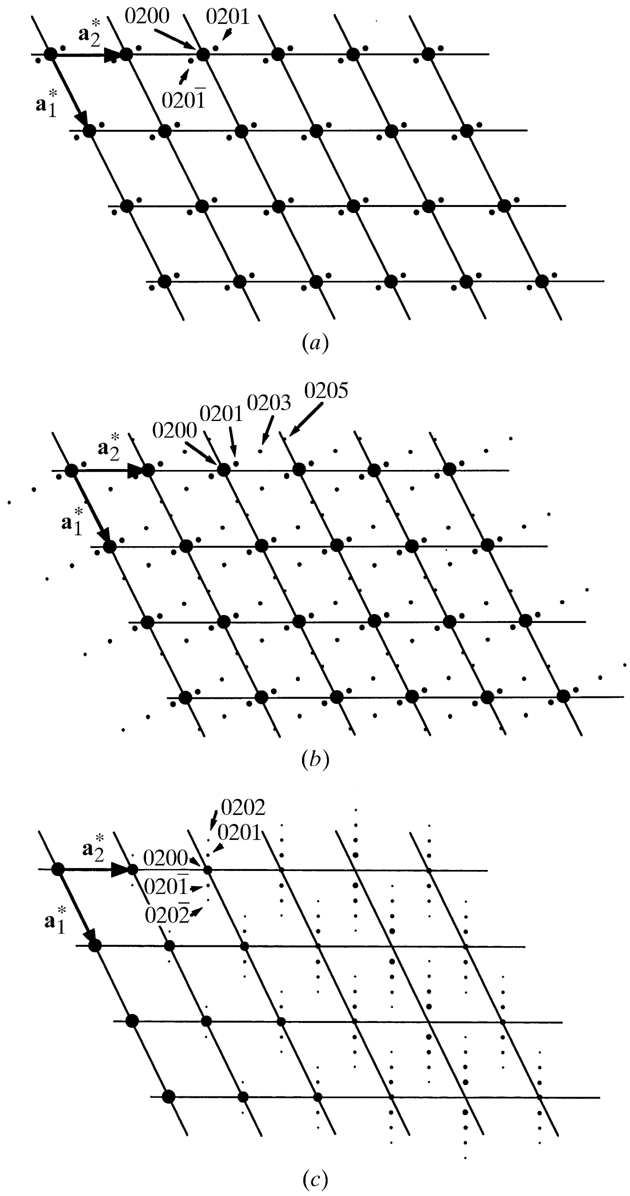

Fig. 4.6.3.3. Schematic diffraction patterns for 3D IMSs with (*a*) 1D harmonic and (*b*) rectangular density modulation. The modulation direction is parallel to $\mathbf{a}_2$. In (*a*) only first-order satellites exist; in (*b*), all odd-order satellites can be present. In (*c*), the diffraction pattern 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.

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

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

The structure-factor magnitudes of the *m*th-order satellite reflections are a function of the *m*th-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).

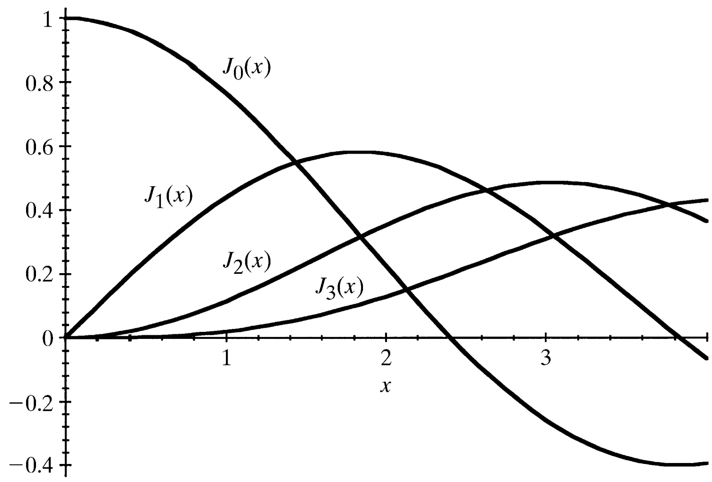

Fig. 4.6.3.4. The relative structure-factor magnitudes of *m*th-order satellite reflections for a harmonic displacive modulation are proportional to the values of the *m*th-order Bessel function $J_m(x)$.

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 $\mathbf{a}_{i\nu}^* = \sum_{k=1}^{3+d} Z_{ik\nu} \mathbf{a}_k^*$, $i = 1, \ldots, 3$. In the general case, each subsystem will be modulated with the periods of the others due to their mutual interactions. Thus, in general, CSs consist of several intergrown incommensurately modulated substructures. The satellite vectors $\mathbf{q}_{j\nu}$, $j = 1, \ldots, d$, referred to the νth subsystem can be obtained from M^* by applying the $d \times (3 + d)$ integer matrices $V_{jk\nu}$: $\mathbf{q}_{j\nu} = \sum_{k=1}^{3+d} V_{jk\nu} \mathbf{a}_k^*$, $j = 1, \ldots, d$. The matrices consisting of the components σ_ν of the satellite vectors $\mathbf{q}_{j\nu}$ with regard to the reciprocal sublattices Λ_ν^* can be calculated by $\sigma_\nu = (V_{3\nu} + V_{d\nu}\sigma)(Z_{3\nu} + Z_{d\nu}\sigma)^{-1}$, where the subscript 3 refers to the 3×3 submatrix of physical space and the subscript *d* to the $d \times d$ matrix of the internal space. The juxtaposition of the $3 \times (3 + d)$ matrix Z_ν and the $d \times (3 + d)$ matrix V_ν defines the non-singular $(3 + d) \times (3 + d)$ matrix W_ν,

$$W_\nu = \begin{pmatrix} Z_\nu \\ V_\nu \end{pmatrix}.$$

This matrix allows the reinterpretation of the Fourier module M^* as the Fourier module $M_\nu^* = M^* W_\nu$ of a *d*-dimensionally modulated subsystem ν. It also describes the coordinate transformation between the superspace basis Σ and Σ_ν.

The superspace description is obtained analogously to that for IMSs (see Section 4.6.3.1) by considering the 3D Fourier module M^* of rank $3 + d$ as the projection of a $(3 + d)$D reciprocal lattice Σ^* upon the physical space. Thus, one obtains for the definition