International Tables for Crystallography (2006). Vol. B, Figure 4.6.3.12, p. 503.

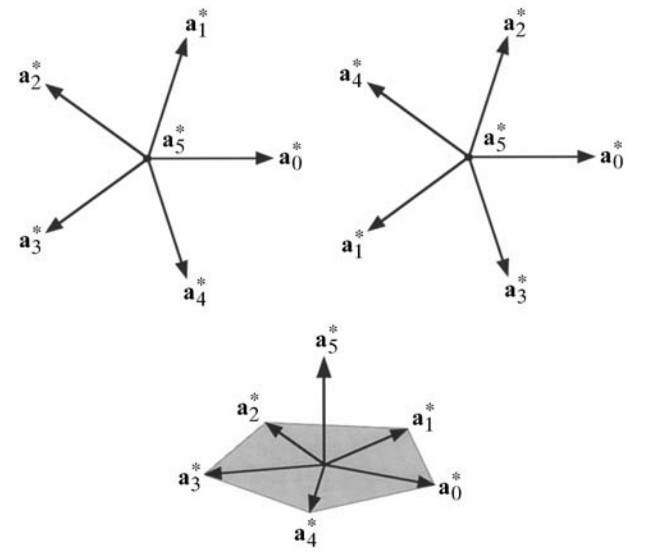

Fig. 4.6.3.12. Reciprocal basis of the decagonal phase in the 5D description projected upon $\mathbf{V}^{\|}$ (above left) and $\mathbf{V}^{\perp}$ (above right). Below, a perspective physical-space view is shown.

4.6.3.3.2. *Decagonal phases*

A structure quasiperiodic in two dimensions, periodic in the third dimension and with decagonal diffraction symmetry is called a decagonal phase. Its holohedral Laue symmetry group is $K = 10/mmm$. All reciprocal-space vectors $\mathbf{H} \in M^*$ can be represented on a basis (V basis) $\mathbf{a}_i^* = a_i^*\,(\cos 2\pi i/5, \sin 2\pi i/5, 0)$, $i = 1, \ldots, 4$ and $\mathbf{a}_5^* = a_5^*(0, 0, 1)$ (Fig. 4.6.3.12) as $\mathbf{H} = \sum_{i=1}^{5} h_i \mathbf{a}_i^*$. The vector components refer to a Cartesian coordinate system in physical (parallel) space. Thus, from the number of independent reciprocal-basis vectors necessary to index the Bragg reflections with integer numbers, the dimension of the embedding space has to be at least five. This can also be shown in a different way (Hermann, 1949).

The set M^* of all vectors $\mathbf{H}$ remains invariant under the action of the symmetry operators of the point group $10/mmm$. The symmetry-adapted matrix representations for the point-group generators, the tenfold rotation $\alpha = 10$, the reflection plane $\beta = m_2$ (normal of the reflection plane along the vectors $\mathbf{a}_i^*\mathbf{a}_{i+3}^*$ with $i = 1, \ldots, 4$ modulo 5) and the inversion operation $\Gamma(\gamma) = \bar{1}$ may be written in the form

$$\Gamma(\alpha) = \begin{pmatrix} 0 & 1 & \bar{1} & 0 & 0 \\ 0 & 1 & 0 & \bar{1} & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \bar{1} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D \quad \Gamma(\beta) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_D$$

$$\Gamma(\gamma) = \begin{pmatrix} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & \bar{1} \end{pmatrix}_D .$$

By block-diagonalization, these reducible symmetry matrices can be decomposed into non-equivalent irreducible representations. These can be assigned to the two orthogonal subspaces forming the 5D embedding space $\mathbf{V} = \mathbf{V}^{\|} \oplus \mathbf{V}^{\perp}$, the 3D parallel (physical) subspace $\mathbf{V}^{\|}$ and the perpendicular 2D subspace $\mathbf{V}^{\perp}$. Thus, using $W\Gamma W^{-1} = \Gamma_V = \Gamma_V^{\|} \oplus \Gamma_V^{\perp}$, we obtain

$$\Gamma_V(\alpha) = \left(\begin{array}{ccc|cc} \cos(\pi/5) & -\sin(\pi/5) & 0 & 0 & 0 \\ \sin(\pi/5) & \cos(\pi/5) & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & \cos(3\pi/5) & -\sin(3\pi/5) \\ 0 & 0 & 0 & \sin(3\pi/5) & \cos(3\pi/5) \end{array}\right)_V$$

$$= \left(\begin{array}{c|c} \Gamma^{\|}(\alpha) & 0 \\ \hline 0 & \Gamma^{\perp}(\alpha) \end{array}\right)_V ,$$

$$\Gamma_V(\beta) = \left(\begin{array}{ccc|cc} 1 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right)_V , \quad \Gamma_V(\gamma) \left(\begin{array}{ccc|cc} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 \\ \hline 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & \bar{1} \end{array}\right)_V ,$$

where

$$W = \left(\begin{array}{ccccc} a_1^*\cos(2\pi/5) & a_2^*\cos(4\pi/5) & a_3^*\cos(6\pi/5) & a_4^*\cos(8\pi/5) & 0 \\ a_1^*\sin(2\pi/5) & a_2^*\sin(4\pi/5) & a_3^*\sin(6\pi/5) & a_4^*\sin(8\pi/5) & 0 \\ 0 & 0 & 0 & 0 & a_5^* \\ \hline a_1^*\cos(6\pi/5) & a_2^*\cos(2\pi/5) & a_3^*\cos(8\pi/5) & a_4^*\cos(4\pi/5) & 0 \\ a_1^*\sin(6\pi/5) & a_2^*\sin(2\pi/5) & a_3^*\sin(8\pi/5) & a_4^*\sin(4\pi/5) & 0 \end{array}\right).$$

The column vectors of the matrix W give the parallel- (above the partition line) and perpendicular-space components (below the partition line) of a reciprocal basis in V space. Thus, W can be rewritten using the physical-space reciprocal basis defined above as

$$W = (\mathbf{d}_1^*, \quad \mathbf{d}_2^*, \quad \mathbf{d}_3^*, \quad \mathbf{d}_4^*, \quad \mathbf{d}_5^*),$$

yielding the reciprocal basis $\mathbf{d}_i^*, i = 1, \ldots, 5$, in the 5D embedding space (D space):

$$\mathbf{d}_i^* = a_i^* \begin{pmatrix} \cos(2\pi i/5) \\ \sin(2\pi i/5) \\ 0 \\ \cos(6\pi i/5) \\ \sin(6\pi i/5) \end{pmatrix}_V , \; i = 1, \ldots, 4 \text{ and } \mathbf{d}_5^* = a_5^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}_V .$$

The 5×5 symmetry matrices can each be decomposed into a 3×3 matrix and a 2×2 matrix. The first one, $\Gamma^{\|}$, acts on the parallel-space component, the second one, $\Gamma^{\perp}$, on the perpendicular-space component. In the case of $\Gamma(\alpha)$, the coupling factor between a rotation in parallel and perpendicular space is 3. Thus, a $\pi/5$ rotation in physical space is related to a $3\pi/5$ rotation in perpendicular space (Fig. 4.6.3.12).

With the condition $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$, a basis in direct 5D space is obtained:

$$\mathbf{d}_i = \frac{2}{5a_i^*} \begin{pmatrix} \cos(2\pi i/5) - 1 \\ \sin(2\pi i/5) \\ 0 \\ \cos(6\pi i/5) - 1 \\ \sin(6\pi i/5) \end{pmatrix}, \; i = 1, \ldots, 4, \text{ and } \mathbf{d}_5 = \frac{1}{a_5^*} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

The metric tensors G, G^* are of the type

$$\begin{pmatrix} A & C & C & C & 0 \\ C & A & C & C & 0 \\ C & C & A & C & 0 \\ C & C & C & A & 0 \\ 0 & 0 & 0 & 0 & B \end{pmatrix}$$

with $A = 2a_1^{*2}, B = a_5^{*2}, C = -(1/2)a_1^{*2}$ for the reciprocal space and $A = 4/5a_1^{*2}, B = 1/a_5^{*2}, C = 2/5a_1^{*2}$ for the direct space. Thus, for the lattice parameters in reciprocal space we obtain