where $p_j(x) = p_j(x+1)$. By g_s, the position $\mathbf{n}+\mathbf{r}_j$ is transformed to the equivalent position $\mathbf{n}'+\mathbf{r}_{j'} = R\mathbf{n}+R\mathbf{r}_j+\mathbf{v}$. As the crystal is left invariant by the superspace group, the occupation probability on equivalent points has to be the same:

$$P_A(\mathbf{n}', j', t) = P_A[\mathbf{n}, j, \varepsilon(t-\upsilon_I)]. \tag{9.8.4.38}$$

This implies that for the structure in the three-dimensional space one has the relation

$$P_A(\mathbf{n}', j', 0) = P_A(\mathbf{n}, j, -\varepsilon\upsilon_I). \tag{9.8.4.39}$$

In terms of the modulation function p_j this means

$$p_{j'}[\mathbf{q}\cdot(\mathbf{n}'+\mathbf{r}_{j'})] = p_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)-\varepsilon\upsilon_I]. \tag{9.8.4.40}$$

In the same way, one derives the following property of the modulation function:

$$p_{j'}(x) = p_j[\varepsilon(x-\delta)+\mathbf{K}\cdot(\mathbf{r}_{j'}-\mathbf{v})], \quad \text{where } R\mathbf{q} = \varepsilon\mathbf{q}+\mathbf{K}. \tag{9.8.4.41}$$

Analogously, for a displacive modulation, the position $\mathbf{n}+\mathbf{r}_j$ with displacement $\mathbf{u}_j(t_o)$, where $t_o = \mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)$, is transformed to $\mathbf{n}'+\mathbf{r}_{j'}$ with displacement

$$\mathbf{u}_{j'}(t_o') = R\mathbf{u}_j(t_o-\varepsilon\upsilon_I). \tag{9.8.4.42}$$

To be invariant, the displacement function has to satisfy the relation

$$\mathbf{u}_{j'}(x) = R\mathbf{u}_j[\varepsilon x-\varepsilon\delta+\mathbf{K}\cdot(\mathbf{r}_{j'}-\mathbf{v})], \quad \text{where } R\mathbf{q} = \varepsilon\mathbf{q}+\mathbf{K}. \tag{9.8.4.43}$$

The expressions for $d > 1$ are straightforward generalizations of these.

9.8.4.4.3. *Structure factor*

The scattering from a set of atoms at positions $\mathbf{r}_n$ is described in the kinematic approximation by the structure factor:

$$S_{\mathbf{H}} = \sum_n f_n(\mathbf{H})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_n), \tag{9.8.4.44}$$

where $f_n(\mathbf{H})$ is the atomic scattering factor. For an incommensurate crystal phase, this structure factor $S_{\mathbf{H}}$ is equal to the structure factor S_{H_s} of the crystal structure embedded in $3+d$ dimensions, where $\mathbf{H}$ is the projection of H_s on V_E. This structure factor is expressed by a sum of the products of atomic scattering factors f_n and phase factors $\exp(2\pi i H_s\cdot r_{sn})$ over all particles in the unit cell of the higher-dimensional lattice. For an incommensurate phase, the number of particles in such a unit cell is infinite: for a given atom in space, the embedded positions form a dense set on lines or hypersurfaces of the higher-dimensional space. Disregarding pathological cases, the sum may be replaced by an integral. Including the possibility of an occupation modulation, the structure factor becomes (up to a normalization factor)

$$S_{\mathbf{H}} = \sum_A\sum_j\int_\Omega \mathrm{d}\mathbf{t}\, f_A(\mathbf{H})P_{Aj}(\mathbf{t}) \times \exp\{2\pi i(\mathbf{H},\mathbf{H}_I)\cdot[\mathbf{r}_j+\mathbf{u}_j(\mathbf{t}),\mathbf{t}]\}, \tag{9.8.4.45}$$

where the first sum is over the different species, the second over the positions in the unit cell of the basic structure, the integral over a unit cell of the lattice spanned by $\mathbf{d}_1,\ldots,\mathbf{d}_d$ in V_I; f_A is the atomic scattering factor of species A, $P_{Aj}(\mathbf{t})$ is the probability of atom j being of species A when the internal position is $\mathbf{t}$.

In particular, for a given atomic species, without occupational modulation and a sinusoidal one-dimensional displacive modulation

$$P_j(t) = 1; \quad \mathbf{u}_j(t) = \mathbf{U}_j\sin[2\pi(\mathbf{q}\cdot\mathbf{r}_j+t+\varphi_j)]. \tag{9.8.4.46}$$

According to (9.8.4.45), the structure factor is

$$S_{\mathbf{H}} = \sum_j\int_0^1 \mathrm{d}t f_j(\mathbf{H})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_j)\exp(2\pi imt) \times \exp[2\pi i\mathbf{H}\cdot\mathbf{U}_j\sin 2\pi(\mathbf{q}\cdot\mathbf{r}_j+t+\varphi_j)]. \tag{9.8.4.47}$$

For a diffraction vector $\mathbf{H} = \mathbf{K}+m\mathbf{q}$, this reduces to

$$S_{\mathbf{H}} = \sum_j f_j(\mathbf{H})\exp(2\pi i\mathbf{K}\cdot\mathbf{r}_j)J_{-m}(2\pi\mathbf{H}\cdot\mathbf{U}_j) \times \exp(-2\pi im\varphi_j). \tag{9.8.4.48}$$

For a general one-dimensional modulation with occupation modulation function $p_j(t)$ and displacement function $\mathbf{u}_j(t)$, the structure factor becomes

$$S_{\mathbf{H}} = \sum_j\int_0^1 \mathrm{d}t\, f_j(\mathbf{H})p_j(\mathbf{q}\cdot\mathbf{r}_j+t+\psi_j)\exp[2\pi i(\mathbf{H}\cdot\mathbf{r}_j+mt)] \times \exp[2\pi i\mathbf{H}\cdot\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}_j+t+\varphi_j)]. \tag{9.8.4.49}$$

Because of the periodicity of $p_j(t)$ and $\mathbf{u}_j(t)$, one can expand the Fourier series:

$$p_j(\mathbf{q}\cdot\mathbf{r}_j+t+\psi_j)\exp[2\pi i\mathbf{H}\cdot\mathbf{u}_j(\mathbf{q}\cdot\mathbf{r}_j+t+\varphi_j)] = \sum_k C_{j,k}(\mathbf{H})\exp[2\pi ik(\mathbf{q}\cdot\mathbf{r}_j+t)], \tag{9.8.4.50}$$

and consequently the structure factor becomes

$$S_{\mathbf{H}} = \sum_j f_j(\mathbf{H})\exp(2\pi i\mathbf{K}\cdot\mathbf{r}_j)C_{j,-m}(\mathbf{H}), \quad \text{where } \mathbf{H} = \mathbf{K}+m\mathbf{q}. \tag{9.8.4.51}$$

The diffraction from incommensurate crystal structures has been treated by de Wolff (1974), Yamamoto (1982*a*,*b*), Paciorek & Kucharczyk (1985), Petricek, Coppens & Becker (1985), Petříček & Coppens (1988), Perez-Mato *et al*. (1986, 1987), and Steurer (1987).

9.8.5. Generalizations

9.8.5.1. *Incommensurate composite crystal structures*

The basic structure of a modulated crystal does not always have space-group symmetry. Consider, for example, composite crystals (also called intergrowth crystals). Disregarding modulations, one can describe these crystals as composed of a finite number of subsystems, each with its own space-group symmetry. The lattices of these subsystems can be mutually incommensurate. In that case, the overall symmetry is not a space group, the composite crystal is incommensurate and so also is its basic structure. The superspace approach can also be applied to such crystals. Let the subsystems be labelled by an index ν. For the subsystem ν, we denote the lattice by Λ_ν with basis vectors $\mathbf{a}_{\nu i}$ $(i = 1, 2, 3)$, its reciprocal lattice by Λ_ν^* with basis vectors $\mathbf{a}_{\nu i}^*$ $(i = 1, 2, 3)$, and the space group by G_ν. The atomic positions of the basic structure are given by

$$\mathbf{n}_\nu+\mathbf{r}_{\nu j}, \tag{9.8.5.1}$$

where $\mathbf{n}_\nu$ is a lattice vector belonging to Λ_ν. In the special case that the subsystems are mutually commensurate, there are three basis vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ such that all vectors $\mathbf{a}_{\nu i}^*$ are integral linear combinations of them. In general, however, more than three basis vectors are needed, but never more than three times the number of subsystems. Suppose that the vectors $\mathbf{a}_i^*$ $(i = 1,\ldots,n)$

references