**, 1–26.
- Namba, K., Yamashita, I. & Vonderviszt, F. (1989). *Structure of the core and central channel of bacterial flagella*. *Nature (London)*, **342**, 648–654.
- Nambudripad, R., Stark, W. & Makowski, L. (1991). *Neutron diffraction studies of the structure of filamentous bacteriophage Pfl*. *J. Mol. Biol.* **220**, 359–379.
- Park, H., Arnott, S., Chandrasekaran, R., Millane, R. P. & Campagnari, F. (1987). *Structure of the α -form of poly-(dA)-poly(dT) and related polynucleotide duplexes*. *J. Mol. Biol.* **197**, 513–523.
- Perez, S. & Chanzy, H. (1989). *Electron crystallography of linear polysaccharides*. *J. Electron Microsc. Tech.* **11**, 280–285.
- Rickert, S. E., Lando, J. B., Hopfinger, A. J. & Baer, E. (1979). *Epitaxial polymerization of (SN)_x I. Structure and morphology of single crystals on alkali halide substrates*. *Macromolecules*, **12**, 1053–1057.
- Rybnikar, F., Liu, J. & Geil, P. H. (1994). *Thin film melt-polymerized single crystals of poly(p-oxybenzoate)*. *Makromol. Chem. Phys.* **195**, 81–104.
- Sayre, D. (1952). *The squaring method: a new method for phase determination*. *Acta Cryst.* **5**, 60–65.
- Schneider, A. I., Blackwell, J., Pielartzik, H. & Karbach, A. (1991). *Structure analysis of copoly(ester carbonate)*. *Macromolecules*, **24**, 5676–5682.
- Shotton, M. W., Denny, R. C. & Forsyth, V. T. (1998). *CCP13 software development*. *Fiber Diffr. Rev.* **7**, 40–44.
- Sim, G. A. (1960). *A note on the heavy atom method*. *Acta Cryst.* **13**, 511–512.
- Squire, J. M., Al-Khayat, H. A. & Yagi, N. (1993). *Muscle thin-filament structure and regulation. Actin sub-domain movements and the tropomyosin shift modelled from low-angle X-ray diffraction*. *J. Chem. Soc. Faraday Trans.* **89**, 2717–2726.
- Squire, J., Cantino, M., Chew, M., Denny, R., Harford, J., Hudson, L. & Luther, P. (1998). *Myosin rod-packing schemes in vertebrate muscle thick filaments*. *J. Struct. Biol.* **122**, 128–138.
- Squire, J. M. & Vibert, P. J. (1987). *Editors. Fibrous protein structure*. London: Academic Press.
- Stanley, E. (1986). *'Peakiness' test functions*. *Acta Cryst. A* **42**, 297–299.
- Stark, W., Glucksman, M. J. & Makowski, L. (1988). *Conformation of the coat protein of filamentous bacteriophage Pfl determined by neutron diffraction from magnetically oriented gels of specifically deuterated virions*. *J. Mol. Biol.* **199**, 171–182.
- Storks, K. H. (1938). *An electron diffraction examination of some linear high polymers*. *J. Am. Chem. Soc.* **60**, 1753–1761.
- Stroud, W. J. & Millane, R. P. (1995a). *Analysis of disorder in biopolymer fibres*. *Acta Cryst. A* **51**, 790–800.

REFERENCES

4.5 (cont.)

- Stroud, W. J. & Millane, R. P. (1995b). *Diffraction by disordered polycrystalline fibres*. *Acta Cryst.* **A51**, 771–790.
- Stroud, W. J. & Millane, R. P. (1996a). *Cylindrically averaged diffraction by distorted lattices*. *Proc. R. Soc. London*, **452**, 151–173.
- Stroud, W. J. & Millane, R. P. (1996b). *Diffraction by polycrystalline fibres with correlated disorder*. *Acta Cryst.* **A52**, 812–829.
- Stubbs, G. (1987). *The Patterson function in fibre diffraction*. In *Patterson and Pattersons*, edited by J. P. Glusker, B. K. Patterson & M. Rossi, pp. 548–557. Oxford University Press.
- Stubbs, G. (1989). *The probability distributions of X-ray intensities in fibre diffraction: largest likely values for fibre diffraction R factors*. *Acta Cryst.* **A45**, 254–258.
- Stubbs, G. (1999). *Developments in fiber diffraction*. *Curr. Opin. Struct. Biol.* **9**, 615–619.
- Stubbs, G., Warren, S. & Holmes, K. (1977). *Structure of RNA and RNA binding site in tobacco mosaic virus from a 4 Å map calculated from X-ray fibre diagrams*. *Nature (London)*, **267**, 216–221.
- Stubbs, G. J. (1974). *The effect of disorientation on the intensity distribution of non-crystalline fibres. II. Applications*. *Acta Cryst.* **A30**, 639–645.
- Stubbs, G. J. & Diamond, R. (1975). *The phase problem for cylindrically averaged diffraction patterns. Solution by isomorphous replacement and application to tobacco mosaic virus*. *Acta Cryst.* **A31**, 709–718.
- Stubbs, G. J. & Makowski, L. (1982). *Coordinated use of isomorphous replacement and layer-line splitting in the phasing of fibre diffraction data*. *Acta Cryst.* **A38**, 417–425.
- Tadokoro, H. (1979). *Structure of crystalline polymers*. New York: Wiley.
- Tanaka, S. & Naya, S. (1969). *Theory of X-ray scattering by disordered polymer crystals*. *J. Phys. Soc. Jpn*, **26**, 982–993.
- Tatarinova, L. I. & Vainshtein, B. K. (1962). *Issledovanie poli- γ -metil-L-glutamata v α -forme metodom difraktsi elektronov. (Electron diffraction study of poly- γ -methyl-L-glutamate in the α -form.)* *Visokomol. Soed.* **4**, 261–269. (In Russian.)
- Tirion, M., ben Avraham, D., Lorenz, M. & Holmes, K. C. (1995). *Normal modes as refinement parameters for the F-actin model*. *Biophys. J.* **68**, 5–12.
- Tsujii, M. (1989). *Electron microscopy*. In *Comprehensive polymer science*, Vol. 1. *Polymer characterization*, edited by G. A. Allen, pp. 785–866. Oxford: Pergamon Press.
- Vainshtein, B. K. (1964). *Structure analysis by electron diffraction*. Oxford: Pergamon Press.
- Vainshtein, B. K. (1966). *Diffraction of X-rays by chain molecules*. Amsterdam: Elsevier.
- Vainshtein, B. K. & Tatarinova, L. I. (1967). *The β -form of poly- γ -methyl-L-glutamate*. *Sov. Phys. Crystallogr.* **11**, 494–498.
- Vibert, P. J. (1987). *Fibre diffraction methods*. In *Fibrous protein structure*, edited by J. M. Squire & P. J. Vibert, pp. 23–45. New York: Academic Press.
- Wang, H., Culver, J. N. & Stubbs, G. (1997). *Structure of ribgrass mosaic virus at 2.9 Å resolution: evolution and taxonomy of tobamoviruses*. *J. Mol. Biol.* **269**, 769–779.
- Wang, H. & Stubbs, G. (1993). *Molecular dynamics refinement against fibre diffraction data*. *Acta Cryst.* **A49**, 504–513.
- Wang, H. & Stubbs, G. J. (1994). *Structure determination of cucumber green mottle mosaic virus by X-ray fibre diffraction. Significance for the evolution of tobamoviruses*. *J. Mol. Biol.* **239**, 371–384.
- Welberry, T. R., Miller, G. H. & Carroll, C. E. (1980). *Paracrystals and growth-disorder models*. *Acta Cryst.* **A36**, 921–929.
- Welsh, L. C., Symmons, M. F. & Marvin, D. A. (2000). *The molecular structure and structural transition of the α -helical capsid in filamentous bacteriophage Pf1*. *Acta Cryst.* **D56**, 137–150.

- Welsh, L. C., Symmons, M. F., Sturtevant, J. M., Marvin, D. A. & Perham, R. N. (1998). *Structure of the capsid of Pf3 filamentous phage determined from X-ray fiber diffraction data at 3.1 Å resolution*. *J. Mol. Biol.* **283**, 155–177.
- Wilson, A. J. C. (1950). *Largest likely values for the reliability index*. *Acta Cryst.* **3**, 397–399.
- Wittmann, J. C. & Lotz, B. (1985). *Polymer decoration: the orientation of polymer folds as revealed by the crystallization of polymer vapor*. *J. Polym. Sci. Polym. Phys. Ed.* **23**, 205–226.
- Wittmann, J. C. & Lotz, B. (1990). *Epitaxial crystallization of polymers on organic and polymeric substrates*. *Prog. Polym. Sci.* **15**, 909–948.
- Wunderlich, B. (1973). *Macromolecular physics*, Vol. 1. *Crystal structure, morphology, defects*. New York: Academic Press.
- Yamashita, I., Hasegawa, K., Suzuki, H., Vonderviszt, F., Mimori-Kiyosue, Y. & Namba, K. (1998). *Structure and switching of bacterial flagellar filaments studied by X-ray fiber diffraction*. *Nature Struct. Biol.* **5**, 125–132.
- Zugenmaier, P. & Sarko, A. (1980). *The variable virtual bond*. In *Fibre diffraction methods*, ACS Symposium Series Vol. 141, edited by A. D. French & K. H. Gardner, pp. 225–237. Washington DC: American Chemical Society.

4.6

- Axel, F. & Gratias, D. (1995). *Beyond quasicrystals*. Les Ulis: Les Editions de Physique and Berlin: Springer-Verlag.
- Bancel, P. A., Heiney, P. A., Stephens, P. W., Goldman, A. I. & Horn, P. M. (1985). *Structure of rapidly quenched Al-Mn*. *Phys. Rev. Lett.* **54**, 2422–2425.
- Böhm, H. (1977). *Eine erweiterte Theorie der Satellitenreflexe und die Bestimmung der modulierten Struktur des Natriumnitrits*. Habilitation thesis, University of Munster.
- Cummins, H. Z. (1990). *Experimental studies of structurally incommensurate crystal phases*. *Phys. Rep.* **185**, 211–409.
- Dehlinger, U. (1927). *Über die Verbreiterung der Debyelinien bei kaltbearbeiteten Metallen*. *Z. Kristallogr.* **65**, 615–631.
- Dräger, J. & Mermin, N. D. (1996). *Superspace groups without the embedding: the link between superspace and Fourier-space crystallography*. *Phys. Rev. Lett.* **76**, 1489–1492.
- Estermann, M., Haibach, T. & Steurer, W. (1994). *Quasicrystal versus twinned approximant: a quantitative analysis with decagonal Al₇₀Co₁₅Ni₁₅*. *Philos. Mag. Lett.* **70**, 379–384.
- Goldman, A. I. & Kelton, K. F. (1993). *Quasicrystals and crystalline approximants*. *Rev. Mod. Phys.* **65**, 213–230.
- Gouyet, J. F. (1996). *Physics and fractal structures*. Paris: Masson and Berlin: Springer-Verlag.
- Hausdorff, F. (1919). *Dimension und äusseres Mass*. *Math. Ann.* **79**, 157–179.
- Hermann, C. (1949). *Kristallographie in Räumen beliebiger Dimensionszahl. I. Die Symmetrioperationen*. *Acta Cryst.* **2**, 139–145.
- Ishihara, K. N. & Yamamoto, A. (1988). *Penrose patterns and related structures. I. Superstructure and generalized Penrose patterns*. *Acta Cryst.* **A44**, 508–516.
- Janner, A. (1992). *Decagrammatic symmetry of decagonal Al₇₈Mn₂₂ quasicrystal*. *Acta Cryst.* **A48**, 884–901.
- Janner, A. & Janssen, T. (1979). *Superspace groups*. *Physica A*, **99**, 47–76.
- Janner, A. & Janssen, T. (1980a). *Symmetry of incommensurate crystal phases. I. Commensurate basic structures*. *Acta Cryst.* **A36**, 399–408.
- Janner, A. & Janssen, T. (1980b). *Symmetry of incommensurate crystal phases. II. Incommensurate basic structures*. *Acta Cryst.* **A36**, 408–415.
- Janner, A., Janssen, T. & de Wolff, P. M. (1983a). *Bravais classes for incommensurate crystal phases*. *Acta Cryst.* **A39**, 658–666.
- Janner, A., Janssen, T. & de Wolff, P. M. (1983b). *Determination of the Bravais class for a number of incommensurate crystals*. *Acta Cryst.* **A39**, 671–678.
- Janot, Chr. (1994). *Quasicrystals. A primer*. Oxford: Clarendon Press.