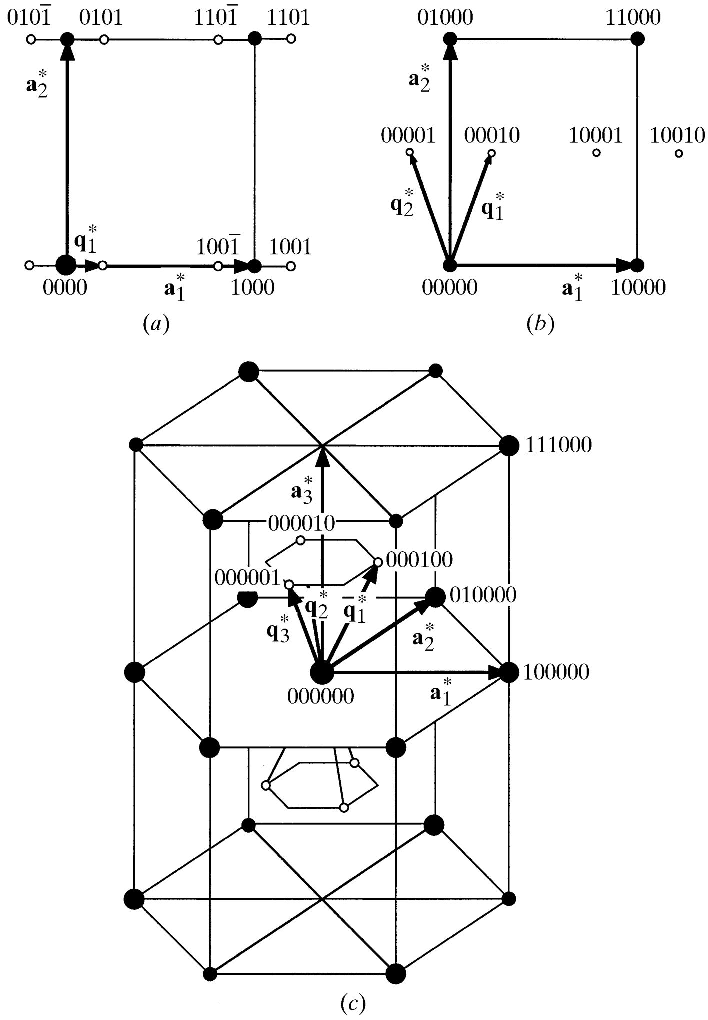

Fig. 4.6.3.1. Schematic diffraction patterns for IMSs with (*a*) 1D, (*b*) 2D and (*c*) 3D modulation. The satellite vectors correspond to $\mathbf{q} = \alpha_1\mathbf{a}_1^*$ in (*a*), $\mathbf{q}_1 = \alpha_{11}\mathbf{a}_1^* + (1/2)\mathbf{a}_2^*$ and $\mathbf{q}_2 = -\alpha_{12}\mathbf{a}_1^* + (1/2)\mathbf{a}_2^*$, where $\alpha_{11} = \alpha_{12}$, in (*b*), and $\mathbf{q}_1 = \alpha_{11}\mathbf{a}_1^* + \alpha_{31}\mathbf{a}_3^*$, $\mathbf{q}_2 = \alpha_{12}(-\mathbf{a}_1^* + \mathbf{a}_2^*) + \alpha_{32}\mathbf{a}_3^*$, $\mathbf{q}_3 = -\alpha_{13}\mathbf{a}_2^* + \alpha_{33}\mathbf{a}_3^*$, where $\alpha_{11} = \alpha_{12} = \alpha_{13}$ and $\alpha_{31} = \alpha_{32} = \alpha_{33}$, in (*c*). The areas of the circles are proportional to the reflection intensities. Main (filled circles) and satellite (open circles) reflections are indexed (after Janner *et al.*, 1983*b*).

IMS, at least one entry to σ has to be irrational. The wavelength of the modulation function is $\lambda_j = 1/q_j$. The set of vectors $\mathbf{H}$ forms a Fourier module $M^* = \{\mathbf{H} = \sum_{i=1}^{3+d} h_i\mathbf{a}_i^* | h_i \in \mathbb{Z}\}$ of rank $n = 3 + d$, which can be decomposed into a rank 3 and a rank d submodule $M^* = M_1^* \oplus M_2^*$. $M_1^* = \{h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*\}$ corresponds to a $\mathbb{Z}$ module of rank 3 in a 3D subspace (the physical space), $M_2^* = \{h_4\mathbf{a}_4^* + \ldots + h_{3+d}\mathbf{a}_{3+d}^*\}$ corresponds to a $\mathbb{Z}$ module of rank d in a dD subspace (perpendicular space). The submodule M_1 is identical to the 3D reciprocal lattice Λ^* of the average structure. M_2 results from the projection of the perpendicular-space component of the $(3 + d)$D reciprocal lattice Σ^* upon the physical space. Owing to the coincidence of one subspace with the physical space, the dimension of the embedding space is given as $(3 + d)$D and not as nD. This terminology points out the special role of the physical space.

Hence the reciprocal-basis vectors $\mathbf{a}_i^*, i = 1, \ldots, 3 + d$, can be considered to be physical-space projections of reciprocal-basis vectors $\mathbf{d}_i^*, i = 1, \ldots, 3 + d$, spanning a $(3 + d)$D reciprocal lattice Σ^*:

$$\Sigma^* = \left\{\mathbf{H} = \sum_{i=1}^{3+d} h_i\mathbf{d}_i^* \middle| h_i \in \mathbb{Z}\right\},$$

$$\mathbf{d}_i^* = (\mathbf{a}_i^*, \mathbf{0}),\ i = 1, \ldots, 3 \text{ and } \mathbf{d}_{3+j}^* = (\mathbf{a}_{3+j}^*, c\mathbf{e}_j^*),\ j = 1, \ldots, d.$$

The first vector component of $\mathbf{d}_i^*$ refers to the physical space, the second to the perpendicular space spanned by the mutually orthogonal unit vectors $\mathbf{e}_j$. c is an arbitrary constant which can be set to 1 without loss of generality.

A direct lattice Σ with basis $\mathbf{d}_i$, $i = 1, \ldots, 3 + d$ and $\mathbf{d}_i \cdot \mathbf{d}_j^* = \delta_{ij}$, can be constructed according to

$$\Sigma = \left\{\mathbf{r} = \sum_{i=1}^{3+d} m_i\mathbf{d}_i \middle| m_i \in \mathbb{Z}\right\},$$

$$\mathbf{d}_i = \left(\mathbf{a}_i, -\sum_{j=1}^{d} \alpha_{ij}(1/c)\mathbf{e}_j\right),\ i = 1, \ldots, 3$$

$$\text{and } \mathbf{d}_{3+j} = \left(\mathbf{0}, (1/c)\mathbf{e}_j^*\right),\ j = 1, \ldots, d.$$

Consequently, the aperiodic structure in physical space $\mathbf{V}^{\parallel}$ is equivalent to a 3D section of the $(3 + d)$D hypercrystal.

4.6.3.1.1. *Indexing*

The 3D reciprocal space M^* of a $(3 + d)$D IMS consists of two separable contributions,

$$M^* = \left\{\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^* + \sum_{j=1}^{d} m_j\mathbf{q}_j\right\},$$

the set of main reflections ($m_j = 0$) and the set of satellite reflections ($m_j \neq 0$) (Fig. 4.6.3.1). In most cases, the modulation is only a weak perturbation of the crystal structure. The main reflections are related to the average structure, the satellites to the difference between the average and actual structure. Consequently, the satellite reflections are generally much weaker than the main reflections and can be easily identified. Once the set of main reflections has been separated, a conventional basis $\mathbf{a}_i^*, i = 1, \ldots, 3$, for Λ^* is chosen.

The only ambiguity is in the assignment of rationally independent satellite vectors $\mathbf{q}_i$. They should be chosen inside the reciprocal-space unit cell (Brillouin zone) of Λ^* in such a way as to give a minimal number d of additional dimensions. If satellite vectors reach the Brillouin-zone boundary, centred $(3 + d)$D Bravais lattices are obtained. The star of satellite vectors has to be invariant under the point-symmetry group of the diffraction pattern. There should be no contradiction to a reasonable physical modulation model concerning period or propagation direction of the modulation wave. More detailed information on how to find the optimum basis and the correct setting is given by Janssen *et al.* (2004) and Janner *et al.* (1983*a*,*b*).

4.6.3.1.2. *Diffraction symmetry*

The Laue symmetry group $K^{\mathrm{L}} = \{R\}$ of the Fourier module M^*,

$$M^* = \left\{\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^* + \sum_{j=1}^{d} m_j\mathbf{q}_j = \sum_{i=1}^{3+d} h_i\mathbf{a}_i^*\right\},\ \Lambda^* = \left\{\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^*\right\},$$

is isomorphous to or a subgroup of one of the 11 3D crystallographic Laue groups leaving Λ^* invariant. The action of the point-group symmetry operators R on the reciprocal basis $\mathbf{a}_i^*, i = 1, \ldots, 3 + d$, can be written as

$$R\mathbf{a}_i^* = \sum_{j=1}^{3+d} \Gamma_{ij}^T(R)\mathbf{a}_j^*,\ i = 1, \ldots, 3 + d.$$