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

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

*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.

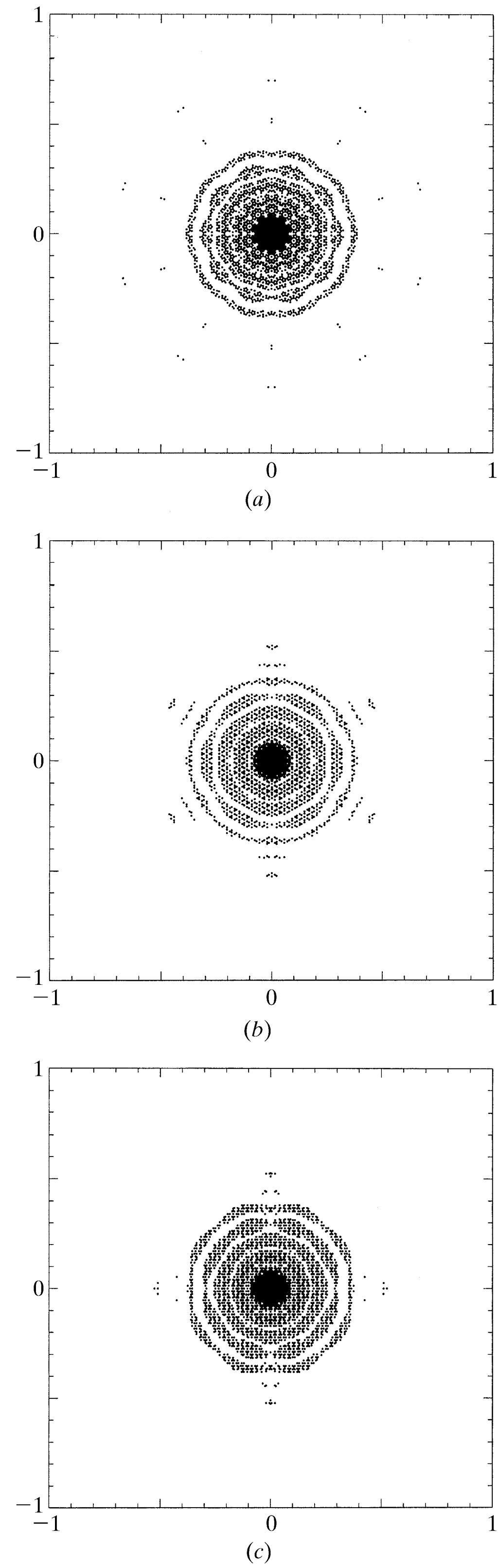


Fig. 4.6.3.34. Perpendicular-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0$ Å). Sections with (*a*) five-, (*b*) three- and (*c*) twofold symmetry are shown for the primitive 6D analogue of Bravais type *P*. All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

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