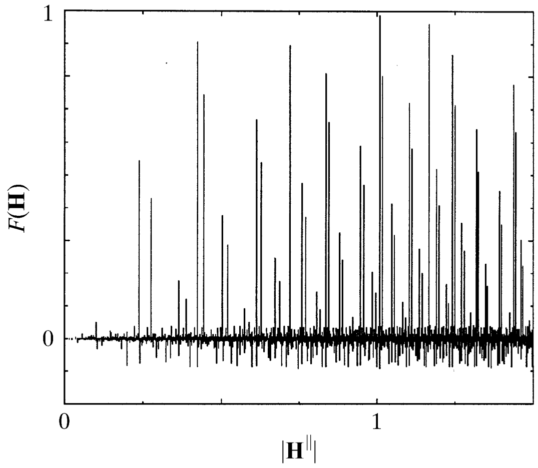

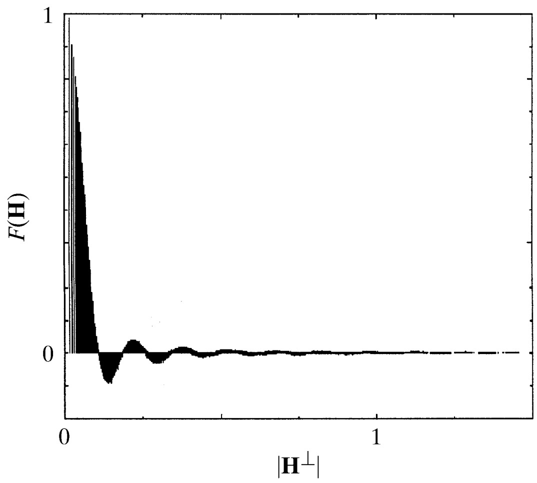

Fig. 4.6.3.35. Radial distribution function of the structure factors $F(\mathbf{H})$ of the 3D Penrose tiling (edge lengths of the Penrose unit rhombohedra $a_r = 5.0$ Å) decorated with point atoms as a function of $|\mathbf{H}^{\parallel}|$ (above) and $|\mathbf{H}^{\perp}|$ (below). All reflections are shown within $10^{-6}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \le h_i \le 6, i = 1, \ldots, 6$.

4.6.3.3.3.3. Structure factor

The structure factor of the icosahedral phase corresponds to the Fourier transform of the 6D unit cell,

$$F(\mathbf{H}) = \sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel}) T_k(\mathbf{H}^{\parallel}, \mathbf{H}^{\perp}) g_k(\mathbf{H}^{\perp}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_k),$$

with 6D diffraction vectors $\mathbf{H} = \sum_{i=1}^{6} h_i \mathbf{d}_i^*$, parallel-space atomic scattering factor $f_k(H^{\parallel})$, temperature factor $T_k(\mathbf{H}^{\parallel}, \mathbf{H}^{\perp})$ and perpendicular-space geometric form factor $g_k(\mathbf{H}^{\perp})$. $T_k(\mathbf{H}^{\parallel}, \mathbf{0})$ is equivalent to the conventional Debye–Waller factor and $T_k(\mathbf{0}, \mathbf{H}^{\perp})$ describes random fluctuations in perpendicular space. These fluctuations cause characteristic jumps of vertices (*phason flips*) in the physical space. Even random phason flips map the vertices onto positions that can still be described by physical-space vectors of the type $\mathbf{r} = \sum_{i=1}^{6} n_i \mathbf{a}_i$. Consequently, the set $M = \{\mathbf{r} = \sum_{i=1}^{6} n_i \mathbf{a}_i | n_i \in \mathbb{Z}\}$ of all possible vectors forms a $\mathbb{Z}$ module. The shape of the atomic surfaces corresponds to a selection rule for the positions actually occupied. The geometric form factor $g_k(\mathbf{H}^{\perp})$ is equivalent to the Fourier transform of the *atomic surface*, *i.e.* the 3D perpendicular-space component of the 6D *hyperatoms*.

For the example of the canonical 3D Penrose tiling, $g_k(\mathbf{H}^{\perp})$ corresponds to the Fourier transform of a triacontahedron:

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

where $A_{\rm UC}^{\perp}$ is the volume of the 6D unit cell projected upon $\mathbf{V}^{\perp}$ and A_k is the volume of the triacontahedron. $A_{\rm UC}^{\perp}$ and A_k are equal in the present case and amount to the volumes of ten prolate and ten oblate rhombohedra: $A_{\rm UC}^{\perp} = 8a_r^3[\sin(2\pi/5) + \sin(\pi/5)]$. 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 $\mathbf{e}_i$, $i = 1, \ldots, 3$, one obtains

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

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

$$\begin{aligned} g_k(\mathbf{H}^{\perp}) = {} & -iV_r[A_2A_3A_4 \exp(iA_1) + A_1A_3A_5 \exp(iA_2) \\ & + A_1A_2A_6 \exp(iA_3) + A_4A_5A_6] \\ & \times (A_1A_2A_3A_4A_5A_6)^{-1}, \end{aligned}$$

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

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 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 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 $K = m\bar{3}\bar{5}$. It is invariant under the action of the scaling matrix S^3:

$$S = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \end{pmatrix}_D, \quad S^3 = \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & -1 & -1 & 1 \\ 1 & 1 & 2 & 1 & -1 & -1 \\ 1 & -1 & 1 & 2 & 1 & -1 \\ 1 & -1 & -1 & 1 & 2 & 1 \\ 1 & 1 & -1 & -1 & 1 & 2 \end{pmatrix}_D,$$

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

references