International Tables for Crystallography (2010). Vol. B, Figure 4.6.3.2, p. 601.

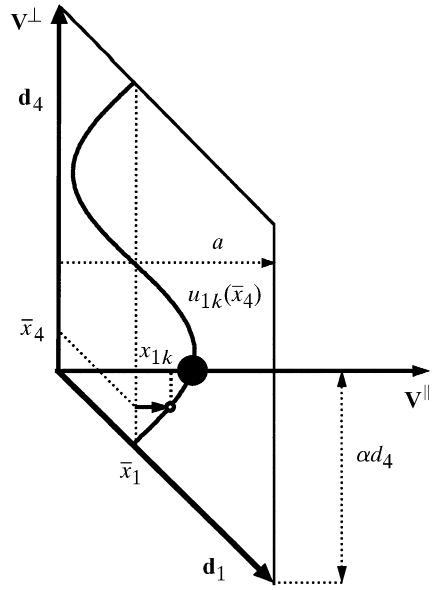

Fig. 4.6.3.2. The relationships between the coordinates $x_{1k}, x_{4k}, \bar{x}_1, \bar{x}_4$ and the modulation function u_{1k} in a special section of the $(3+d)$D space.

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

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 $p_k(\bar{x}_4, \ldots, \bar{x}_{3+d})$:

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

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

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

The resulting structure-factor formula is

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

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 for a harmonic modulation of the occupancy factor

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

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

$$
\begin{aligned}
F_0(\mathbf{H}) &= (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_k),\\
F_m(\mathbf{H}) &= (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})(p_k^0/2)^{|m|}\exp\left[2\pi i\left(\sum_{i=1}^{3} h_i x_{ik} + m\varphi_k\right)\right].
\end{aligned}
$$

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,

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

and the resulting structure factor of the mth order satellite is

$$
\begin{aligned}
F_0(\mathbf{H}) &= (1/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})\exp\left(2\pi i\sum_{i=1}^{3} h_i x_{ik}\right),\\
F_m(\mathbf{H}) &= (1/\pi m)\sin(m\pi/2)\sum_{k=1}^{N} f_k(\mathbf{H}^{\parallel})T_k(\mathbf{H}^{\parallel})p_k^0\\
&\quad \times \exp\left[2\pi i\left(\sum_{i=1}^{3} h_i x_{ik} + m\varphi_k\right)\right].
\end{aligned}
$$

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

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

and the structure factor by

references