

4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

reduced when using a low-resolution diffraction data set. A combination of high-resolution electron microscopy, lattice imaging and diffraction techniques allows a good characterization of the local and global order even in these cases. For a more detailed analysis of these problems see Steurer (1995).

4.6.4.2. Commensurability versus incommensurability

The question whether an aperiodic crystal is really aperiodic or rather a high-order approximant is of different importance depending on the point of view. As far as real finite crystals are considered, definitions of *periodic* and *aperiodic real crystals* and of *periodic* and *aperiodic perfect crystals* have to be given first. *Real crystals*, despite periodicity or aperiodicity, are the actual samples under investigation. Partial information about their actual structure can be obtained today by imaging methods (scanning tunnelling microscopy, atomic force microscopy, high-resolution transmission electron microscopy, ...). Basically, the real crystal structure can be determined using full diffraction information from Bragg and diffuse scattering. In practice, however, only 'Bragg reflections' are included in a structure analysis. 'Bragg reflections' result from the integration of diffraction intensities from extended volumes around a limited number of Bragg-reflection positions (\mathbb{Z} module). This process of intensity condensation at Bragg points corresponds in direct space to an averaging process. The real crystal structure is projected upon one unit cell in direct space defined by the \mathbb{Z} module in reciprocal space. Generally, the identification of appropriate reciprocal-space metrics is not a problem in the case of crystals. It can be problematic, however, in the case of aperiodic crystals, in particular quasicrystals (see Lancon *et al.*, 1994). The metrics, and to some extent the global order in the case of quasicrystals, are fixed by assigning the reciprocal basis. The spatial resolution of a diffraction experiment defines the accuracy of the resulting metrics. The decision whether the rational number obtained for the relative length of a satellite vector indicates a commensurate or an incommensurate modulation can only be made considering temperature- and pressure-dependent chemical and physical properties of the material. The same is valid for other types of aperiodic crystals.

4.6.4.3. Twinning and nanodomain structures

High-order approximants of quasicrystals often occur in orientationally twinned form or, on a smaller scale, as oriented nanodomain structures. These structures can be identified by electron microscopy, and, in certain cases, also by high-resolution X-ray diffractometry (Kalning *et al.*, 1994). If the intensity and spatial resolution is sufficient, characteristic reflection splitting and diffuse diffraction phenomena can be observed. It has been demonstrated that for the determination of the local structure (structure-building elements) it does not matter greatly whether one uses a data set for a real quasicrystal or one for a twinned approximant (Estermann *et al.*, 1994). Examples of reciprocal-space images of an approximant, a twinned approximant and the related decagonal phase are shown schematically in Fig. 4.6.4.1 and for real samples in Fig. 4.6.4.2.

References

- Axel, F. & Gratias, D. (1995). Editors. *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 $Al_{70}Co_{15}Ni_{15}$* . *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 $Al_{78}Mn_{22}$ 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.
- Janssen, T. (1986). *Crystallography of quasicrystals*. *Acta Cryst.* **A42**, 261–271.
- Janssen, T. (1988). *Aperiodic crystals: a contradictio in terminis?* *Phys. Rep.* **168**, 55–113.
- Janssen, T. (1995). *From quasiperiodic to more complex systems*. In *Beyond Quasicrystals*, edited by F. Axel & D. Gratias, pp. 75–140. Les Ulis: Les Editions de Physique and Berlin: Springer-Verlag.
- Janssen, T., Janner, A., Looijenga-Vos, A. & de Wolff, P. M. (2004). *Incommensurate and commensurate modulated crystal structures*. In *International Tables for Crystallography*, Vol. C, edited by E. Prince, ch. 9.8. Dordrecht: Kluwer Academic Publishers.
- Jaric, M. V. (1986). *Diffraction from quasicrystals: geometric structure factor*. *Phys. Rev. B*, **34**, 4685–4698.
- Kalning, M., Kek, S., Burandt, B., Press, W. & Steurer, W. (1994). *Examination of a multiple twinned periodic approximant of the decagonal phase $Al_{70}Co_{15}Ni_{15}$* . *J. Phys. Condens. Matter*, **6**, 6177–6187.
- Kato, K. (1990). *Strukturverfeinerung des Kompositkristalls im mehrdimensionalen Raum*. *Acta Cryst.* **B46**, 39–44.
- Kelton, K. F. (1995). *Quasicrystals and related structures*. In *Intermetallic Compounds. Principles and Practice*, Vol. 1, edited by J. H. Westbrook & R. L. Fleischer, pp. 453–491. Chichester: John Wiley & Sons.
- Korekawa, M. (1967). *Theorie der Satellitenreflexe*. Habilitation thesis, University of Munich.
- Lancon, F., Billard, L., Burkov, S. & DeBoissieu, M. (1994). *On choosing a proper basis for determining structures of quasicrystals*. *J. Phys. I France*, **4**, 283–301.
- Levine, D. & Steinhardt, P. J. (1986). *Quasicrystals. I. Definition and structure*. *Phys. Rev. B*, **34**, 596–616.
- Levitov, L. S. & Rhyner, J. (1988). *Crystallography of quasicrystals; application to icosahedral symmetry*. *J. Phys. France*, **49**, 1835–1849.
- Luck, J. M., Godréche, C., Janner, A. & Janssen, T. (1993). *The nature of the atomic surfaces of quasiperiodic self-similar structures*. *J. Phys. A Math. Gen.* **26**, 1951–1999.
- Paciorek, W. A. & Chapuis, G. (1994). *Generalized Bessel functions in incommensurate structure analysis*. *Acta Cryst.* **A50**, 194–203.
- Pavlovitch, A. & Kleman, M. (1987). *Generalized 2D Penrose tilings: structural properties*. *J. Phys. A Math. Gen.* **20**, 687–702.
- Penrose, R. (1974). *The role of aesthetics in pure and applied mathematical research*. *Bull. Math. Appl.* **10**, 266–271.
- Penrose, R. (1979). *Pentaplexity. A class of non-periodic tilings of the plane*. *Math. Intell.* **2**, 32–37.

4. DIFFUSE SCATTERING AND RELATED TOPICS

- Petricek, V., Maly, K. & Cisarova, I. (1991). *The computing system 'JANA'*. In *Methods of Structural Analysis of Modulated Structures and Quasicrystals*, edited by J. M. Pérez-Mato, F. J. Zuniga & G. Madriaga, pp. 262–267. Singapore: World Scientific.
- Petricek, V., Maly, K., Coppens, P., Bu, X., Cisarova, I. & Frost-Jensen, A. (1991). *The description and analysis of composite crystals*. *Acta Cryst.* **A47**, 210–216.
- Rabson, D. A., Mermin, N. D., Rokhsar, D. S. & Wright, D. C. (1991). *The space groups of axial crystals and quasicrystals*. *Rev. Mod. Phys.* **63**, 699–733.
- Rokhsar, D. S., Wright, D. C. & Mermin, N. D. (1988). *Scale equivalence of quasicrystallographic space groups*. *Phys. Rev. B*, **37**, 8145–8149.
- Senechal, M. (1995). *Quasicrystals and Geometry*. Cambridge University Press.
- 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.
- Smaalen, S. van (1991). *Symmetry of composite crystals*. *Phys. Rev. B*, **43**, 11330–11341.
- Smaalen, S. van (1992). *Superspace description of incommensurate intergrowth compounds and the application to inorganic misfit layer compounds*. *Mater. Sci. Forum*, **100 & 101**, 173–222.
- Smaalen, S. van (1995). *Incommensurate crystal structures*. *Crystallogr. Rev.* **4**, 79–202.
- Socolar, J. E. S. & Steinhardt, P. J. (1986). *Quasicrystals. II. Unit-cell configurations*. *Phys. Rev. B*, **34**, 617–647.
- Steurer, W. (1990). *The structure of quasicrystals*. *Z. Kristallogr.* **190**, 179–234.
- Steurer, W. (1995). *Experimental aspects of the structure analysis of aperiodic materials*. In *Beyond Quasicrystals*, edited by F. Axel & D. Gratias, pp. 203–228. Les Ulis: Les Editions de Physique and Berlin: Springer-Verlag.
- Steurer, W. (1996). *The structure of quasicrystals*. In *Physical Metallurgy*, Vol. I, edited by R. W. Cahn & P. Haasen, pp. 371–411. Amsterdam: Elsevier.
- Willis, B. T. M. & Pryor, A. W. (1975). *Thermal Vibrations in Crystallography*. Cambridge University Press.
- Wolff, P. M. de (1974). *The pseudo-symmetry of modulated crystal structures*. *Acta Cryst.* **A30**, 777–785.
- Wolff, P. M. de (1977). *Symmetry operations for displacively modulated structures*. *Acta Cryst.* **A33**, 493–497.
- Wolff, P. M. de (1984). *Dualistic interpretation of the symmetry of incommensurate structures*. *Acta Cryst.* **A40**, 34–42.
- 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.
- Yamamoto, A. (1982). *Structure factor of modulated crystal structures*. *Acta Cryst.* **A38**, 87–92.
- Yamamoto, A. (1992a). *Unified setting and symbols of superspace groups for composite crystals*. *Acta Cryst.* **A48**, 476–483.
- Yamamoto, A. (1992b). *Ideal structure of icosahedral Al–Cu–Li quasicrystals*. *Phys. Rev. B*, **45**, 5217–5227.
- Zobetz, E. (1993). *One-dimensional quasilattices: fractally shaped atomic surfaces and homometry*. *Acta Cryst.* **A49**, 667–676.