

4. DIFFUSE SCATTERING AND RELATED TOPICS

 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
$\frac{10\ 2\ 2}{m\ m\ m}$	40	$P\frac{10\ 2\ 2}{m\ m\ m}$	No condition
		$P\frac{10\ 2\ 2}{m\ c\ c}$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$ $h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
		$P\frac{10_5\ 2\ 2}{m\ m\ c}$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
		$P\frac{10_5\ 2\ 2}{m\ c\ m}$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
$\frac{10}{m}$	20	$P\frac{10}{m}$	No condition
		$P\frac{10_5}{m}$	$0000h_5: h_5 = 2n$
1022	20	$P1022$	No condition
		$P10_22$	$0000h_5: jh_5 = 10n$
10mm	20	$P10mm$	No condition
		$P10cc$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$ $h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
		$P10_5mc$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
		$P10_5cm$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
$\overline{10}m2$	20	$P\overline{10}m2$	No condition
		$P\overline{10}c2$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
		$P\overline{10}2m$	No condition
		$P\overline{10}2c$	$h_1 h_2 h_2 h_1 h_5: h_5 = 2n$
$\overline{10}$	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:

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

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

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

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

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

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

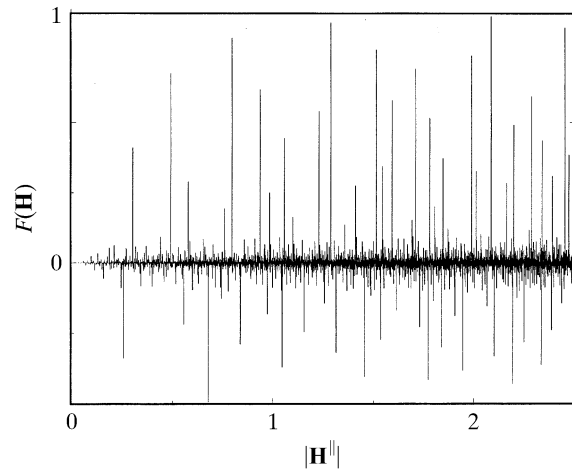


Fig. 4.6.3.21. Radial distribution function of the structure factors $F(\mathbf{H})$ of the Penrose tiling (edge length of the Penrose unit rhombs $a_r = 4.04 \text{ \AA}$) decorated with point atoms as a function of \mathbf{H}^\parallel . All structure factors within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2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

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

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 n D unit cell. Thus, for the Penrose tiling, three special reflection classes can be distinguished: for $|\sum_{i=1}^4 h_i| = m \pmod{5}$ and $m = 0$ the class of strong main reflections is obtained, and for $m = \pm 1, \pm 2$ 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 $\sum_{i=1}^4 h_i = m \pmod{5}$ 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