International Tables for Crystallography (2010). Vol. B, Section 4.6.3.3.3.1, pp. 616–618.

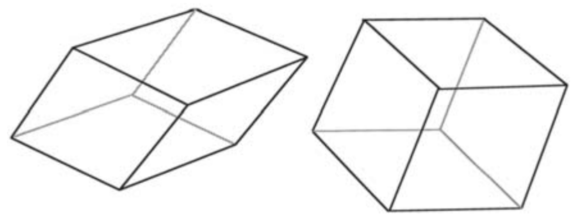

Fig. 4.6.3.30. The two unit tiles of the 3D Penrose tiling: a prolate $[\alpha_p = \arccos(5^{-1/2}) \simeq 63.44^\circ]$ and an oblate $(\alpha_o = 180^\circ - \alpha_p)$ rhombohedron with equal edge lengths a_r.

$$\begin{pmatrix} A & B & B & B & B & B \\ B & A & B & -B & -B & B \\ B & B & A & B & -B & -B \\ B & -B & B & A & B & -B \\ B & -B & -B & B & A & B \\ B & B & -B & -B & B & A \end{pmatrix},$$

with $A = (1 + c^2)a^{*2}$, $B = [(5)^{1/2}/5](1 - c^2)a^{*2}$ for the reciprocal space and $A = (1 + c^2)/[4(ca^*)^2]$, $B = [(5)^{1/2}(c^2 - 1)]/[20(ca^*)^2]$ for the direct space. For $c = 1$ we obtain hypercubic direct and reciprocal 6D lattices.

The lattice parameters in reciprocal and direct space are $d_i^* = a^*(2)^{1/2}$ and $d_i = 1/[(2)^{1/2}a^*]$ with $i = 1, \ldots, 6$, respectively. The volume of the 6D unit cell can be calculated from the metric tensor G. For $c = 1$ it is simply $V = [\det(G)]^{1/2} = \{1/[(2)^{1/2}a^*]\}^6$.

The best known example of a 3D quasiperiodic structure is the canonical 3D *Penrose tiling* (see Janssen, 1986). It can be constructed from two unit tiles: a prolate and an oblate rhombohedron with equal edge lengths a_r (Fig. 4.6.3.30). Each face of the rhombohedra is a rhomb with acute angles $\alpha_r = \arccos[1/(5)^{1/2}] \simeq 63.44^\circ$. Their volumes are $V_p = (4/5)a_r^3 \sin(2\pi/5)$, $V_o = (4/5)a_r^3 \sin(\pi/5) = V_p/\tau$, and their frequencies $\nu_p{:}\nu_o = \tau{:}1$. The resulting point density (number of vertices per unit volume) is $\rho_p = (\tau + 1)/(\tau V_p + V_o) = (\tau/a_r^3)\sin(2\pi/5)$. Ten prolate and ten oblate rhombohedra can be packed to form a rhombic triacontahedron. The icosahedral symmetry of this zonohedron is broken by the many possible decompositions into the rhombohedra. Removing one zone of the triacontahedron gives a rhomb-icosahedron consisting of five prolate and five oblate rhombohedra. Again, the singular fivefold axis of the rhomb-icosahedron is broken by the decomposition into rhombohedra. Removing one zone again gives a rhombic dodecahedron consisting of two prolate and two oblate rhombohedra. Removing the last remaining zone leads finally to a single prolate rhombohedron. Using these zonohedra as elementary clusters, a matching rule can be derived for the 3D construction of the 3D Penrose tiling (Levine & Steinhardt, 1986; Socolar & Steinhardt, 1986).

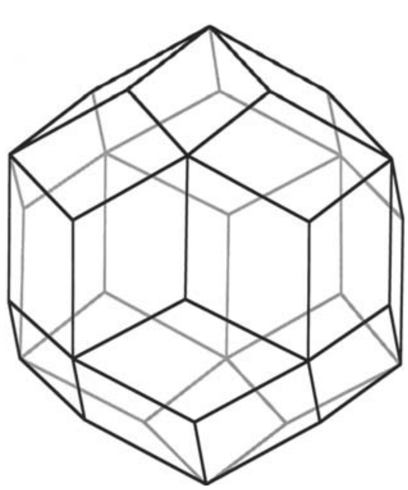

Fig. 4.6.3.31. Atomic surface of the 3D Penrose tiling in the 6D hypercubic description. The projection of the 6D hypercubic unit cell upon $\mathbf{V}^\perp$ gives a rhombic triacontahedron.

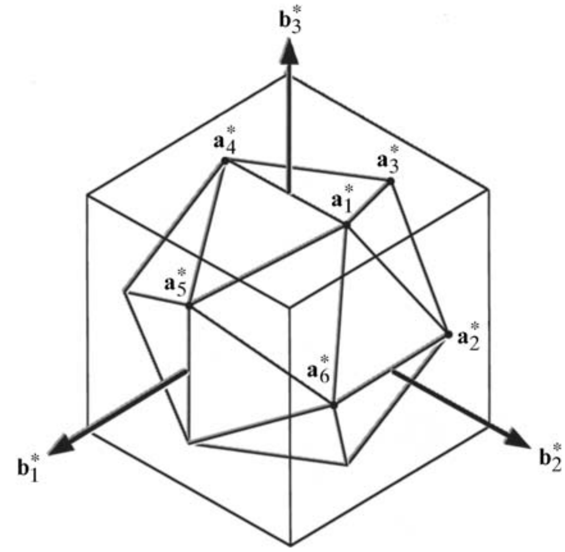

Fig. 4.6.3.32. Perspective parallel-space view of the two alternative reciprocal bases of the 3D Penrose tiling: the cubic and the icosahedral setting, represented by the bases $\mathbf{b}_i^*$, $i = 1, \ldots, 3$, and $\mathbf{a}_i^*$, $i = 1, \ldots, 6$, respectively.

The 3D Penrose tiling can be embedded in the 6D space as shown above. The 6D hypercubic lattice is decorated on the lattice nodes with 3D triacontahedra obtained from the projection of a 6D unit cell upon the perpendicular space $\mathbf{V}^\perp$ (Fig. 4.6.3.31). Thus the edge length of the rhombs covering the triacontahedron is equivalent to the length $\pi^\perp(\mathbf{d}_i) = 1/2a^*$ of the perpendicular-space component of the vectors spanning the 6D hypercubic lattice $\Sigma = \{\mathbf{r} = \sum_{i=1}^6 n_i \mathbf{d}_i | n_i \in \mathbb{Z}\}$.

4.6.3.3.3.1. *Indexing*

There are several indexing schemes in use. The generic one uses a set of six rationally independent reciprocal-basis vectors pointing to the corners of an icosahedron, $\mathbf{a}_1^* = a^*(0, 0, 1)$, $\mathbf{a}_i^* = a^*[\sin\theta\cos(2\pi i/5), \sin\theta\sin(2\pi i/5), \cos\theta]$, $i = 2, \ldots, 6$, $\sin\theta = 2/(5)^{1/2}$, $\cos\theta = 1/(5)^{1/2}$, with $\theta \simeq 63.44^\circ$, the angle between two neighbouring fivefold axes (setting 1) (Fig. 4.6.3.28). In this case, the physical-space basis corresponds to a simple projection of the 6D reciprocal basis $\mathbf{d}_i^*$, $i = 1, \ldots, 6$. Sometimes, the same set of six reciprocal-basis vectors is referred to a differently oriented Cartesian reference system (C basis, with basis vectors $\mathbf{e}_i$ along the twofold axes) (Bancel *et al.*, 1985). The reciprocal basis is

$$\begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix} = \frac{a^*}{(1+\tau^2)^{1/2}} \begin{pmatrix} 0 & 1 & \tau \\ -1 & \tau & 0 \\ -\tau & 0 & 1 \\ 0 & -1 & \tau \\ \tau & 0 & 1 \\ 1 & \tau & 0 \end{pmatrix}_C \begin{pmatrix} \mathbf{e}_1^C \\ \mathbf{e}_2^C \\ \mathbf{e}_3^C \end{pmatrix}.$$

An alternate way of indexing is based on a 3D set of cubic reciprocal-basis vectors $\mathbf{b}_i^*$, $i = 1, \ldots, 3$ (setting 2) (Fig. 4.6.3.32):

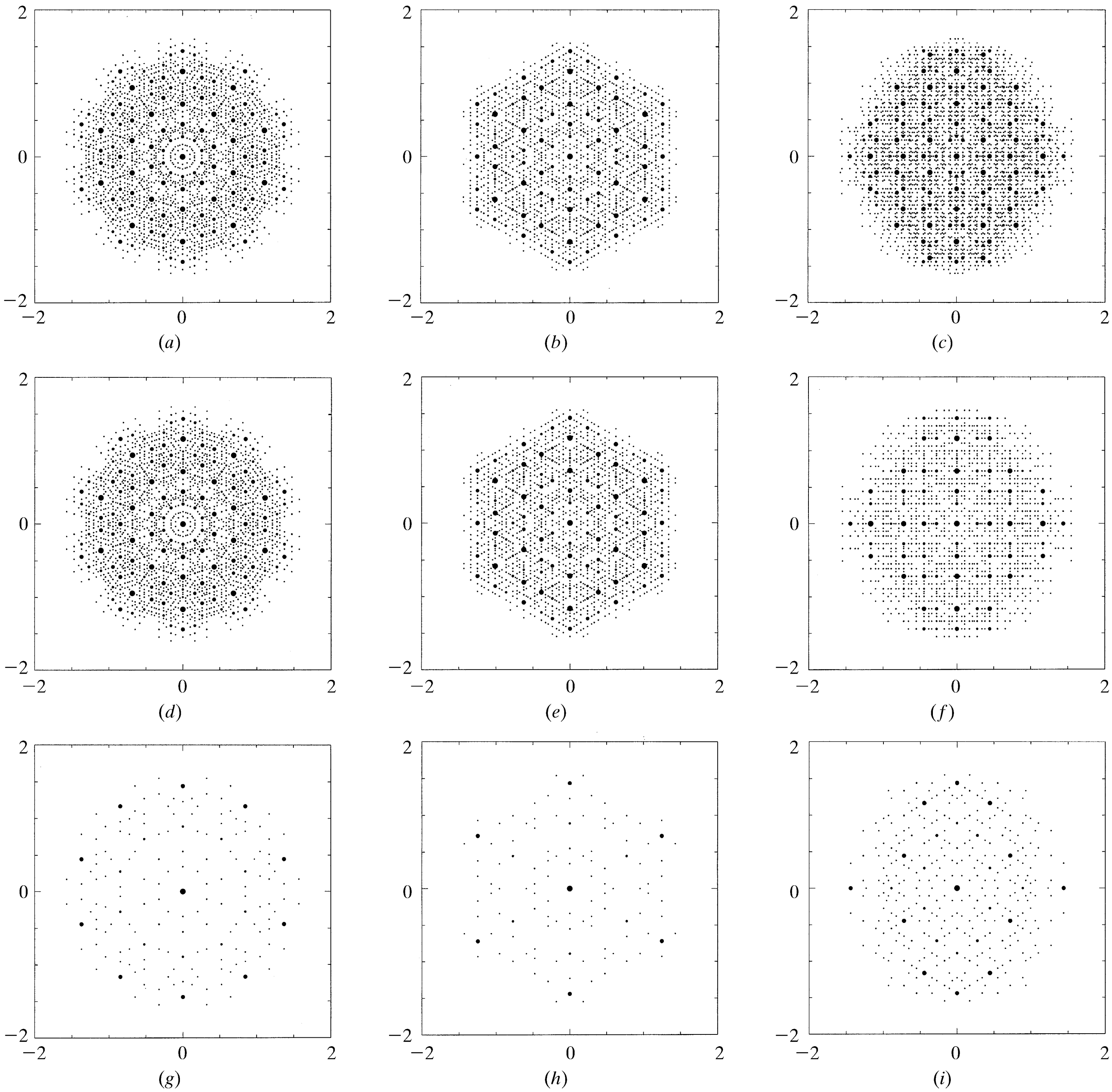

Fig. 4.6.3.33. Physical-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0$ Å). Sections with five-, three- and twofold symmetry are shown for the primitive 6D analogue of Bravais type P in (a, b, c), the body-centred 6D analogue to Bravais type I in (d, e, f) and the face-centred 6D analogue to Bravais type F in (g, h, i). All reflections are shown within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \le h_i \le 6, i = 1, \ldots, 6$.

$$\begin{pmatrix}\mathbf{b}_1^*\\ \mathbf{b}_2^*\\ \mathbf{b}_3^*\end{pmatrix} = \tfrac{1}{2}\begin{pmatrix}0&\bar{1}&0&0&0&1\\ 1&0&0&\bar{1}&0&0\\ 0&0&1&0&1&0\end{pmatrix}_D \begin{pmatrix}\mathbf{a}_1^*\\ \mathbf{a}_2^*\\ \mathbf{a}_3^*\\ \mathbf{a}_4^*\\ \mathbf{a}_5^*\\ \mathbf{a}_6^*\end{pmatrix} = \frac{a^*}{(1+\tau^2)^{1/2}}\begin{pmatrix}\mathbf{e}_1^C\\ \mathbf{e}_2^C\\ \mathbf{e}_3^C\end{pmatrix}.$$

The Cartesian C basis is related to the V basis by a $\theta/2$ rotation around $[100]_C$, yielding $[001]_V$, followed by a $\pi/10$ rotation around $[001]_C$:

$$\begin{pmatrix}\mathbf{e}_1^C\\ \mathbf{e}_2^C\\ \mathbf{e}_3^C\end{pmatrix} = \begin{pmatrix}\cos(\pi/10) & \sin(\pi/10) & 0\\ -\cos(\theta/2)\sin(\pi/10) & \cos(\theta/2)\cos(\pi/10) & \sin(\theta/2)\\ \sin(\theta/2)\sin(\pi/10) & -\sin(\theta/2)\cos(\pi/10) & \cos(\theta/2)\end{pmatrix}_V \begin{pmatrix}\mathbf{e}_1^V\\ \mathbf{e}_2^V\\ \mathbf{e}_3^V\end{pmatrix}.$$

Thus, indexing the diffraction pattern of an icosahedral phase with integer indices, one obtains for setting 1 $\mathbf{H} = \sum_{i=1}^{6} h_i \mathbf{a}_i^*$, $h_i \in \mathbb{Z}$. These indices ($h_1\ h_2\ h_3\ h_4\ h_5\ h_6$) transform into the second setting to ($h/h'\ k/k'\ l/l'$) with the fractional cubic indices $h_1^c = h + h'\tau$, $h_2^c = k + k'\tau$, $h_3^c = l + l'\tau$. The transformation matrix is

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
$\frac{2}{m}\bar{3}\bar{5}$	120	$P\frac{2}{m}\bar{3}\bar{5}$	No condition
		$P\frac{2}{n}\bar{3}\bar{5}$	$h_1h_2\overline{h_1h_2}h_5h_6$: $h_5-h_6=2n$
		$I\frac{2}{m}\bar{3}\bar{5}$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i=1}^{6}h_i=2n$
		$F\frac{2}{m}\bar{3}\bar{5}$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i\neq j=1}^{6}h_i+h_j=2n$
		$F\frac{2}{n}\bar{3}\bar{5}$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i\neq j=1}^{6}h_i+h_j=2n$ $h_1h_2\overline{h_1h_2}h_5h_6$: $h_5-h_6=4n$
235	60	$P235$	No condition
		$P235_1$	$h_1h_2h_2h_2h_2h_2$: $h_1=5n$
		$I235$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i=1}^{6}h_i=2n$
		$I235_1$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i=1}^{6}h_i=2n$ $h_1h_2h_2h_2h_2h_2$: $h_1+5h_2=10n$
		$F235$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i\neq j=1}^{6}h_i+h_j=2n$
		$F235_1$	$h_1h_2h_3h_4h_5h_6$: $\sum_{i\neq j=1}^{6}h_i+h_j=2n$ $h_1h_2h_2h_2h_2h_2$: $h_1+5h_2=10n$

$$\begin{pmatrix} h \\ h' \\ k \\ k' \\ l \\ l' \end{pmatrix}_C = \begin{pmatrix} 0 & \bar{1} & 0 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 & 1 & 0 \\ 1 & 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \end{pmatrix}_D = \begin{pmatrix} h_6-h_2 \\ h_5-h_3 \\ h_1-h_4 \\ h_6+h_2 \\ h_5+h_3 \\ h_1+h_4 \end{pmatrix}_D .$$

4.6.3.3.3.2. Diffraction symmetry

The diffraction symmetry of icosahedral phases can be described by the Laue group $K = m\bar{3}\bar{5}$. The set of all vectors $\mathbf{H}$ forms a Fourier module $M^* = \{\mathbf{H}^{\parallel} = \sum_{i=1}^{6} h_i\mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ of rank 6 in physical space. Consequently, it can be considered as a projection from a 6D reciprocal lattice, $M^* = \pi^{\parallel}(\Sigma^*)$. The parallel and perpendicular reciprocal-space sections of the 3D Penrose tiling decorated with equal point scatterers on its vertices are shown in Figs. 4.6.3.33 and 4.6.3.34. The diffraction pattern in perpendicular space is the Fourier transform of the triacontahedron. All Bragg reflections within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ are depicted. Without intensity-truncation limit, the diffraction pattern would be densely filled with discrete Bragg reflections.

The 6D icosahedral space groups that are relevant to the description of icosahedral phases (six symmorphous and five non-symmorphous groups) are listed in Table 4.6.3.2. These space groups are a subset of all 6D icosahedral space groups fulfilling the condition that the 6D point groups they are associated with are isomorphous to the 3D point groups $\frac{2}{m}\bar{3}\bar{5}$ and 235 describing the diffraction symmetry. From 826 6D (analogues to) Bravais groups (Levitov & Rhyner, 1988), only three fulfil the condition that the projection of the 6D hypercubic lattice upon the 3D physical space is compatible with the icosahedral point groups $\frac{2}{m}\bar{3}\bar{5}$, 235: the primitive hypercubic Bravais lattice P, the body-centred Bravais lattice I with translation 1/2(111111), and the face-centred Bravais lattice F with translations $1/2(110000) + 14$ further cyclic permutations. Hence, the I lattice is twofold primitive (*i.e.* it contains two vertices per unit cell) and the F lattice is 16-fold primitive. The orientation of the symmetry elements in the 6D space is defined by the isomorphism of the 3D and 6D point groups. The action of the fivefold rotation, however, is different in the subspaces $\mathbf{V}^{\parallel}$ and $\mathbf{V}^{\perp}$: a rotation of $2\pi/5$ in $\mathbf{V}^{\parallel}$ is correlated with a rotation of $4\pi/5$ in $\mathbf{V}^{\perp}$. The reflection and inversion operations are equivalent in both subspaces.

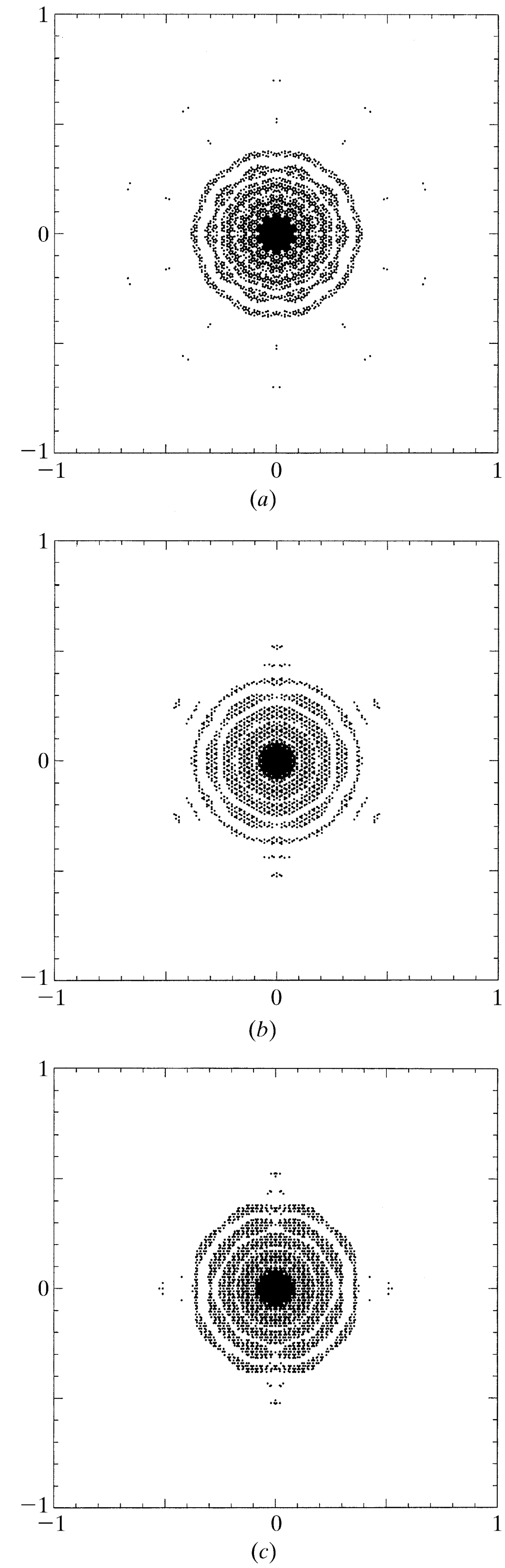

Fig. 4.6.3.34. Perpendicular-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra a_r = 5.0 Å). Sections with (*a*) five-, (*b*) three- and (*c*) twofold symmetry are shown for the primitive 6D analogue of Bravais type *P*. All reflections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