International Tables for Crystallography (2010). Vol. B, Figure 4.6.3.32, p. 616.

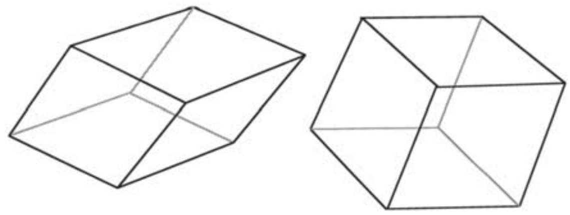

Fig. 4.6.3.30. The two unit tiles of the 3D Penrose tiling: a prolate $[\alpha_{\rm p} = \arccos(5^{-1/2}) \simeq 63.44^\circ]$ and an oblate $(\alpha_{\rm o} = 180^\circ - \alpha_{\rm p})$ rhombohedron with equal edge lengths $a_{\rm r}$.

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

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 $a_{\rm r}$ (Fig. 4.6.3.30). Each face of the rhombohedra is a rhomb with acute angles $\alpha_{\rm r} = \arccos[1/(5)^{1/2}] \simeq 63.44^\circ$. Their volumes are $V_{\rm p} = (4/5)a_{\rm r}^3 \sin(2\pi/5)$, $V_{\rm o} = (4/5)a_{\rm r}^3 \sin(\pi/5) = V_{\rm p}/\tau$, and their frequencies $\nu_{\rm p}{:}\nu_{\rm o} = \tau{:}1$. The resulting point density (number of vertices per unit volume) is $\rho_{\rm p} = (\tau+1)/(\tau V_{\rm p} + V_{\rm o}) = (\tau/a_{\rm r}^3)\sin(2\pi/5)$. 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).

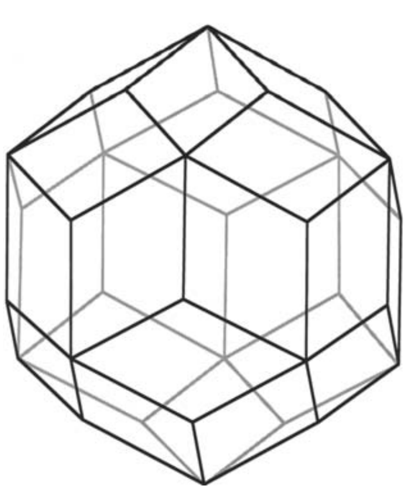

Fig. 4.6.3.31. Atomic surface of the 3D Penrose tiling in the 6D hypercubic description. The projection of the 6D hypercubic unit cell upon $\mathbf{V}^\perp$ gives a rhombic triacontahedron.

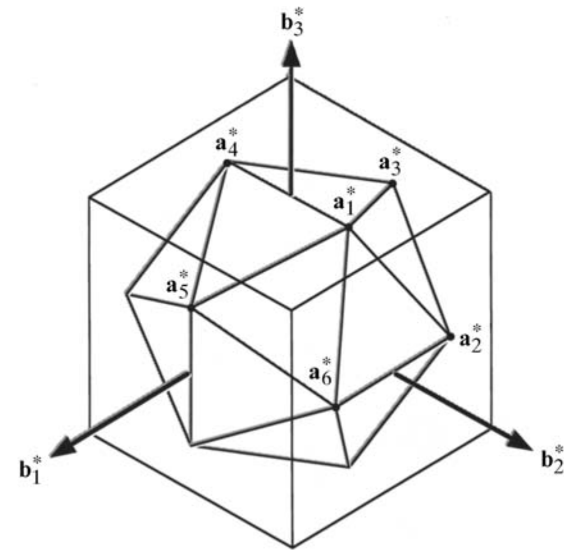

Fig. 4.6.3.32. Perspective parallel-space view of the two alternative reciprocal bases of the 3D Penrose tiling: the cubic and the icosahedral setting, represented by the bases $\mathbf{b}_i^*$, $i = 1, \ldots, 3$, and $\mathbf{a}_i^*$, $i = 1, \ldots, 6$, respectively.

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):

references