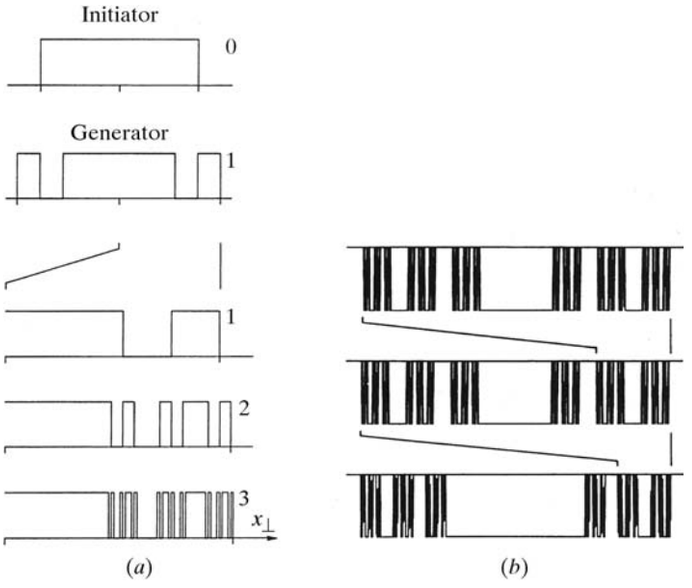

Fig. 4.6.2.12. (*a*) Three steps in the development of the fractal atomic surface of the squared Fibonacci sequence starting from an initiator and a generator. The action of the generator is to cut a piece from each side of the initiator and to add it where the initiator originally ended. This is repeated, cutting thinner and thinner pieces each time from the generated structures. (*b*) Magnification sequence of the fractal atomic surface illustrating its self-similarity. Each successive figure represents a magnification of a selected portion of the previous figure (from Zobetz, 1993).

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ \tau \end{pmatrix} = \begin{pmatrix} \tau+1 \\ 2\tau+1 \end{pmatrix} = \begin{pmatrix} \tau^2 \\ \tau^3 \end{pmatrix} = \tau^2\begin{pmatrix} 1 \\ \tau \end{pmatrix}.$$

Identifying the eigenvector $\begin{pmatrix} 1 \\ \tau \end{pmatrix}$ with $\begin{pmatrix} \mathrm{S} \\ \mathrm{L} \end{pmatrix}$ shows that the infinite 1D sequence $s(\mathbf{r})$ multiplied by powers of its eigenvalue τ^2 (scaling operation) remains invariant (each new lattice point coincides with one of the original lattice):

$$s(\tau^2\mathbf{r}) = s(\mathbf{r}).$$

The fractal sequence can be described on the same reciprocal and direct bases as the Fibonacci sequence. The only difference in the 2D direct-space description is the fractal character of the perpendicular-space component of the hyperatoms (Fig. 4.6.2.12) (see Zobetz, 1993).

4.6.3. Reciprocal-space images

4.6.3.1. *Incommensurately modulated structures (IMSs)*

One-dimensionally modulated structures are the simplest representatives of IMSs. The vast majority of the one hundred or so IMSs known so far belong to this class (Cummins, 1990). However, there is also an increasing number of IMSs with 2D or 3D modulation. The dimension d of the modulation is defined by the number of rationally independent modulation wave vectors (satellite vectors) $\mathbf{q}_i$ (Fig. 4.6.3.1). The electron-density function of a dD modulated 3D crystal can be represented by the Fourier series

$$\rho(\mathbf{r}) = (1/V)\sum_{\mathbf{H}} F(\mathbf{H})\exp(-2\pi i\mathbf{H}\cdot\mathbf{r}).$$

The Fourier coefficients (*structure factors*) $F(\mathbf{H})$ differ from zero only for reciprocal-space vectors $\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^* + \sum_{j=1}^{d} m_j\mathbf{q}_j = \sum_{i=1}^{3+d} h_i\mathbf{a}_i^*$ with $h_i, m_j \in \mathbb{Z}$. The d satellite vectors are given by $\mathbf{q}_j = \mathbf{a}_{3+j}^* = \sum_{i=1}^{3}\alpha_{ij}\mathbf{a}_i^*$, with α_{ij} a $3\times d$ matrix σ. In the case of an 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

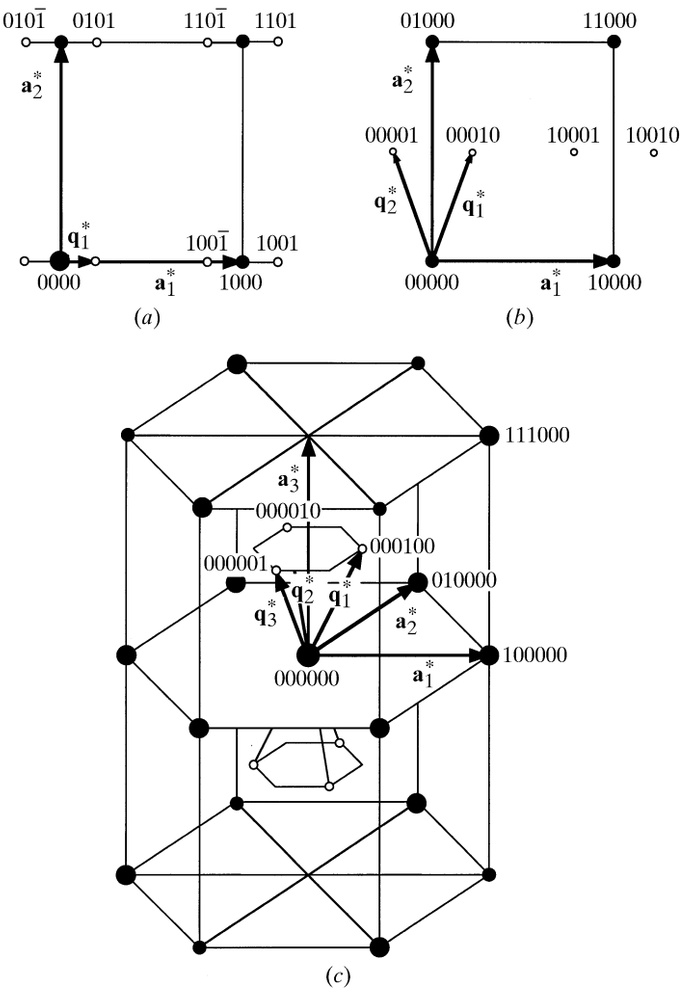

Fig. 4.6.3.1. Schematic diffraction patterns for IMSs with (*a*) 1D, (*b*) 2D and (*c*) 3D modulation. The satellite vectors correspond to $\mathbf{q} = \alpha_1\mathbf{a}_1^*$ in (*a*), $\mathbf{q}_1 = \alpha_{11}\mathbf{a}_1^* + (1/2)\mathbf{a}_2^*$ and $\mathbf{q}_2 = -\alpha_{12}\mathbf{a}_1^* + (1/2)\mathbf{a}_2^*$, 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*).

vectors $\mathbf{d}_i^*, i = 1, \ldots, 3+d$, spanning a $(3+d)$D reciprocal lattice Σ^*:

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

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

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

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

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

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

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 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.* (1999) and Janner *et al.* (1983*a*,*b*).

4.6.3.1.2. *Diffraction symmetry*

The Laue symmetry group $K^L = \{R\}$ 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

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

The $(3+d) \times (3+d)$ matrices $\Gamma^T(R)$ form a finite group of integral matrices which are reducible, since R is already an orthogonal transformation in 3D physical space. Consequently, R can be expressed as pair of orthogonal transformations $(R^{\parallel}, R^{\perp})$ in 3D physical and dD perpendicular space, respectively. Owing to their mutual orthogonality, no symmetry relationship exists between the set of main reflections and the set of satellite reflections. $\Gamma^T(R)$ is the transpose of $\Gamma(R)$ which acts on vector components in direct space.

For the $(3+d)$D direct-space (*superspace*) symmetry operator $(R_s, \mathbf{t}_s)$ and its matrix representation $\Gamma(R_s, \mathbf{t}_s)$ on Σ, the following decomposition can be performed:

$$\Gamma(R_s) = \begin{pmatrix} \Gamma^{\parallel}(R) & 0 \\ \Gamma^M(R) & \Gamma^{\perp}(R) \end{pmatrix} \text{ and } \mathbf{t}_s = (\mathbf{t}_3, \mathbf{t}_d).$$

$\Gamma^{\parallel}(R)$ is a 3×3 matrix, $\Gamma^{\perp}(R)$ is a $d \times d$ matrix and $\Gamma^M(R)$ is a $d \times 3$ matrix. The translation operator $\mathbf{t}_s$ consists of a 3D vector $\mathbf{t}_3$ and a dD vector $\mathbf{t}_d$. According to Janner & Janssen (1979), $\Gamma^M(R)$ can be derived from $\Gamma^M(R) = \sigma\Gamma^{\parallel}(R) - \Gamma^{\perp}(R)\sigma$. $\Gamma^M(R)$ has integer elements only as it contains components of primitive-lattice vectors of Λ^*, whereas σ in general consists of a rational and an irrational part: $\sigma = \sigma^i + \sigma^r$. Thus, only the rational part gives rise to nonzero entries in $\Gamma^M(R)$. With the order of the Laue group denoted by N, one obtains $\sigma^i \equiv (1/N)\sum_R \Gamma^{\perp}(R)\sigma\Gamma^{\parallel}(R)^{-1}$, where $\Gamma^{\perp}(R)\sigma^i\Gamma^{\parallel}(R)^{-1} = \sigma^i$, implying that $\Gamma^M(R) = \sigma^r\Gamma^{\parallel}(R) - \Gamma^{\perp}(R)\sigma^r$ and $0 = \sigma^i\Gamma^{\parallel}(R) - \Gamma^{\perp}(R)\sigma^i$.

Example: In the case of a 3D IMS with 1D modulation $(d = 1)$ the $3 \times d$ matrix

$$\sigma = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$$

has the components of the wavevector $\mathbf{q} = \sum_{i=1}^{3} \alpha_i \mathbf{a}_i^* = \mathbf{q}^i + \mathbf{q}^r$. $\Gamma^{\perp}(R) = \varepsilon = \pm 1$ because for $d = 1$, $\mathbf{q}$ can only be transformed into $\pm\mathbf{q}$. Corresponding to $\mathbf{q}^i \equiv (1/N)\sum_R \varepsilon R\mathbf{q}$, one obtains $R^T\mathbf{q}^i \equiv \varepsilon\mathbf{q}^i$ (modulo Λ^*). The 3×1 row matrix $\Gamma^M(R)$ is equivalent to the difference vector between $R^T\mathbf{q}$ and $\varepsilon\mathbf{q}$ (Janssen *et al.*, 1999).

For a monoclinic modulated structure with point group $2/m$ for M^* (unique axis $\mathbf{a}_3$) and satellite vector $\mathbf{q} = (1/2)\mathbf{a}_1{}^* + \alpha_3\mathbf{a}_3{}^*$, with α_3 an irrational number, one obtains

$$\begin{aligned} \mathbf{q}^i &\equiv (1/N)\sum_R \varepsilon R\mathbf{q} \\ &= \frac{1}{4}\left(+1 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/2 \\ 0 \\ \alpha_3 \end{pmatrix} \right. \\ &\quad + 1 \cdot \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/2 \\ 0 \\ \alpha_3 \end{pmatrix} - 1 \cdot \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 1/2 \\ 0 \\ \alpha_3 \end{pmatrix} \\ &\quad \left. -1 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 1/2 \\ 0 \\ \alpha_3 \end{pmatrix} \right) \\ &= \begin{pmatrix} 0 \\ 0 \\ \alpha_3 \end{pmatrix}. \end{aligned}$$

From the relations $R^T\mathbf{q}^i \equiv \varepsilon\mathbf{q}^i$ (modulo Λ^*), it can be shown that

the symmetry operations 1 and 2 are associated with the perpendicular-space transformations $\varepsilon = 1$, and m and $\bar{1}$ with $\varepsilon = -1$. The matrix $\Gamma^M(R)$ is given by

$$\Gamma^M(2) = \sigma^r \Gamma^{\parallel}(2) - \Gamma^{\perp}(2)\sigma^r = \begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} - (+1) \begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \bar{1} \\ 0 \\ 0 \end{pmatrix}$$

for the operation 2, for instance.

The matrix representations $\Gamma^T(R_s)$ of the symmetry operators R in reciprocal $(3+d)$D superspace decompose according to

$$\Gamma^T(R_s) = \begin{pmatrix} \Gamma^{\parallel T}(R) & \Gamma^{MT}(R) \\ 0 & \Gamma^{\perp T}(R) \end{pmatrix}.$$

Phase relationships between modulation functions of symmetry-equivalent atoms can give rise to systematic extinctions of different classes of satellite reflections. The extinction rules may include indices of both main and satellite reflections. A full list of systematic absences is given in the table of $(3+1)$D superspace groups (Janssen *et al.*, 1999). Thus, once point symmetry and systematic absences are found, the superspace group can be obtained from the tables in a way analogous to that used for regular 3D crystals. A different approach for the symmetry description of IMSs from the 3D Fourier-space perspective has been given by Dräger & Mermin (1996).

4.6.3.1.3. *Structure factor*

The structure factor of a periodic structure is defined as the Fourier transform of the density distribution $\rho(\mathbf{r})$ of its unit cell (UC):

$$F(\mathbf{H}) = \int_{\mathrm{UC}} \rho(\mathbf{r}) \exp(2\pi i \mathbf{H}\cdot\mathbf{r})\, \mathrm{d}\mathbf{r}.$$

The same is valid in the case of the $(3+d)$D description of IMSs. The parallel- and perpendicular-space components are orthogonal to each other and can be separated. The Fourier transform of the parallel-space component of the electron-density distribution of a single atom gives the usual atomic scattering factors $f_k(\mathbf{H}^{\parallel})$. For the structure-factor calculation, one does not need to use $\rho(\mathbf{r})$ explicitly. The hyperatoms correspond to the convolution of the electron-density distribution in 3D physical space with the modulation function in dD perpendicular space. Therefore, the Fourier transform of the $(3+d)$D hyperatoms is simply the product of the Fourier transform $f_k(\mathbf{H}^{\parallel})$ of the physical-space component with the Fourier transform of the perpendicular-space component, the modulation function.

For a general *displacive modulation* one obtains for the ith coordinate x_{ik} of the kth atom in 3D physical space

$$x_{ik} = \bar{x}_{ik} + u_{ik}(\bar{x}_4, \ldots, \bar{x}_{3+d}),\ i = 1, \ldots, 3,$$

where $\bar{x}_{ik}$ are the basic-structure coordinates and $u_{ik}(\bar{x}_4, \ldots, \bar{x}_{3+d})$ are the modulation functions with unit periods in their arguments (Fig. 4.6.3.2). The arguments are $\bar{x}_{3+j} = \alpha_{ij}\bar{x}^0_{ik} + t_j$, $j = 1, \ldots, d$, where $\bar{x}^0_{ik}$ are the coordinates of the kth atom referred to the origin of its unit cell and t_j are the phases of the modulation functions. The modulation functions $u_{ik}(\bar{x}_4, \ldots, \bar{x}_{3+d})$ themselves can be expressed in terms of a Fourier series as

$$u_{ik}(\bar{x}_4, \ldots, \bar{x}_{3+d}) = \sum_{n_1=1}^{\infty} \ldots \sum_{n_d=1}^{\infty} \left\{ {}^{u}C_{ik}^{n_1\ldots n_d} \cos[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] + {}^{u}S_{ik}^{n_1\ldots n_d} \sin[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] \right\},$$

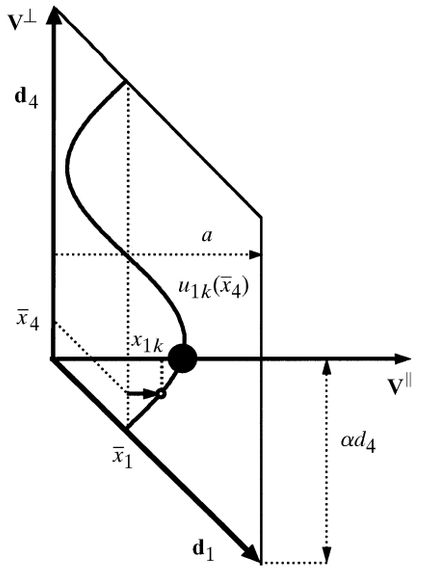

Fig. 4.6.3.2. The relationships between the coordinates $x_{1k}, x_{4k}, \bar{x}_1, \bar{x}_4$ and the modulation function u_{1k} in a special section of the $(3+d)$D space.

where n_j are the orders of harmonics for the jth modulation wave of the ith component of the kth atom and their amplitudes are ${}^{u}C_{ik}^{n_1\ldots n_d}$ and ${}^{u}S_{ik}^{n_1\ldots n_d}$.

Analogous expressions can be derived for a *density modulation*, *i.e.*, the modulation of the occupation probability $p_k(\bar{x}_4, \ldots, \bar{x}_{3+d})$:

$$p_k(\bar{x}_4, \ldots, \bar{x}_{3+d}) = \sum_{n_1=1}^{\infty} \ldots \sum_{n_d=1}^{\infty} \left\{ {}^{p}C_{k}^{n_1\ldots n_d} \cos[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] + {}^{p}S_{k}^{n_1\ldots n_d} \sin[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] \right\},$$

and for the modulation of the tensor of thermal parameters $B_{ijk}(\bar{x}_4, \ldots, \bar{x}_{3+d})$:

$$B_{ijk}(\bar{x}_4, \ldots, \bar{x}_{3+d}) = \sum_{n_1=1}^{\infty} \ldots \sum_{n_d=1}^{\infty} \left\{ {}^{B}C_{ijk}^{n_1\ldots n_d} \cos[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] + {}^{B}S_{ijk}^{n_1\ldots n_d} \sin[2\pi(n_1\bar{x}_4 + \ldots + n_d\bar{x}_{3+d})] \right\}.$$

The resulting structure-factor formula is

$$F(\mathbf{H}) = \sum_{k=1}^{N'} \sum_{(R,\,t)} \int_0^1 \mathrm{d}\bar{x}_{4,\,k} \ldots \int_0^1 \mathrm{d}\bar{x}_{3+d,\,k} f_k(\mathbf{H}^{\parallel}) p_k \times \exp\left(-\sum_{i,\,j=1}^{3+d} h_i \left[RB_{ijk}R^T\right] h_j + 2\pi i \sum_{j=1}^{3+d} h_j R x_{jk} + h_j t_j \right)$$

for summing over the set $(R, \mathbf{t})$ of superspace symmetry operations and the set of N' atoms in the asymmetric unit of the $(3+d)$D unit cell (Yamamoto, 1982). Different approaches without numerical integration based on analytical expressions including Bessel functions have also been developed. For more information see Paciorek & Chapuis (1994), Petricek, Maly & Cisarova (1991), and references therein.

For illustration, some fundamental IMSs will be discussed briefly (see Korekawa, 1967; Böhm, 1977).

Harmonic density modulation. A harmonic density modulation can result on average from an ordered distribution of vacancies on atomic positions. For an IMS with N atoms per unit cell one obtains

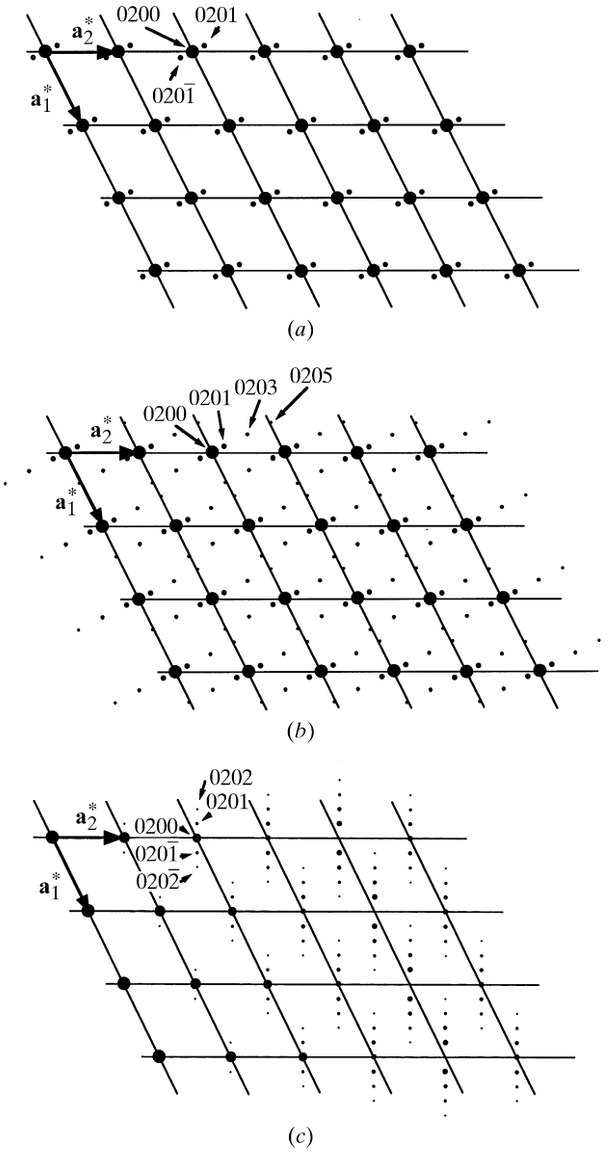

Fig. 4.6.3.3. Schematic diffraction patterns for 3D IMSs with (*a*) 1D harmonic and (*b*) rectangular density modulation. The modulation direction is parallel to $\mathbf{a}_2$. In (*a*) only first-order satellites exist; in (*b*), all odd-order satellites can be present. In (*c*), the diffraction pattern of a harmonic displacive modulation along $\mathbf{a}_1$ with amplitudes parallel to $\mathbf{a}_2^*$ is depicted. Several reflections are indexed. The areas of the circles are proportional to the reflection intensities.

for a harmonic modulation of the occupancy factor

$$p_k = (p_k^0/2)\{1 + \cos[2\pi(\bar{x}_{4,\,k} + \varphi_k)]\}, \quad 0 \le p_k^0 \le 1,$$

the structure-factor formula for the mth order satellite $(0 \le m \le 1)$

$$F_0(\mathbf{H}) = (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_k),$$

$$F_m(\mathbf{H}) = (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})(p_k^0/2)^{|m|}\exp\left[2\pi i\left(\sum_{i=1}^{3} h_i x_{ik} + m\varphi_k\right)\right].$$

Thus, a linear correspondence exists between the structure-factor magnitudes of the satellite reflections and the amplitude of the density modulation. Furthermore, only first-order satellites exist, since the modulation wave consists only of one term. An important criterion for the existence of a density modulation is that a pair of satellites around the origin of the reciprocal lattice exists (Fig. 4.6.3.3).

Symmetric rectangular density modulation. The box-function-like modulated occupancy factor can be expanded into a Fourier series,

$$p_k = p_k^0(4/\pi)\left\{\sum_{n=1}^{\infty}[(-1)^{n+1}/(2n-1)]\cos[2\pi(2n-1)(\bar{x}_{4,\,k} + \varphi_k)]\right\}, \quad 0 \le p_k^0 \le 1,$$

and the resulting structure factor of the mth order satellite is

$$F_0(\mathbf{H}) = (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})\exp\left(2\pi i\sum_{i=1}^{3} h_i x_{ik}\right),$$

$$F_m(\mathbf{H}) = (1/\pi m)\sin(m\pi/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})p_k^0 \times \exp\left[2\pi i\left(\sum_{i=1}^{3} h_i x_{ik} + m\varphi_k\right)\right].$$

According to this formula, only odd-order satellites occur in the diffraction pattern. Their structure-factor magnitudes decrease linearly with the order $|m|$ (Fig. 4.6.3.3*b*)

Harmonic displacive modulation. The displacement of the atomic coordinates is given by the function

$$x_{ik} = x_{ik}^0 + A_{ik}\cos[2\pi(\bar{x}_{4,\,k} + \varphi_k)], \quad i = 1, \ldots, 3,$$

and the structure factor by

$$F_0(\mathbf{H}) = \sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})J_0(2\pi\mathbf{H}^{\parallel}\cdot\mathbf{A}_k)\exp\left(2\pi i\sum_{i=1}^{3} h_i x_{ik}\right),$$

$$F_m(\mathbf{H}) = \sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})J_m(2\pi\mathbf{H}^{\parallel}\cdot\mathbf{A}_k) \times \exp\left[2\pi i\left(\sum_{i=1}^{3} h_i x_{ik} + m\varphi_k\right)\right].$$

The structure-factor magnitudes of the mth-order satellite reflections are a function of the mth-order Bessel functions. The arguments of the Bessel functions are proportional to the scalar products of the amplitude and the diffraction vector. Consequently, the intensity of the satellites will vary characteristically as a function of the length of the diffraction vector. Each main reflection is accompanied by an infinite number of satellite reflections (Figs. 4.6.3.3*c* and 4.6.3.4).

4.6.3.2. *Composite structures (CSs)*

Composite structures consist of N mutually incommensurate substructures with N basic sublattices $\Lambda_\nu = \{\mathbf{a}_{1\nu}, \mathbf{a}_{2\nu}, \mathbf{a}_{3\nu}\}$, with $\nu = 1, \ldots, N$. The reciprocal sublattices $\Lambda_\nu^* = \{\mathbf{a}_{1\nu}^*, \mathbf{a}_{2\nu}^*, \mathbf{a}_{3\nu}^*\}$, with $\nu = 1, \ldots, N$, have either only the origin of the reciprocal lattice or one or two reciprocal-lattice directions in common. Thus, one needs $(3 + d) < 3N$ reciprocal-basis vectors for integer indexing of diffraction patterns that show Bragg reflections at positions given by the Fourier module M^*. The CSs discovered to date have at least one lattice direction in common and consist of a maximum number of $N = 3$ substructures. They can be divided in three main classes: channel structures, columnar packings and layer packings (see van Smaalen, 1992, 1995).

In the following, the approach of Janner & Janssen (1980*b*) and van Smaalen (1992, 1995, and references therein) for the description of CSs is used. The set of diffraction vectors of a CS, *i.e.* its Fourier module $M^* = \{\sum_{i=1}^{3+d} h_i \mathbf{a}_i^*\}$, can be split into the contributions of the ν subsystems by employing $3 \times (3 + d)$ matrices $Z_{ik\nu}$ with integer coefficients $\mathbf{a}_{i\nu}^* = \sum_{k=1}^{3+d} Z_{ik\nu}\mathbf{a}_k^*$,

references