International Tables for Crystallography (2010). Vol. B, Section 4.6.3.3.2.4, pp. 612–613.

Table 4.6.3.1. *3D point groups of order k describing the diffraction symmetry and corresponding 5D decagonal space groups with reflection conditions (see Rabson et al., 1991)*

3D point group	k	5D space group	Reflection condition
$\frac{10}{m}\frac{2}{m}\frac{2}{m}$	40	$P\frac{10}{m}\frac{2}{m}\frac{2}{m}$	No condition
		$P\frac{10}{m}\frac{2}{c}\frac{2}{c}$	$h_1h_2h_2h_1h_5$: $h_5 = 2n$ $h_1h_2\overline{h_2h_1}h_5$: $h_5 = 2n$
		$P\frac{10_5}{m}\frac{2}{m}\frac{2}{c}$	$h_1h_2\overline{h_2h_1}h_5$: $h_5 = 2n$
		$P\frac{10_5}{m}\frac{2}{c}\frac{2}{m}$	$h_1h_2h_2h_1h_5$: $h_5 = 2n$
$\frac{10}{m}$	20	$P\frac{10}{m}$	No condition
		$P\frac{10_5}{m}$	$0000h_5$: $h_5 = 2n$
1022	20	$P1022$	No condition
		$P10_j22$	$0000h_5$: $jh_5 = 10n$
$10mm$	20	$P10mm$	No condition
		$P10cc$	$h_1h_2h_2h_1h_5$: $h_5 = 2n$ $h_1h_2\overline{h_2h_1}h_5$: $h_5 = 2n$
		$P10_5mc$	$h_1h_2\overline{h_2h_1}h_5$: $h_5 = 2n$
		$P10_5cm$	$h_1h_2h_2h_1h_5$: $h_5 = 2n$
$\overline{10}m2$	20	$P\overline{10}m2$	No condition
		$P\overline{10}c2$	$h_1h_2h_2h_1h_5$: $h_5 = 2n$
		$P\overline{10}2m$	No condition
		$P\overline{10}2c$	$h_1h_2\overline{h_2h_1}h_5$: $h_5 = 2n$
$\overline{10}$	10	$P\overline{10}$	No condition
10	10	$P10$	No condition
		$P10_j$	$0000h_5$: $jh_5 = 10n$

Fourier transform of the *atomic surface*, *i.e.* the 2D perpendicular-space component of the 5D *hyperatoms*.

For example, the canonical Penrose tiling $g_k(\mathbf{H}^\perp)$ corresponds to the Fourier transform of pentagonal atomic surfaces:

$$g_k(\mathbf{H}^\perp) = (1/A_{\rm UC}^\perp)\int\limits_{A_k} \exp(2\pi i\mathbf{H}^\perp\cdot\mathbf{r})\,{\rm d}\mathbf{r},$$

where $A_{\rm UC}^\perp$ is the area of the 5D unit cell projected upon $\mathbf{V}^\perp$ and A_k is the area of the kth atomic surface. The area $A_{\rm UC}^\perp$ can be calculated using the formula

$$A_{\rm UC}^\perp = (4/25a_i^{*2})[(7+\tau)\sin(2\pi/5) + (2+\tau)\sin(4\pi/5)].$$

Evaluating the integral by decomposing the pentagons into triangles, one obtains

$$g_k(\mathbf{H}^\perp) = \frac{1}{A_{\rm UC}^\perp}\sin\left(\frac{2\pi}{5}\right) \times \sum_{j=0}^{4}\frac{A_j[\exp(iA_{j+1}\lambda_k)-1] - A_{j+1}[\exp(iA_j\lambda_k)-1]}{A_jA_{j+1}(A_j - A_{j+1})}$$

with $j = 0, \ldots, 4$ running over the five triangles, where the radii of the pentagons are λ_j, $A_j = 2\pi\mathbf{H}^\perp\mathbf{e}_j$,

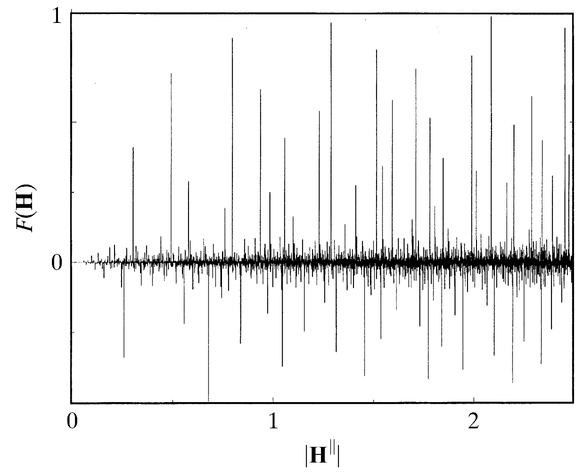

Fig. 4.6.3.21. Radial distribution function of the structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length of the Penrose unit rhombs a_r = 4.04 Å) decorated with point atoms as a function of $\mathbf{H}^\parallel$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \le |\mathbf{H}^\parallel| \le 2.5$ Å^{-1} have been used and normalized to $F(0000) = 1$.

$$\mathbf{H}^\perp = \pi^\perp(\mathbf{H}) = \sum_{j=0}^{4} h_j a_j^* \begin{pmatrix} 0 \\ 0 \\ 0 \\ \cos(6\pi j/5) \\ \sin(6\pi j/5) \end{pmatrix}$$

and the vectors

$$\mathbf{e}_j = \frac{1}{a_j^*}\begin{pmatrix} 0 \\ 0 \\ 0 \\ \cos(2\pi j/5) \\ \sin(2\pi j/5) \end{pmatrix} \text{ with } j = 0, \ldots, 4.$$

As shown by Ishihara & Yamamoto (1988), the Penrose tiling can be considered to be a superstructure of a pentagonal tiling with only one type of pentagonal atomic surface in the nD unit cell. Thus, for the Penrose tiling, three special reflection classes can be distinguished: for $|\sum_{i=1}^4 h_i| = m$ mod 5 and $m = 0$ the class of strong main reflections is obtained, and for $m = \pm1, \pm2$ the classes of weaker first- and second-order satellite reflections are obtained (see Fig. 4.6.3.18).

4.6.3.3.2.4. *Intensity statistics*

This section deals with the reciprocal-space characteristics of the 2D quasiperiodic component of the 3D structure, namely the Fourier module M_1^*. The radial structure-factor distributions of the Penrose tiling decorated with point scatterers are plotted in Figs. 4.6.3.21 and 4.6.3.22 as a function of parallel and perpendicular space. The distribution of $|F(\mathbf{H})|$ as a function of their frequencies clearly resembles a centric distribution, as can be expected from the centrosymmetric 4D subunit cell. The shape of the distribution function depends on the radius of the limiting sphere in reciprocal space. The number of weak reflections increases to the power of four, that of strong reflections only quadratically (strong reflections always have small $\mathbf{H}^\perp$ components). The radial distribution of the structure-factor amplitudes as a function of perpendicular space clearly shows three branches, corresponding to the reflection classes $\sum_{i=1}^4 h_i = m$ mod 5 with $|m| = 0$, $|m| = 1$ and $|m| = 2$ (Fig. 4.6.3.23).

The weighted reciprocal space of the Penrose tiling contains an infinite number of Bragg reflections within a limited region of the physical space. Contrary to the diffraction pattern of a periodic

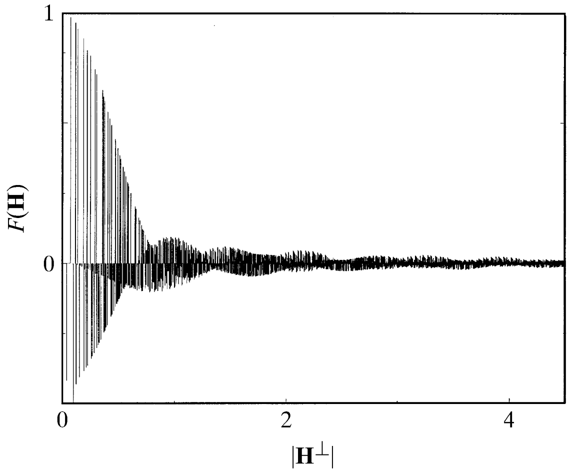

Fig. 4.6.3.22. Radial distribution function of the structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length of the Penrose unit rhombs a_r = 4.04 Å) decorated with point atoms as a function of $\mathbf{H}^{\perp}$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \leq |\mathbf{H}^{\parallel}| \leq 2.5$ Å^{-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 τ^{-n} by employing the matrix S^{-n} scales at the same time its reciprocal space by a factor τ^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 τ 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:

$$\left|F(S^n\mathbf{H})\right| > \left|F(S^{n-1}\mathbf{H})\right| > \ldots > \left|F(S^1\mathbf{H})\right| > \left|F(\mathbf{H})\right|,$$
$$\left|F(\tau^n\mathbf{H}^{\parallel})\right| > \left|F(\tau^{n-1}\mathbf{H}^{\parallel})\right| > \ldots > \left|F(\tau\mathbf{H}^{\parallel})\right| > \left|F(\mathbf{H})\right|.$$

The scaling operations S^n, $n \in \mathbb{Z}$, the rotoscaling 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).

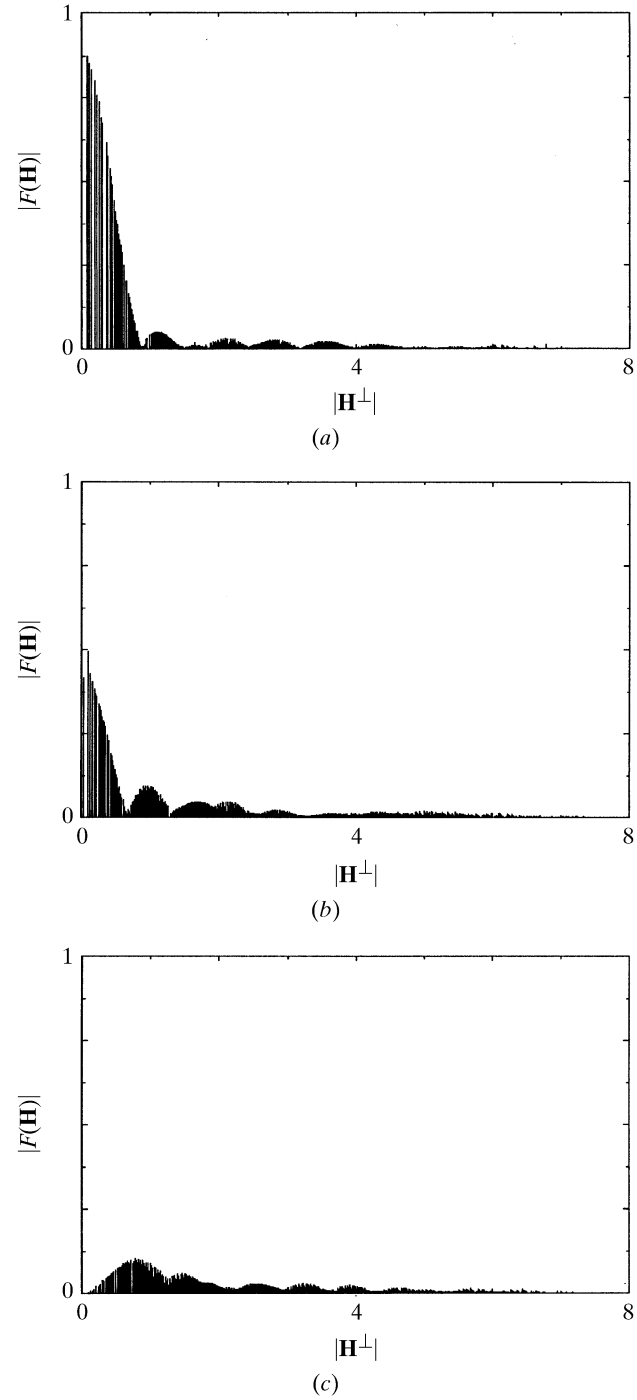

Fig. 4.6.3.23. Radial distribution function of the structure-factor magnitudes $|F(\mathbf{H})|$ of the Penrose tiling (edge length of the Penrose unit rhombs a_r = 4.04 Å) decorated with point atoms as a function of $\mathbf{H}^{\perp}$. All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $0 \leq |\mathbf{H}^{\parallel}| \leq 2.5$ Å^{-1} have been used and normalized to $F(0000) = 1$. The branches with (*a*) $|\sum_{i=1}^{4} h_i| = 0 \bmod 5$, (*b*) $|\sum_{i=1}^{4} h_i| = 1 \bmod 5$ and (*c*) $|\sum_{i=1}^{4} h_i| = 2 \bmod 5$ 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 $K = m\bar{3}\bar{5}$. All reciprocal-space vectors $\mathbf{H} = \sum_{i=1}^{6} h_i \mathbf{a}_i^* \in M^*$ can be represented on a basis $\mathbf{a}_1^* = a^*(0, 0, 1)$, $\mathbf{a}_i^* = a^*[\sin\theta\cos(2\pi i/5), \sin\theta\sin(2\pi i/5), \cos\theta]$, $i = 2, \ldots, 6$ where $\sin\theta = 2/(5)^{1/2}$, $\cos\theta = 1/(5)^{1/2}$ and $\theta \simeq 63.44°$, the angle between two neighbouring fivefold axes (Fig. 4.6.3.28). This can be rewritten as

references