Janner & Janssen, 1977) to *enlarging the class of symmetry transformations* admitted, from Euclidean in three dimensions to Euclidean in n dimensions (here $n = 4$). A four-dimensional Euclidean operation transforms the three-dimensional structure but does not leave distances invariant in general. To illustrate this phenomenon, consider the effect of a lattice translation of the basic structure on the modulation: it gives rise to a shift of the phase. Combining such a translation with an appropriate (compensating) shift of the phase, one obtains a transformation that leaves the basic structure *and* the modulation invariant. Such a transformation corresponds precisely to a lattice translation in four dimensions for the embedded crystal structure. In the real space, however, a shift of the phase is not an admitted Euclidean transformation as it does not leave invariant the distance between the particles, so that the combination of lattice translation and (compensating) phase shift also is not admitted as such, even if for an incommensurate modulation it simply corresponds to a relabelling of the atoms leaving the global structure invariant.

From what has been said, it should be apparent that the four-dimensional embedding of the modulated structure according to the superspace approach can also be obtained directly by considering as additional coordinate the phase t of the modulation. The positions in three dimensions are then the intersection of the lines of the atomic positions (parametrized by t) with the hyperplane $t = 0$. For the modulated structure of (9.8.1.4), these lines are given by

$$(\mathbf{n} + \mathbf{r}_j + \mathbf{U}_j \sin\{2\pi[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)+t]+\varphi_j\}, t) \quad \text{any real } t, \qquad (9.8.1.10a)$$

and for a more general, not necessarily sinusoidal, modulation by

$$(\mathbf{n} + \mathbf{r}_j + \mathbf{u}_j\{\mathbf{q}\cdot[\mathbf{n}+\mathbf{r}_j]+t\}, t), \qquad (9.8.1.10b)$$

where $\mathbf{u}_j(x)$ is a periodic vector function: $\mathbf{u}_j(x+1) = \mathbf{u}_j(x)$. A general point in four-dimensional space is $r_s = (\mathbf{r}, t)$ with $\mathbf{r} = (x, y, z)$.

The notation adopted here for the $(3+1)$-dimensional embedding of the modulated structure is a shorthand notation intended to stress the double role of the variable t as a parameter in the three-dimensional description of the structure and as a coordinate in the $(3+1)$-dimensional embedding. In the latter case, it implicitly assumes the choice of a fourth basis vector $\mathbf{d}$ perpendicular to the physical space of the crystal, so that the following four-dimensional vector notations are considered to be equivalent:

$$r_s = (\mathbf{r}, \mathbf{t}) = (\mathbf{r}, t\mathbf{d}) = (\mathbf{r}, t).$$

The pattern of lines (9.8.1.10a, b) has lattice periodicity. Indeed, it is invariant under the shift $t \to t+1$ and, for every lattice translation $\mathbf{n}$ from the basic structure, there is a compensating phase shift: the pattern is left invariant under the combination of the translation $\mathbf{n}$ and the phase shift $t \to t - \mathbf{q}\cdot\mathbf{n}$. Therefore, (9.8.1.10$a, b$) is invariant under translations from a four-dimensional lattice with basis

$$\begin{aligned} a_{s1} &= (\mathbf{a}, -\mathbf{q}\cdot\mathbf{a}), \quad a_{s2} = (\mathbf{b}, -\mathbf{q}\cdot\mathbf{b}), \\ a_{s3} &= (\mathbf{c}, -\mathbf{q}\cdot\mathbf{c}), \quad a_{s4} = (0, 1). \end{aligned} \qquad (9.8.1.11)$$

In accordance with the equivalent descriptions given for r_s, equivalent descriptions for a_{s4} are $a_{s4} = (0, 1) = (0, \mathbf{d})$ with dual basis vector $a^*_{s4} = (\mathbf{q}, 1) = (\mathbf{q}, \mathbf{d}^*)$, where $\mathbf{d}^*$ is reciprocal to $\mathbf{d}$ in the fourth direction. With respect to the axes (9.8.1.11), a general point in four dimensions can be written as

$$r_s = \sum_{i=1}^{4} x_i a_{si} = (\mathbf{r}, r_I),$$

with

$$\mathbf{r} = x_1\mathbf{a} + x_2\mathbf{b} + x_3\mathbf{c}, \quad \text{and} \quad r_I = t = x_4 - \mathbf{q}\cdot\mathbf{r}. \qquad (9.8.1.12)$$

Some, or sometimes all, transformations of the space group of the basic structure give rise to a symmetry transformation for the modulated structure when combined with an appropriate phase shift, possibly together with an inversion of the phase. If $\{R|\mathbf{v}\}$ is an element of the space group of the basic structure, Δ is a phase shift and $\varepsilon = \pm 1$, then the point $(\mathbf{r}, t)$ is transformed to $(R\mathbf{r} + \mathbf{v}, \varepsilon t + \Delta)$. The pattern (9.8.1.10$b$) is left invariant by $(\{R|\mathbf{v}\}, \{\varepsilon|\Delta\})$ if

$$\begin{aligned} &(R\mathbf{n} + R\mathbf{r}_j + \mathbf{v} + R\mathbf{u}_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j) + \varepsilon t - \varepsilon\Delta], t) \\ &\quad = (\mathbf{n}' + \mathbf{r}_{j'} + \mathbf{u}_{j'}[\mathbf{q}\cdot(\mathbf{n}'+\mathbf{r}_{j'}) + t], t). \end{aligned} \qquad (9.8.1.13)$$

The position $\mathbf{n}' + \mathbf{r}_{j'}$ is the transform of $\mathbf{n} + \mathbf{r}_j$ in the basic structure and therefore also belongs to the basic structure.

One can conclude that the pattern has as symmetry transformations all elements $(\{R|\mathbf{v}\}, \{\varepsilon|\Delta\})$ satisfying (9.8.1.13). These form a space group in four dimensions.

The reciprocal to the basis (9.8.1.11) is

$$\begin{aligned} a^*_{s1} &= (\mathbf{a}^*, 0), \quad a^*_{s2} = (\mathbf{b}^*, 0), \\ a^*_{s3} &= (\mathbf{c}^*, 0), \quad a^*_{s4} = (\mathbf{q}, 1). \end{aligned} \qquad (9.8.1.14)$$

A general reciprocal-lattice vector is now

$$H_s = \sum_{i=1}^{4} h_i a^*_{si} = (h_1\mathbf{a}^* + h_2\mathbf{b}^* + h_3\mathbf{c}^* + h_4\mathbf{q}, h_4).$$

The projection of this reciprocal-lattice vector is of the form (9.8.1.7), as it should be. Moreover, the projection of the four-dimensional Fourier transform on the hyperplane $t = 0$ is exactly the Fourier transform of the structure in this hyperplane. If, as a consequence of the four-dimensional space-group symmetry, the four-dimensional diffraction pattern shows systematic extinctions, the same extinctions are present in the diffraction pattern of the three-dimensional structure.

There are also other ways to describe the symmetry relations of incommensurate modulated structures. One is based on representation theory. This method has in particular been used when the modulation occurs as a consequence of a soft mode. Then the irreducible representation of the space group to which the soft mode belongs gives information on the modulation function as well. Heine & McConnell have treated the symmetry with a method related to the Landau theory of phase transitions (Heine & McConnell, 1981; McConnell & Heine, 1984). Perez-Mato *et al*. have given a formulation in terms of three-dimensional structures parametrized by what are here the additional coordinates (Perez-Mato, Madariaga & Tello, 1984, 1986; Perez-Mato, Madariaga, Zuñiga & Garcia Arribas, 1987). Other treatments of the problem can be found in Koptsik (1978), Lifshitz (1996), and de Wolff (1984).

9.8.1.4. *Basic symmetry considerations*

9.8.1.4.1. *Bravais classes of vector modules*

For a modulated crystal structure with a one-dimensional modulation, the positions of the diffraction spots are given by vectors

$$\mathbf{H} = \sum_{i=1}^{3} h_i \mathbf{a}^*_i + m\mathbf{q}. \qquad (9.8.1.15)$$

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This set of vectors is a vector module M^*. The vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ form a basis of the reciprocal lattice Λ^* of the basic structure and $\mathbf{q}$ is the modulation wavevector. The choice of the basis of Λ^* has the usual freedom, the wavevector $\mathbf{q}$ is only determined up to a sign and up to a reciprocal-lattice vector of the basic structure.

A vector module M^* has point-group symmetry K, which is the subgroup of all elements R of $O(3)$ leaving it invariant.

In the case of an incommensurate one-dimensional modulation, M^* is generated by the lattice Λ^* of main reflections and the modulation wavevector $\mathbf{q}$. It then follows that K is characterized by the following properties:

(1) It leaves Λ^* invariant. (Only in this way are main reflections transformed into main reflections and satellites into satellites.)

(2) Any element R of K then transforms $\mathbf{q}$ into $\pm\mathbf{q}$ (modulo reciprocal-lattice vectors of Λ^*).

An element R of K then transforms the basic vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$, $\mathbf{q}$ into ones of the form (9.8.1.15). If one denotes, as in (9.8.1.2), $\mathbf{q}$ by $\mathbf{a}_4^*$, this implies

$$R\mathbf{a}_i^* = \sum_{j=1}^{4} \Gamma^*(R)_{ji}\mathbf{a}_j^*, \quad i = 1, \ldots, 4, \tag{9.8.1.16}$$

with $\Gamma^*(R)$ a 4×4 matrix with integral entries. In the case of an incommensurate modulated crystal structure, only two vectors with the same length as $\mathbf{q}$ are $\mathbf{q}$ and $-\mathbf{q}$. As Λ^* is left invariant, it follows that for a one-dimensionally modulated structure $\Gamma^*(R)$ has the form

$$\Gamma^*(R) = \begin{pmatrix} \Gamma_E^*(R) & \Gamma_M^*(R) \\ 0 & \varepsilon(R) \end{pmatrix}, \quad \text{where } \varepsilon(R) = \pm 1. \tag{9.8.1.17}$$

This matrix represents the orthogonal transformation R when referred to the basis vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3, 4)$ of the vector module M^*. As in the case of lattices, two vector modules of modulated crystals are equivalent if they have bases (*i.e.* a basis for the reciprocal lattice Λ^* of the basic structure together with a modulation wavevector $\mathbf{q}$) such that the set of matrices $\Gamma^*(K)$ representing their symmetry is the same for both vector modules. Equivalent vector modules form a *Bravais class*.

Again, as in the case of three-dimensional lattices, it is sometimes convenient to consider a vector module that includes as subset the one spanned by all diffraction spots as in (9.8.1.15). Within such a larger vector module, the actual diffraction peaks then obey *centring conditions*. For a vector module associated with a modulated structure, centring may involve main reflections (the basic structure then has a centred lattice), or satellites, or both. For example, if in a structure with primitive orthorhombic basic structure the modulation wavevector is given by $\alpha\mathbf{a}_1^* + \frac{1}{2}\mathbf{a}_2^*$, one may describe the diffraction spots by means of the non-primitive lattice basis $\mathbf{a}_1^*, \frac{1}{2}\mathbf{a}_2^*, \mathbf{a}_3^*$ and by the modulation wavevector $\alpha\mathbf{a}_1^*$.

Crystallographic point groups are denoted generally by the same letter K.

9.8.1.4.2. *Description in four dimensions*

The matrices $\Gamma^*(R)$ form a faithful integral representation of the three-dimensional point group K. It is also possible to consider them as four-dimensional orthogonal transformations leaving a lattice with basis vectors (9.8.1.14) invariant. Indeed, one can consider the vectors (9.8.1.15) as *projections* of four-dimensional lattice vectors $H_s = (\mathbf{H}, H_I)$, which can be written as

$$H_s = \sum_{i=1}^{4} h_i a_{si}^*, \tag{9.8.1.18}$$

where [*cf.* (9.8.1.14)] m has now been replaced by h_4 and

$$a_{si}^* = (\mathbf{a}_i^*, 0), \quad i = 1, 2, 3; \quad a_{s4}^* = (\mathbf{q}, 1). \tag{9.8.1.19}$$

As will be explained in Section 9.8.4, these vectors span the four-dimensional reciprocal lattice for a periodic structure having as three-dimensional intersection (say defined by the hyperplane $t = 0$) the modulated crystal structure (a specific example has been given in Subsection 9.8.1.3). In direct space, the point group K_s in four dimensions with elements R_s of $O(4)$ then acts on the corresponding dual basis vectors (9.8.1.11) of the four-dimensional *direct lattice* as

$$R_s a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj} \quad (i = 1, 2, 3, 4), \tag{9.8.1.20a}$$

where $\Gamma(R)$ is the transpose of the matrix $\Gamma^*(R^{-1})$ appearing in (9.8.1.17) and therefore for incommensurate one-dimensionally modulated structures it has the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \varepsilon(R) \end{pmatrix}. \tag{9.8.1.20b}$$

9.8.1.4.3. *Four-dimensional crystallography*

Let us summarize the results obtained in the previous paragraph. The matrices $\Gamma(R)$ form a faithful integral representation of the three-dimensional point group K with a four-dimensional carrier space V_s. It is a reducible representation having as invariant subspaces the physical three-dimensional space, denoted by V (or sometimes also by V_E), and the additional one-dimensional space, denoted by V_I. In V, the four-dimensional point-group transformation acts as R (sometimes also denoted by R_E), in V_I it acts as one of the two one-dimensional point-group transformations: the identity or the inversion. Therefore, the space V_s can be made Euclidean with $\Gamma(R)$ defining a four-dimensional point-group transformation R_s, which is an element of a crystallographic subgroup K_s of $O(4)$. The four-dimensional point-group transformations are of the form (R, ε), with $\varepsilon = \pm 1$ and they act on the four-dimensional lattice basis as

$$(R, \varepsilon)a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj}, \quad i = 1, \ldots, 4, \tag{9.8.1.21}$$

where ε stands for $\varepsilon(R)$ as in (9.8.1.20*b*). So the point-group symmetry operations are crystallographic and given by pairs of a three-dimensional crystallographic point-group transformation and a one-dimensional $\varepsilon = \pm 1$, respectively. The case $\varepsilon = -1$ corresponds to an *inversion of the phase of the modulation function*.

As in the three-dimensional case, one can define equivalence classes among those four-dimensional point groups.

Two point groups K_s and K_s' belong to the same *geometric crystal class* if their three-dimensional (external) parts (forming the point group K_E and K_E', respectively) are in the same three-dimensional crystal class [*i.e.* are conjugated subgroups of $O(3)$] and their one-dimensional internal parts (forming the point groups K_I and K_I', respectively) are equal. The latter condition implies that corresponding point-group elements have the same value of ε.

Such a geometric crystal class can then be denoted by the symbol of the three-dimensional crystal class together with the values of ε that correspond to the generators.

Also, the notion of *arithmetic equivalence* can be generalized to these four-dimensional point groups, as they admit the same faithful integral representation $\Gamma(K)$ given above. This means

that two such groups are arithmetically equivalent if there is a basis transformation for the reciprocal-vector module, which transforms main reflections into main reflections and satellites into satellites and which transforms one of the matrix groups into the other. The arithmetic classes are determined by the arithmetic equivalence class of the three-dimensional group K_E [*i.e.* by $\Gamma_E(K)$] and by the components of the modulation wavevector with respect to the corresponding reciprocal-lattice basis. This is because the elements ε are fixed by the relation

$$R\mathbf{q} \equiv \varepsilon\mathbf{q} \text{ (modulo reciprocal-lattice vectors of the basic structure).} \qquad (9.8.1.22)$$

Note that these $(3+1)$-dimensional equivalence classes are not simply those one obtains in four-dimensional crystallography, as the relation between the higher-dimensional space V_s and the three-dimensional physical space V plays a fundamental role.

The embedded structures in four dimensions have lattice periodicity. So the symmetry groups are four-dimensional space groups, called *superspace groups*. The new name has been introduced because of the privileged role played by the three-dimensional subspace V. A superspace-group element g_s consists of a point-group transformation (R, ε) and a translation $(\mathbf{v}, \Delta)$. The action of such an element on the four-dimensional space is then given by

$$g_s r_s = \{(R, \varepsilon)|(\mathbf{v}, \Delta)\}(\mathbf{r}, t) = (R\mathbf{r} + \mathbf{v}, \varepsilon t + \Delta). \qquad (9.8.1.23)$$

It is important to realize that a superspace-group symmetry of an embedded crystal induces three-dimensional transformations leaving the original modulated structure invariant. Corresponding to (9.8.1.23), one obtains the following relations [*cf.* (9.8.1.13)]:

$$\boldsymbol{u}_{j'}[\mathbf{q}\cdot(\mathbf{n}' + \mathbf{r}_{j'})] = R\mathbf{u}_j[\mathbf{q}\cdot(\mathbf{n} + \mathbf{r}_j) - \varepsilon\Delta] \qquad (9.8.1.24)$$

with

$$\mathbf{n}' + \mathbf{r}_{j'} = R(\mathbf{n} + \mathbf{r}_j) + \mathbf{v}.$$

These are purely three-dimensional symmetry relations, but of course not Euclidean ones.

In three-dimensional Euclidean space, the types of space-group transformation are translations, rotations, rotoinversions, reflections, central inversion, screw rotations, and glide planes. Only the latter two transformations have intrinsic non-primitive translations. For superspace groups, the types of transformation are determined by the point-group transformations. By an appropriate choice of the basis in V_s, each of the latter can be brought into the form

$$\begin{pmatrix} \cos\varphi & -\sin\varphi & 0 & 0 \\ \sin\varphi & \cos\varphi & 0 & 0 \\ 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}; \quad \varepsilon, \delta = \pm 1. \qquad (9.8.1.25)$$

By a choice of origin, each translational part can be reduced to its intrinsic part, which in combination with the point-group element (R, ε) gives one of the transformations in V indicated above together with the inversion, or the identity, or a shift in V_I. So, for phase inversion (when $\varepsilon = -1$), the intrinsic shift in V_I vanishes. When $\varepsilon = +1$, the intrinsic shift in V_I is given by τ. It will be shown in Subsection 9.8.3.3 that the value of τ is one of

$$0, \frac{1}{2}, \frac{\pm 1}{3}, \frac{\pm 1}{4}, \frac{\pm 1}{6}. \qquad (9.8.1.26)$$

Therefore, a superspace-group element can be denoted by a symbol that consists of a symbol for the three-dimensional part following the conventions given in Volume A of *International Tables for Crystallography*, a symbol that determines ε, and one for the corresponding intrinsic internal translation τ.

9.8.1.4.4. *Generalized nomenclature*

In Section 9.8.4, the theory is extended to structures containing d modulations, with $d \geq 1$. In this case, each point-group transformation in internal space is given by R_I and the associated internal translation by the (d-dimensional) vector $\mathbf{v}_I$. Thus,

$$g_s = \{(R, R_I)|(\mathbf{v}, \mathbf{v}_I)\}.$$

The transformations R and R_I are represented by the matrices $\Gamma_E(R)$ and $\Gamma_I(R)$, respectively. In the following discussion, this nomenclature (but with v_I rather than $\mathbf{v}_I$) is sometimes also applied for the $(3+1)$-dimensional case. The usual formulae are obtained by replacing R_I by ε and v_I by Δ.

9.8.1.4.5. *Four-dimensional space groups*

Four-dimensional space groups were obtained in the $(3+1)$-reducible case by Fast & Janssen (1969) and in the general case by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978). The groups were determined on the basis of algorithms developed by Zassenhaus (1948), Janssen, Janner & Ascher (1969), Brown (1969), and Fast & Janssen (1971). In the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, quoted above, a mathematical characterization of the basic crystallographic concepts is given together with corresponding tables for the dimensions one, two, three, and four. One finds there, in particular, a full list of four–dimensional space groups. The list by Fast & Janssen is restricted to space groups with $(3+1)$-reducible point groups. The four-dimensional groups in the work of Brown *et al.* are labelled by numbers. For these same groups, alternative symbols have been developed by Weigel, Phan, Veysseyre and Grebille generalizing the principles of the notation adopted by *International Tables for Crystallography*, Volume A, for the three-dimensional space groups (Weigel, Phan & Veysseyre, 1987; Veysseyre & Weigel, 1989; Grebille, Weigel, Veysseyre & Phan, 1990).

The difference in the listing of four-dimensional crystallographic groups one finds in Brown *et al.* and in Weigel *et al.* with respect to that in the present tables is not simply a matter of notation. In the first place, here only those groups appear that can occur as symmetry groups of one-dimensional incommensurate modulated phases (there are 371 such space groups). Furthermore, as already mentioned, a finer equivalence relation has been considered that reflects the freedom one has in embedding a three-dimensional modulated structure in a four-dimensional Euclidean space. Instead of 371, one then obtains 775 inequivalent groups for which the name superspace group has been introduced. A $(3+1)$-dimensional superspace group is thus a four-dimensional space group having some additional properties. In Section 9.8.4, the precise definitions are given.

In the commensurate one-dimensionally modulated case, 3833 four-dimensional space groups may occur, out of which 320 already belong to the previous 371. The corresponding additional $(3+1)$-dimensional superspace groups are also present in the listing by Fast & Janssen (1969) and have been considered again (and applied to structure determination) by van Smaalen (1987). The Bravais classes for the commensurate $(3+1)$-dimensional case are given in Table 9.8.3.2(*b*).

The relation between modulated crystals and the superspace groups is treated in a textbook by Opechowski (1986). That between the superspace-group symbols of the present tables and those of Weigel *et al.* is discussed in Grebille *et al.* (1990).

Note that no new names have been introduced for the underlying crystallographic concepts like Bravais classes, geometric and arithmetic crystal classes, even if in those cases also the equivalence relation is not simply that of four-dimensional Euclidean crystallography, an explicit distinction always being possible by specifying the dimension as $(3+1)$ instead of four.

9.8.1.5. *Occupation modulation*

Another type of modulation, the occupation modulation, can be treated in a way similar to the displacive modulation. As an example consider an alloy where the positions of the basic structure have space-group symmetry, but are statistically occupied by either of two types of atoms. Suppose that the position $\mathbf{r}$ is occupied by an atom of type A with probability $p(\mathbf{r})$ and by one of type B with probability $1-p(\mathbf{r})$ and that p is periodic. The probability of finding an A atom at site $\mathbf{n}+\mathbf{r}_j$ is

$$P_A(\mathbf{n}+\mathbf{r}_j) = p_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)], \tag{9.8.1.27}$$

with $p_j(x) = p_j(x+1)$. In this case, the structure factor becomes

$$S_{\mathbf{H}} = \sum_{\mathbf{n}}\sum_{j}\left[\left(f_A p_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)] + f_B\{1-p_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)]\}\right) \times \exp[2\pi i\mathbf{H}\cdot(\mathbf{n}+\mathbf{r}_j)]\right], \tag{9.8.1.28}$$

where f_A and f_B are the atomic scattering factors. Because of the periodicity, one has

$$p_j(x) = \sum_m w_{jm}\exp(2\pi i m x). \tag{9.8.1.29}$$

Hence,

$$S_{\mathbf{H}} = \sum_j\left\{f_B\Delta(\mathbf{H})\exp(2\pi i\mathbf{H}\cdot\mathbf{r}_j) + (f_A - f_B)\sum_m \Delta(\mathbf{H}+m\mathbf{q})w_{jm} \times \exp[2\pi i(\mathbf{H}+m\mathbf{q})\cdot\mathbf{r}_j]\right\}, \tag{9.8.1.30}$$

where $\Delta(\mathbf{H})$ is the sum of δ functions over the reciprocal lattice of the basic structure:

$$\Delta(\mathbf{H}) = \sum_{h_1h_2h_3}\delta\left(\mathbf{H} - \sum_{i=1}^{3} h_i\mathbf{a}_i^*\right).$$

Consequently, the diffraction peaks occur at positions $\mathbf{H}$ given by (9.8.1.7). For a simple sinusoidal modulation [$m=\pm1$ in (9.8.1.29)], there are only main reflections and first-order satellites ($m=\pm1$). One may introduce an additional coordinate t and generalize (9.8.1.27) to

$$P_A(\mathbf{n}+\mathbf{r}_j, t) = p_j[\mathbf{q}\cdot(\mathbf{n}+\mathbf{r}_j)+t], \tag{9.8.1.31}$$

which has $(3+1)$-dimensional space-group symmetry. Generalization to more complex modulation cases is then straightforward.

9.8.2. Outline for a superspace-group determination

In the case of a modulated structure, the diffraction pattern consists of main reflections and satellites. The main reflections span a reciprocal lattice generated by $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$. Considerations are here restricted for simplicity to the one-dimensional modulated case, *i.e.* to the $n=4$ case. Extension to the more general $n=3+d$ case is conceptually not difficult and does not modify the general procedure outlined here.

(1) *The first step* is the determination of the *Laue group* P_L of the diffraction pattern: it is the point group in three dimensions that transforms every diffraction peak into a peak of the same intensity.†

As P_L leaves invariant the subset of main reflections, this Laue group belongs to one of the 11 Laue symmetry classes. Accordingly, the Laue group determines a three-dimensional holohedral point group which determines a crystallographic system.

(2) *The second step* consists of choosing a basis according to the conventions of *IT* A for the main reflections and choosing a modulation wavevector.

From the centring extinctions, one can deduce to which Bravais class the main reflections belong. This is one of the 14 three-dimensional Bravais classes. Notice that the cubic Bravais classes do not occur because a one-dimensional (incommensurate) modulation is incompatible with cubic symmetry. For this same reason, only the nine non-cubic Laue-symmetry classes occur in the one-dimensional incommensurate case.

The main reflections are indexed by $hkl0$ and the satellite reflections by $hklm$. The Fourier wavevector of a general reflection $hklm$ is given by

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q}. \tag{9.8.2.1}$$

Note that this step involves a choice because the system of satellite reflections is only defined modulo the main reflections. When a satellite is in the vicinity of a main reflection, it is reasonable to assign it to that reflection. But one has, especially when deciding whether or not situations are equivalent, to be aware of the fact that each satellite may be assigned to an arbitrary main reflection. It is even possible to assign a satellite to an extinct main reflection. One takes by preference the $\mathbf{q}$ vector along a symmetry axis or in a mirror plane. According to equation (9.8.2.1), the fourth basis vector $\mathbf{a}_4^*$ is equal to the chosen $\mathbf{q}$, the modulation wavevector.

(3) In the *third step*, one determines the space group of the *average structure* (from the main reflections).

The average structure is unique but possibly involves split atoms. The space group of the average structure is often the symmetry group of the undistorted phase. That helps to make a good choice for the basic structure and also gives an insight as to how the satellite reflections split from the main reflections at the phase transition.

(4) *Step four* is the identification of the $(3+1)$-dimensional Bravais lattice type. In superspace also, centring gives rise to *centring extinctions*, and that corresponds to making the choice of a *conventional unit cell* in $(3+1)$ dimensions.

The previous three steps establish $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, the three-dimensional Bravais class and $\mathbf{q} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$, where the components α, β, and γ are given with respect to the three-dimensional conventional basis.

$$\alpha = \mathbf{q}\cdot\mathbf{a}, \quad \beta = \mathbf{q}\cdot\mathbf{b}, \quad \gamma = \mathbf{q}\cdot\mathbf{c}. \tag{9.8.2.2}$$

The $(3+1)$-dimensional Bravais class is fixed by that three-dimensional Bravais class and the components α, β, γ of $\mathbf{q}$.

Just as for three-dimensional lattices, a conventional cell can be chosen for $(3+1)$-dimensional lattices. To this end, the

† Except for deviations from Friedel's law caused by dispersion; see *IT* B (1993, p. 241, Subsection 2.3.4.1).

references