

## 4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

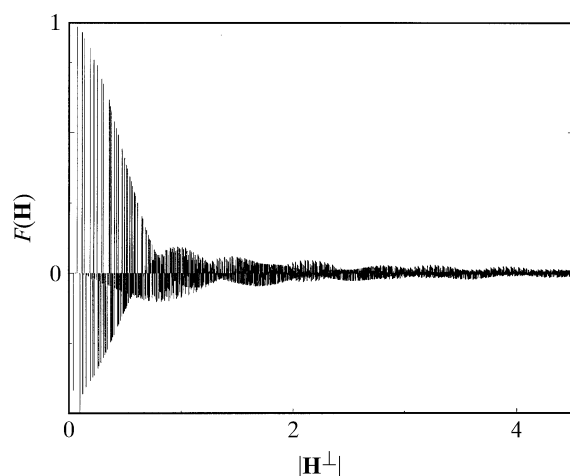


Fig. 4.6.3.22. Radial distribution function of the structure factors  $F(\mathbf{H})$  of the Penrose tiling (edge length of the Penrose unit rhombs  $a_r = 4.04 \text{ \AA}$ ) decorated with point atoms as a function of  $\mathbf{H}^\perp$ . All structure factors within  $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  and  $0 \leq |\mathbf{H}^\perp| \leq 2.5 \text{ \AA}^{-1}$  have been used and normalized to  $F(0000) = 1$ .

structure consisting of point atoms on the lattice nodes, the Bragg reflections show intensities depending on the perpendicular-space components of their diffraction vectors (Figs. 4.6.3.19, 4.6.3.20 and 4.6.3.22).

4.6.3.3.2.5. Relationships between structure factors at symmetry-related points of the Fourier image

Scaling the Penrose tiling by a factor  $\tau^{-n}$  by employing the matrix  $S^{-n}$  scales at the same time its reciprocal space by a factor  $\tau^n$ :

$$S\mathbf{H} = \begin{pmatrix} 0 & 1 & 0 & \bar{1} & 0 \\ 0 & 1 & 1 & \bar{1} & 0 \\ \bar{1} & 1 & 1 & 0 & 0 \\ \bar{1} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \end{pmatrix} = \begin{pmatrix} h_2 - h_4 \\ h_2 + h_3 - h_4 \\ -h_1 + h_2 + h_3 \\ -h_1 + h_3 \\ h_5 \end{pmatrix}.$$

Since this operation increases the lengths of the diffraction vectors by the factor  $\tau$  in parallel space and decreases them by the factor  $1/\tau$  in perpendicular space, the following distribution of structure-factor magnitudes (for point atoms at rest) is obtained:

$$\begin{aligned} |F(S^n \mathbf{H})| &> |F(S^{n-1} \mathbf{H})| > \dots > |F(S^1 \mathbf{H})| > |F(\mathbf{H})|, \\ |F(\tau^n \mathbf{H}^\parallel)| &> |F(\tau^{n-1} \mathbf{H}^\parallel)| > \dots > |F(\tau \mathbf{H}^\parallel)| > |F(\mathbf{H})|. \end{aligned}$$

The scaling operations  $S^n$ ,  $n \in \mathbb{Z}$ , the roto-scaling operations  $(\Gamma(\alpha)S^2)^n$  (Fig. 4.6.3.14) and the tenfold rotation  $(\Gamma(\alpha))^n$ , where

$$(\Gamma(\alpha)S^2)^n = \begin{pmatrix} 1 & 1 & \bar{1} & \bar{1} & 0 \\ 1 & 2 & 0 & \bar{2} & 0 \\ 0 & 2 & 1 & \bar{1} & 0 \\ \bar{1} & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D^n,$$

connect all structure factors with diffraction vectors pointing to the nodes of an infinite series of pentagrams. The structure factors with positive signs are predominantly on the vertices of the pentagram while the ones with negative signs are arranged on circles around the vertices (Figs. 4.6.3.24 to 4.6.3.27).

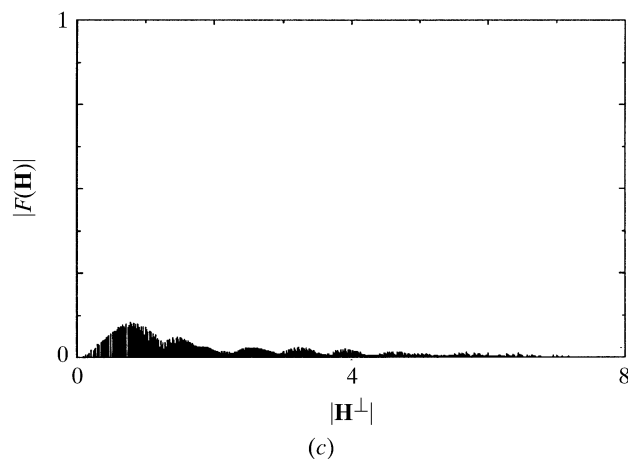
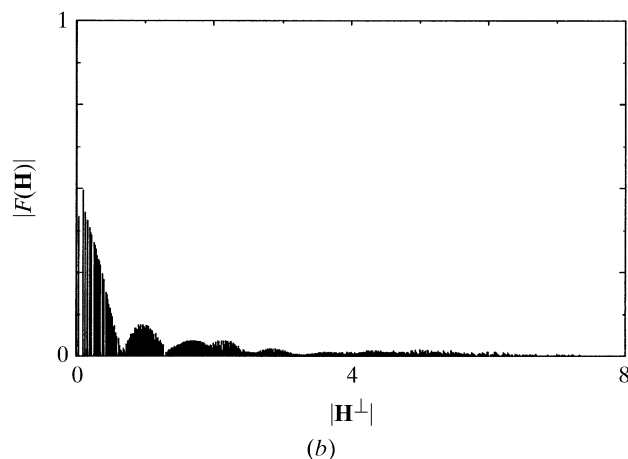
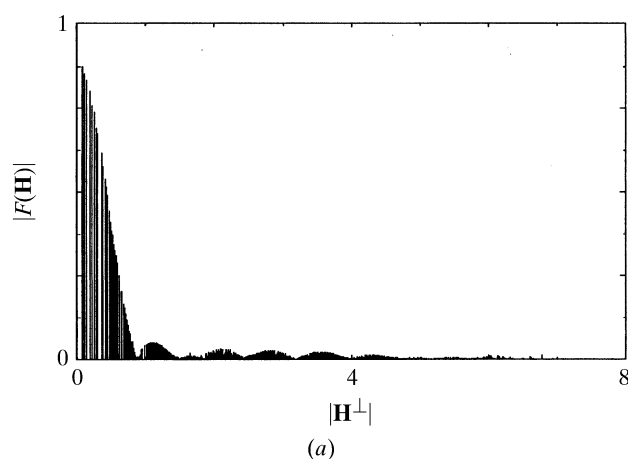


Fig. 4.6.3.23. Radial distribution function of the structure-factor magnitudes  $|F(\mathbf{H})|$  of the Penrose tiling (edge length of the Penrose unit rhombs  $a_r = 4.04 \text{ \AA}$ ) decorated with point atoms as a function of  $\mathbf{H}^\perp$ . All structure factors within  $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$  and  $0 \leq |\mathbf{H}^\perp| \leq 2.5 \text{ \AA}^{-1}$  have been used and normalized to  $F(0000) = 1$ . The branches with (a)  $|\sum_{i=1}^4 h_i| = 0 \pmod{5}$ , (b)  $|\sum_{i=1}^4 h_i| = 1 \pmod{5}$  and (c)  $|\sum_{i=1}^4 h_i| = 2 \pmod{5}$  are shown.

4.6.3.3.3. Icosahedral phases

A structure that is quasiperiodic in three dimensions and exhibits icosahedral diffraction symmetry is called an icosahedral phase. Its holohedral Laue symmetry group is  $K = m\bar{3}5$ . All reciprocal-space vectors  $\mathbf{H} = \sum_{i=1}^6 h_i \mathbf{a}_i^* \in M^*$  can be represented on a basis  $\mathbf{a}_1^* = a^*(0, 0, 1)$ ,  $\mathbf{a}_i^* = a^*[\sin \theta \cos(2\pi i/5), \sin \theta \sin(2\pi i/5), \cos \theta]$ ,  $i = 2, \dots, 6$  where  $\sin \theta = 2/(5)^{1/2}$ ,  $\cos \theta = 1/(5)^{1/2}$  and  $\theta \simeq 63.44^\circ$ , the angle between two neighbouring fivefold axes (Fig. 4.6.3.28). This can be rewritten as