

## 4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

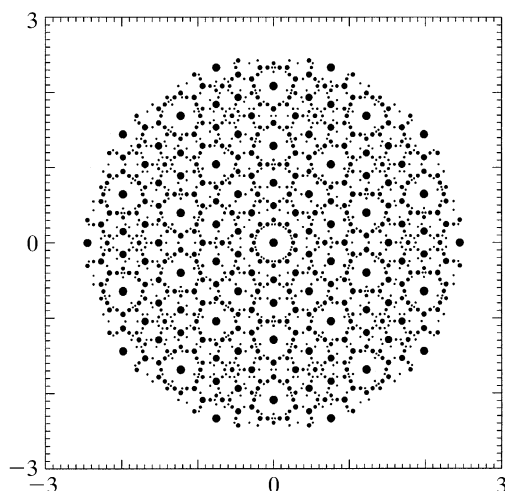


Fig. 4.6.3.17. Schematic diffraction pattern of the Penrose tiling (edge length of the Penrose unit rhombs  $a_r = 4.04 \text{ \AA}$ ). All reflections are shown within  $10^{-2}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  and  $0 \leq |\mathbf{H}^\parallel| \leq 2.5 \text{ \AA}^{-1}$ .

$10^{-2}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  are depicted. Without intensity-truncation limit, the diffraction pattern would be densely filled with discrete Bragg reflections. To illustrate their spatial and intensity distribution, an enlarged section of Fig. 4.6.3.17 is shown in Fig. 4.6.3.18. This picture shows all Bragg reflections within  $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ . The projected 4D reciprocal-lattice unit cell is drawn and several reflections are indexed. All reflections are arranged along lines in five symmetry-equivalent orientations. The perpendicular-space diffraction patterns (Figs. 4.6.3.19 and 4.6.3.20) show a characteristic star-like distribution of the Bragg reflections. This is a consequence of the pentagonal shape of the atomic surfaces: the Fourier transform of a pentagon has a star-like distribution of strong Fourier coefficients.

The 5D decagonal space groups that may be of relevance for the description of decagonal phases are listed in Table 4.6.3.1. These space groups are a subset of all 5D decagonal space groups fulfilling the condition that the 5D point groups they are associated with are isomorphous to the 3D point groups describing the diffraction symmetry. Their structures are comparable to 3D hexagonal groups. Hence, only primitive lattices exist. The orientation of the symmetry elements in the 5D space is defined by the isomorphism of the 3D and 5D point groups. However, the action of the tenfold rotation is different in the subspaces  $\mathbf{V}^\parallel$  and

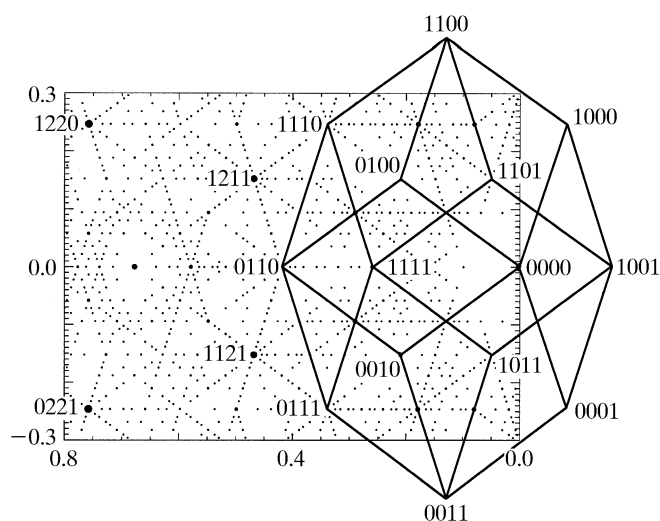


Fig. 4.6.3.18. Enlarged section of Fig. 4.6.3.17. All reflections shown are selected within the given limits from a data set within  $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  and  $0 \leq |\mathbf{H}^\parallel| \leq 2.5 \text{ \AA}^{-1}$ . The projected 4D reciprocal-lattice unit cell is drawn and several reflections are indexed.

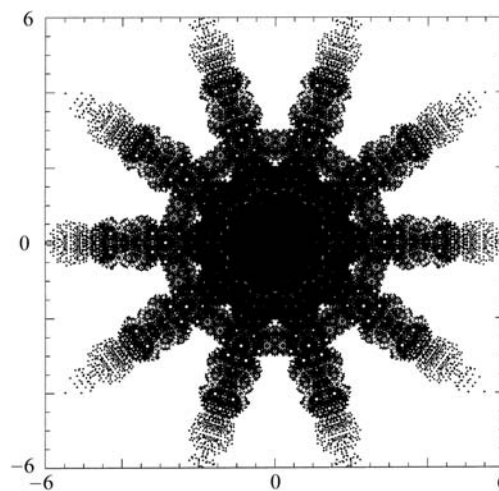


Fig. 4.6.3.19. The perpendicular-space diffraction pattern of the Penrose tiling (edge length of the Penrose unit rhombs  $a_r = 4.04 \text{ \AA}$ ). All reflections are shown within  $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  and  $0 \leq |\mathbf{H}^\parallel| \leq 2.5 \text{ \AA}^{-1}$ .

$\mathbf{V}^\perp$ : a rotation of  $\pi/5$  in  $\mathbf{V}^\parallel$  is correlated with a rotation of  $3\pi/5$  in  $\mathbf{V}^\perp$ . The reflection and inversion operations are equivalent in both subspaces.

## 4.6.3.2.3. Structure factor

The structure factor for the decagonal phase corresponds to the Fourier transform of the 5D unit cell,

$$F(\mathbf{H}) = \sum_{k=1}^N f_k(\mathbf{H}^\parallel) T_k(\mathbf{H}^\parallel, \mathbf{H}^\perp) g_k(\mathbf{H}^\perp) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_k),$$

with 5D diffraction vectors  $\mathbf{H} = \sum_{i=1}^5 h_i \mathbf{d}_i^*$ ,  $N$  hyperatoms, parallel-space atomic scattering factor  $f_k(\mathbf{H}^\parallel)$ , temperature factor  $T_k(\mathbf{H}^\parallel, \mathbf{H}^\perp)$  and perpendicular-space geometric form factor  $g_k(\mathbf{H}^\perp)$ .  $T_k(\mathbf{H}^\parallel, \mathbf{0})$  is equivalent to the conventional Debye-Waller factor and  $T_k(\mathbf{0}, \mathbf{H}^\perp)$  describes random fluctuations along the perpendicular-space coordinate. These fluctuations cause characteristic jumps of vertices in physical space (*phason flips*). Even random phason flips map the vertices onto positions which can still be described by physical-space vectors of the type  $\mathbf{r} = \sum_{i=1}^5 n_i \mathbf{a}_i$ . Consequently, the set  $M = \{\mathbf{r} = \sum_{i=1}^5 n_i \mathbf{a}_i | n_i \in \mathbb{Z}\}$  of all possible vectors forms a  $\mathbb{Z}$  module. The shape of the atomic surfaces corresponds to a selection rule for the positions actually occupied. The geometric form factor  $g_k(\mathbf{H}^\perp)$  is equivalent to the

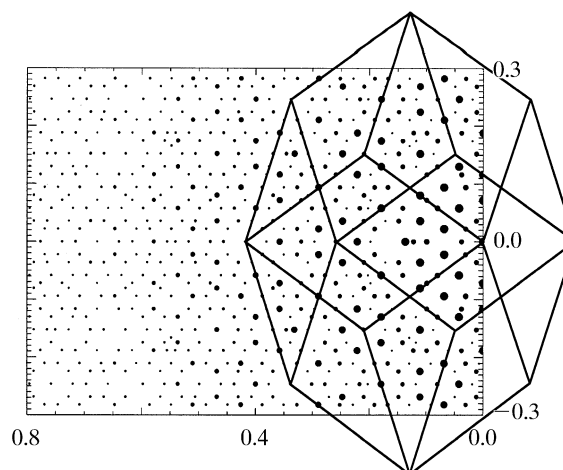


Fig. 4.6.3.20. Enlarged section of Fig. 4.6.3.19 showing the projected 4D reciprocal-lattice unit cell.