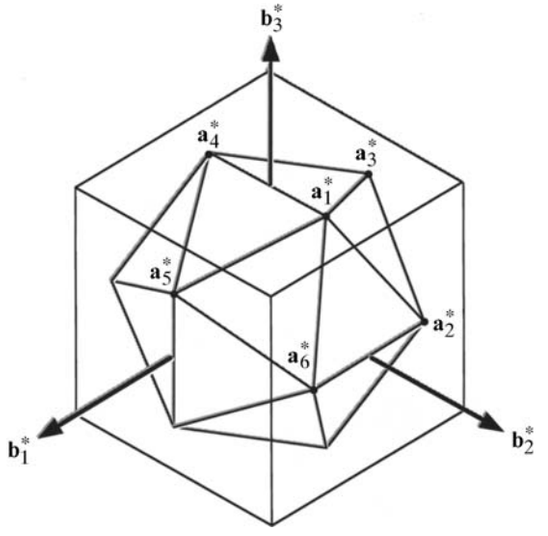

Fig. 4.6.3.32. Perspective parallel-space view of the two alternative reciprocal bases of the 3D Penrose tiling: the cubic and the icosahedral setting, represented by the bases $\mathbf{b}_i^*, i = 1, \ldots, 3$, and $\mathbf{a}_i^*, i = 1, \ldots, 6$, respectively.

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):

$$\begin{pmatrix} \mathbf{b}_1^* \\ \mathbf{b}_2^* \\ \mathbf{b}_3^* \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & \bar{1} & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}_D \begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix}$$

$$= \frac{a^*}{(1+\tau^2)^{1/2}} \begin{pmatrix} \mathbf{e}_1^C \\ \mathbf{e}_2^C \\ \mathbf{e}_3^C \end{pmatrix}.$$

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

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

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.

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:

references