

4. DIFFUSE SCATTERING AND RELATED TOPICS

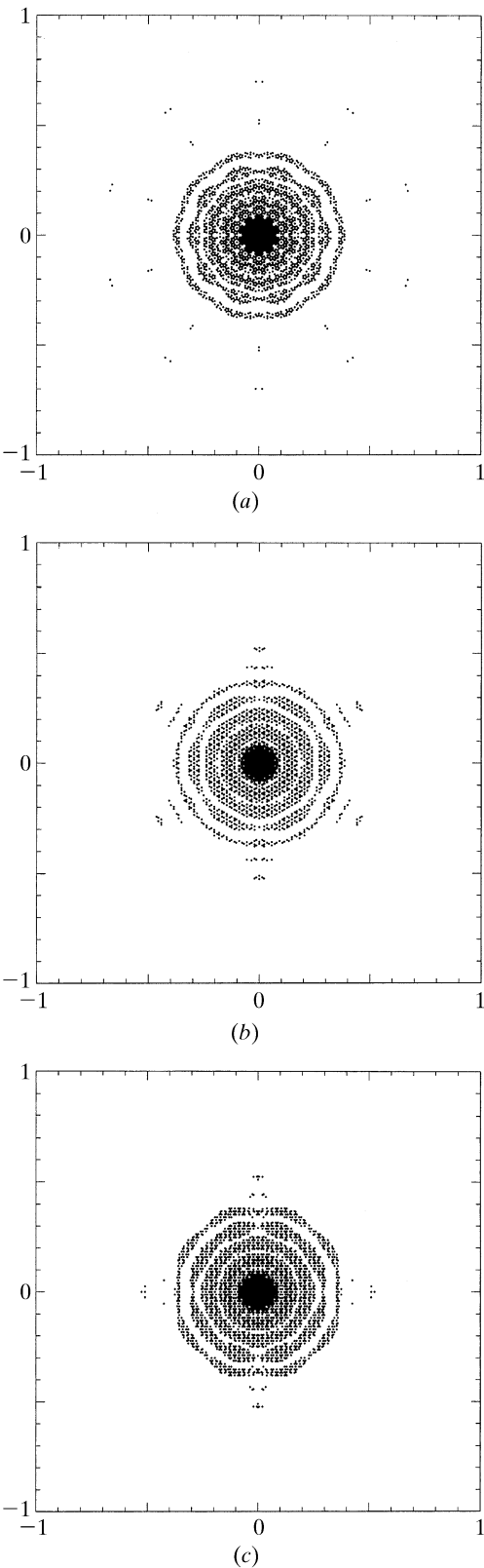


Fig. 4.6.3.34. Perpendicular-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0 \text{ \AA}$). Sections with (a) five-, (b) three- and (c) twofold symmetry are shown for the primitive 6D analogue of Bravais type P . All reflections are shown within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \leq h_i \leq 6, i = 1, \dots, 6$.

distribution, as can be expected from the centrosymmetric unit cell. The shape of the distribution function depends on the radius of the limiting sphere in reciprocal space. The number of weak reflections

Table 4.6.3.2. 3D point groups of order k describing the diffraction symmetry and corresponding 6D decagonal space groups with reflection conditions (see Levitov & Rhyner, 1988; Rokhsar et al., 1988)

3D point group	k	5D space group	Reflection condition
$\frac{2}{m}\bar{3}5$	120	$P\frac{2}{m}\bar{3}5$	No condition
		$P\frac{2}{n}\bar{3}5$	$h_1h_2h_3h_4h_5h_6 : h_5 - h_6 = 2n$
		$I\frac{2}{m}\bar{3}5$	$h_1h_2h_3h_4h_5h_6 : \sum_{i=1}^6 h_i = 2n$
		$F\frac{2}{m}\bar{3}5$	$h_1h_2h_3h_4h_5h_6 : \sum_{i \neq j=1}^6 h_i + h_j = 2n$
		$F\frac{2}{n}\bar{3}5$	$h_1h_2h_3h_4h_5h_6 : \sum_{i \neq j=1}^6 h_i + h_j = 2n$ $h_1h_2h_3h_4h_5h_6 : h_5 - h_6 = 4n$
235	60	$P235$	No condition
		$P235_1$	$h_1h_2h_3h_4h_5h_6 : h_1 = 5n$
		$I235$	$h_1h_2h_3h_4h_5h_6 : \sum_{i=1}^6 h_i = 2n$
		$I235_1$	$h_1h_2h_3h_4h_5h_6 : \sum_{i=1}^6 h_i = 2n$ $h_1h_2h_3h_4h_5h_6 : h_1 + 5h_2 = 10n$
		$F235$	$h_1h_2h_3h_4h_5h_6 : \sum_{i \neq j=1}^6 h_i + h_j = 2n$
		$F235_1$	$h_1h_2h_3h_4h_5h_6 : \sum_{i \neq j=1}^6 h_i + h_j = 2n$ $h_1h_2h_3h_4h_5h_6 : h_1 + 5h_2 = 10n$

increases as the power 6, that of strong reflections only as the power 3 (strong reflections always have small \mathbf{H}^\perp components).

The weighted reciprocal space of the 3D 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 structure consisting of point atoms on the lattice nodes, the Bragg reflections show intensities depending on the perpendicular-space components of their diffraction vectors.

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

The weighted 3D reciprocal space $M^* = \{\mathbf{H}^\parallel = \sum_{i=1}^6 h_i \mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ exhibits the icosahedral point symmetry $K = m\bar{3}5$. It is invariant under the action of the scaling matrix S^3 :

$$S = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \end{pmatrix}_D, S^3 = \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & -1 & -1 & 1 \\ 1 & 1 & 2 & 1 & -1 & -1 \\ 1 & -1 & 1 & 2 & 1 & -1 \\ 1 & -1 & -1 & 1 & 2 & 1 \\ 1 & 1 & -1 & -1 & 1 & 2 \end{pmatrix}_D$$
$$\begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & -1 & -1 & 1 \\ 1 & 1 & 2 & 1 & -1 & -1 \\ 1 & -1 & 1 & 2 & 1 & -1 \\ 1 & -1 & -1 & 1 & 2 & 1 \\ 1 & 1 & -1 & -1 & 1 & 2 \end{pmatrix}_D \begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix} = \tau^3 \begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix}$$

The scaling transformation $(S^{-3})^T$ leaves a primitive 6D reciprocal lattice invariant as can easily be seen from its application on the indices: