

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.

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