

## 4.6. RECIPROCAL-SPACE IMAGES OF APERIODIC CRYSTALS

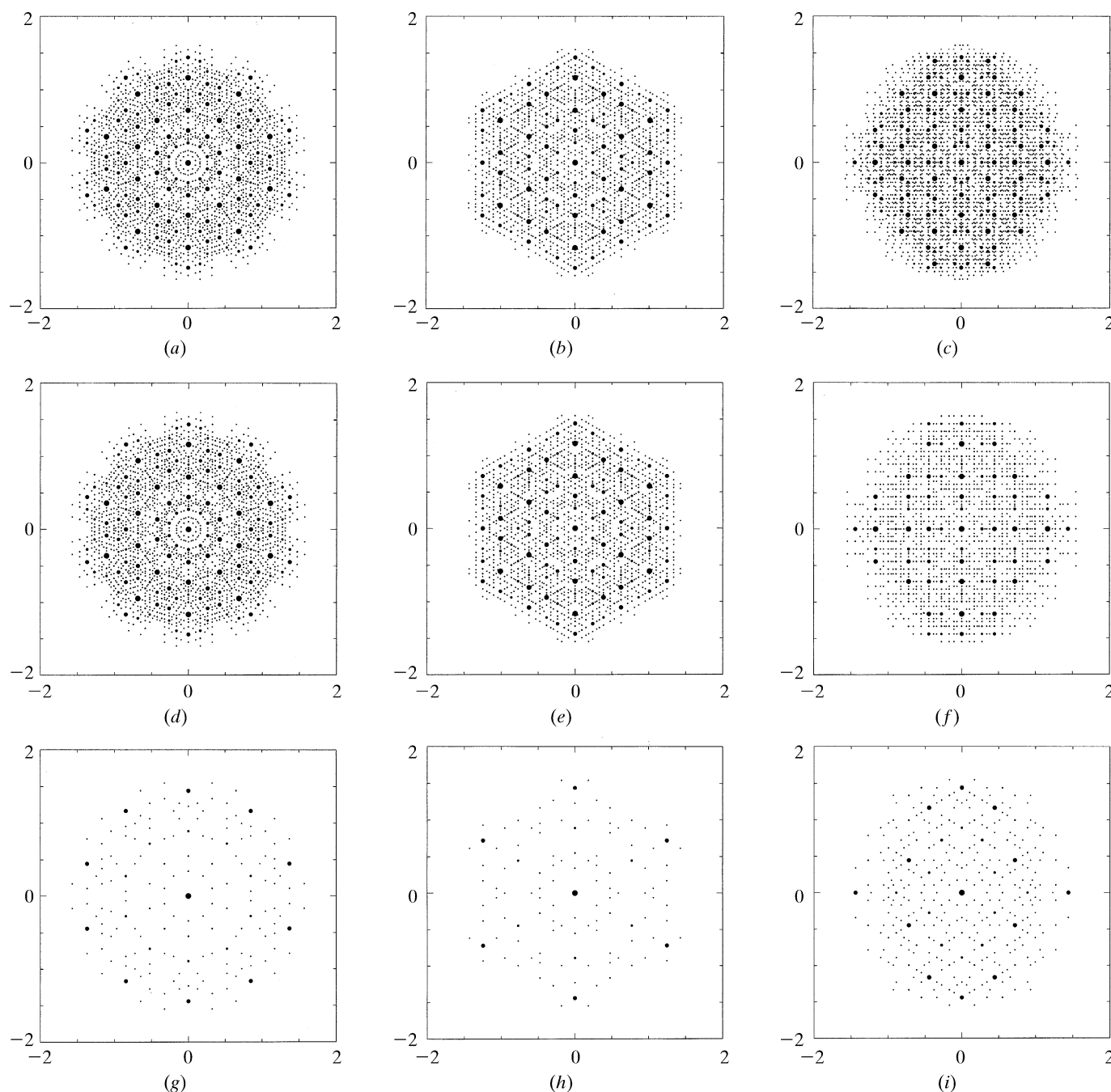


Fig. 4.6.3.33. Physical-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra  $a_r = 5.0 \text{ \AA}$ ). Sections with five-, three- and twofold symmetry are shown for the primitive 6D analogue of Bravais type  $P$  in (a, b, c), 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  $-6 \leq h_i \leq 6, i = 1, \dots, 6$ .

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

where  $A_{\text{UC}}^\perp$  is the volume of the 6D unit cell projected upon  $\mathbf{V}^\perp$  and  $A_k$  is the volume of the triacontahedron.  $A_{\text{UC}}^\perp$  and  $A_k$  are equal in the present case and amount to the volumes of ten prolate and ten oblate rhombohedra:  $A_{\text{UC}}^\perp = 8a_r^3 [\sin(2\pi/5) + \sin(\pi/5)]$ . Evaluating the integral by decomposing the triacontahedron into trigonal pyramids, each one directed from the centre of the triacontahedron to three of its corners given by the vectors  $\mathbf{e}_i, i = 1, \dots, 3$ , one obtains

$$g(\mathbf{H}^\perp) = (1/A_{\text{UC}}^\perp) \sum_R g_k(R^T \mathbf{H}^\perp),$$

with  $k = 1, \dots, 60$  running over all site-symmetry operations  $R$  of the icosahedral group,

$$g_k(\mathbf{H}^\perp) = -iV_r [A_2 A_3 A_4 \exp(iA_1) + A_1 A_3 A_5 \exp(iA_2) + A_1 A_2 A_6 \exp(iA_3) + A_4 A_5 A_6] \times (A_1 A_2 A_3 A_4 A_5 A_6)^{-1},$$

$A_j = 2\pi \mathbf{H}^\perp \cdot \mathbf{e}_j, j = 1, \dots, 3, A_4 = A_2 - A_3, A_5 = A_3 - A_1, A_6 = A_1 - A_2$  and  $V_r = \mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3)$  the volume of the parallelepiped defined by the vectors  $\mathbf{e}_i, i = 1, \dots, 3$  (Yamamoto, 1992b).

## 4.6.3.3.3.4. Intensity statistics

The radial structure-factor distributions of the 3D Penrose tiling decorated with point scatterers are plotted in Fig. 4.6.3.35 as a function of parallel and perpendicular space. The distribution of  $|F(\mathbf{H})|$  as a function of their frequencies clearly resembles a centric