

4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

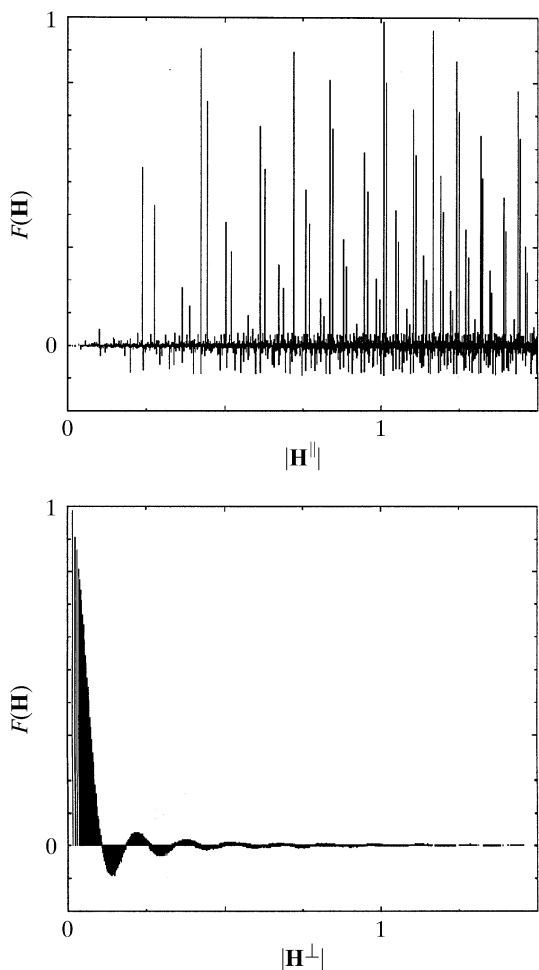


Fig. 4.6.3.35. Radial distribution function of the structure factors $F(\mathbf{H})$ of the 3D Penrose tiling (edge lengths of the Penrose unit rhombohedra $a_r = 5.0 \text{ \AA}$) decorated with point atoms as a function of $|\mathbf{H}^{\parallel}|$ (above) and $|\mathbf{H}^{\perp}|$ (below). All reflections are shown within $10^{-6}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \leq h_i \leq 6, i = 1, \dots, 6$.

$$\begin{pmatrix} h'_1 \\ h'_2 \\ h'_3 \\ h'_4 \\ h'_5 \\ h'_6 \end{pmatrix} = \begin{pmatrix} -2 & 1 & 1 & 1 & 1 & 1 \\ 1 & -2 & 1 & -1 & -1 & 1 \\ 1 & 1 & -2 & 1 & -1 & -1 \\ 1 & -1 & 1 & -2 & 1 & -1 \\ 1 & -1 & -1 & 1 & -2 & 1 \\ 1 & 1 & -1 & -1 & 1 & -2 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \end{pmatrix}.$$

The matrix $(S^{-1})^T$ leaves $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^6 h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ invariant,

$$\begin{pmatrix} h'_1 \\ h'_2 \\ h'_3 \\ h'_4 \\ h'_5 \\ h'_6 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \end{pmatrix},$$

for any $\mathbf{H} = \sum_{i=1}^6 h_i \mathbf{d}_i^*$ with h_i all even or all odd, corresponding to a 6D face-centred hypercubic lattice. In a second case the sum $\sum_{i=1}^6 h_i$ is even, corresponding to a 6D body-centred hypercubic lattice. Block-diagonalization of the matrix S decomposes it into two irreducible representations. With $WSW^{-1} = S_V = S_V^{\parallel} \oplus S_V^{\perp}$ we obtain

$$S_V = \left(\begin{array}{ccc|ccc} \tau & 0 & 0 & 0 & 0 & 0 \\ 0 & \tau & 0 & 0 & 0 & 0 \\ 0 & 0 & \tau & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -1/\tau & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/\tau & 0 \\ 0 & 0 & 0 & 0 & 0 & -1/\tau \end{array} \right)_V = \left(\begin{array}{c|c} S^{\parallel} & 0 \\ \hline 0 & S^{\perp} \end{array} \right)_V,$$

the scaling properties in the two 3D subspaces: scaling by a factor τ in parallel space corresponds to a scaling by a factor $(-\tau)^{-1}$ in perpendicular space. For the intensities of the scaled reflections analogous relationships are valid, as discussed for decagonal phases (Figs. 4.6.3.36 and 4.6.3.37, Section 4.6.3.3.2.5).

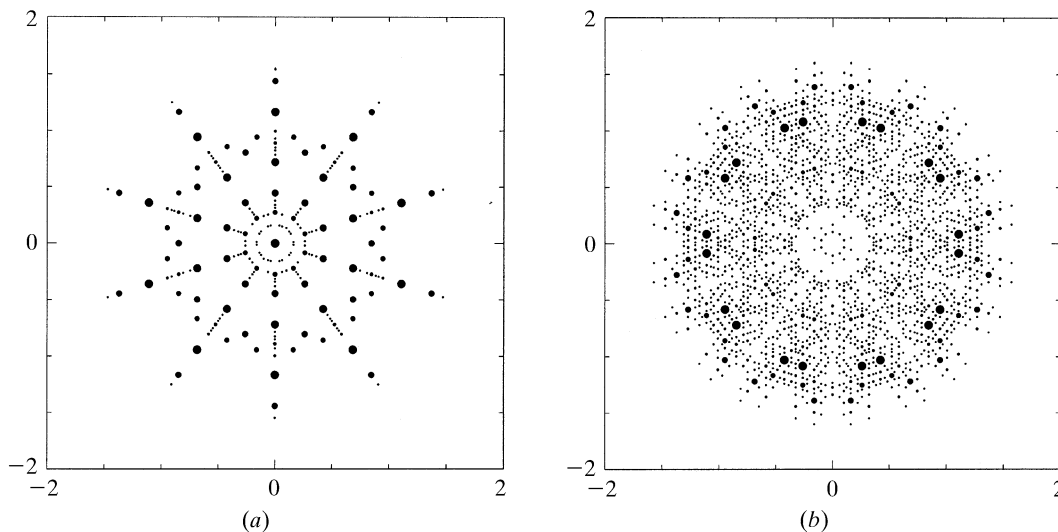


Fig. 4.6.3.36. Parallel-space distribution of (a) positive and (b) negative structure factors of the 3D Penrose tiling of the 6D P lattice type decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0 \text{ \AA}$). The magnitudes of the structure factors are indicated by the diameters of the filled circles. All reflections are shown within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \leq h_i \leq 6, i = 1, \dots, 6$.