9.8 Superspace symmetry for aperiodic crystals, incommensurate and commensurate modulated structures

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9.8.1. Introduction

9.8.1.1. Modulated crystal structures

Lattice periodicity is a fundamental concept in crystallography. This property is widely considered as essential for the characterization of the concept of a crystal. In recent decades, however, more and more long-range-ordered condensed-matter phases have been observed in nature that do not have lattice periodicity, but nevertheless only differ from normal crystal phases in very subtle and not easy to observe structural and physical properties.

It is convenient to extend the concept of a crystal in such a way that it includes these ordered phases as well. If properly applied, crystallographic symmetry concepts are then still valid and of relevance for structural (and physical) investigation. Instead of limiting the validity of crystallographic notions, these developments show how rich the crystallographic ordering can be.

Incommensurate crystals are characterized by Bragg reflection peaks in the diffraction pattern that are well separated but do not belong to a lattice and cannot be indexed by three integer indices. This means that the description in terms of three-dimensional point and space groups, as given in *International Tables of Crystallography*, Volume A (1992), breaks down. It is possible, however, to generalize the crystallographic concepts on which the usual description is based. The ensuing symmetry groups and their equivalence classes are different from those of three-dimensional crystallography. The main properties of these new groups and the specific problems posed by their application to incommensurate crystal structures form the subject of the following sections.

The earliest discovered incommensurate crystals were *modulated structures*. These can be seen as originating from a structure with three-dimensional space group symmetry (the basic structure), but having a modulation that destroys the lattice periodicity. This modulation may be an ordered displacement of the atoms, or an ordered distribution of atoms of different species over the sites of the original structure. There are, however, more complicated cases. *Incommensurate composites* can be seen as systems with two or more subsystems, each of which is an incommensurate crystal, but without common space group for the basic structures. Again different are quasicrystals. The earliest examples showed five-fold symmetry axes. Such a symmetry is incompatible with lattice periodicity in three dimensions. Nevertheless, these quasicrystals are perfectly ordered. Similar compounds

[1]Co-author P.M. de Wolff passed away in 1998. The title of the original chapter was *Incommensurate and commensurate modulated structures.*

without 'forbidden' symmetry were discovered later, but they all can be described using the generalization of crystallographic concepts mentioned above. The tables presented here, and their explanation, have been restricted to cover mainly the simplest case, the modulated crystal phases (in particular, those with a single modulation wave). However, it turns out to be very difficult to draw a sharp separation line between the different classes of incommensurate crystals. Therefore, we shall briefly discuss the other types as well.

As said above, a modulation is here considered to be a periodic deformation of a 'basic structure' having space-group symmetry. If the periodicity of the modulation does not belong to the periodicities of the basic structure, the modulated crystal structure is called incommensurate.

That description is based on the observation, in the diffraction pattern of modulated structures, of main reflections, situated on a reciprocal lattice, and additional reflections, generally of weaker intensity, called satellites.

As far as we know, the first indications that complex crystal structures could exist not having normal lattice periodicity came, at the end of the 19th century, from studies of the morphology of the mineral calaverite. It was found that the faces of this compound do not obey the law of rational indices (Smith, 1903; Goldschmidt, Palache & Peacock, 1931). Donnay (1935) showed that faces that could not be indexed correspond to additional reflections in the X-ray diffraction pattern. From the experience with manufacturing of optical gratings, it was already known that periodic perturbation gives rise to additional diffraction spots. Dehlinger (1927) used this theory of '*Gittergeister*' (lattice ghosts) to explain line broadening in Debye-Scherrer diagrams of metals and alloys. Preston (1938) called the '*Gittergeister*' he found in diffraction from an aluminium-copper alloy 'satellites'. Periodic displacement (modulation) waves were considered by Daniel & Lipson (1943) as the origin of satellites in a copper-iron-nickel alloy. Complex magnetic ordering giving rise to satellites was found in magnetic crystals (Herpin, Meriel & Villain, 1960; Koehler, Cable, Wollan & Wilkinson, 1962). In the early 1970's, the importance of the irrationality was realized and the term 'incommensurate phase' was introduced for modulated crystal phases with wave vectors that have irrational components. Such phases were found in insulators as well (Tanisaki, 1961, 1963; Brouns, Visser & de Wolff, 1964). The remarkable morphological properties of calaverite could also be related to the existence of an incommensurate modulation (Dam, Janner & Donnay, 1985). Structures that are well ordered, show sharp incommensurate spots in the diffraction pattern, but cannot be described as a modulation of a lattice periodic system, were also discovered, indicating that incommensurability is not restricted to modulated crystals. Examples are the composite (or intergrowth) crystals (Jellinek, 1972) and, more recently, quasicrystals (Shechtman, Blech, Gratias & Cahn, 1984). For a review, see Janssen & Janner (1987) and Janssen, Chapuis & de Boissieu (2007).

We denote a basis for the lattice of main reflections by $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$. The satellites are separated from the main reflections by vectors that are integral linear combinations of some basic modulation vectors denoted by $\mathbf{q}_j$ $(j = 1, 2, \ldots, d)$. Accordingly, the positions

of the Bragg reflections are given by

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m_1\mathbf{q}_1 + m_2\mathbf{q}_2 + \ldots + m_d\mathbf{q}_d. \qquad (9.8.1.1)$$

If the modulation is incommensurate, the set of all positions (9.8.1.1) does not form a lattice. Mathematically, it has the structure of a $\mathbb{Z}$-module, and its elements are three-dimensional vectors (of the reciprocal space). Accordingly we shall call it a (reciprocal) *vector module* or *Fourier module*. A structure or function with a Fourier transform different from zero on positions (9.8.1.1) is called *quasiperiodic*. The number of basis vectors ($n = 3 + d$) is called the *rank* of the Fourier module. If $d = 0$, the rank is 3, and the structure is lattice periodic. A periodic function then is a special case of a quasiperiodic function.

The modulation that gives rise to the satellites can be:
(i) a displacive modulation, consisting of a (quasi)periodic displacement from the atomic positions of the basic structure;
(ii) an occupation modulation, in which the atomic positions of the basic structure are occupied with a (quasi)periodic probability function.

Mixed forms also occur. Other modulation phenomena found are, for example, out-of-phase structures and interface modulated structures. The satellite reflections of modulated structures for the various types of modulation were systematically studied by Korekawa (1967).

For an incommensurate structure, at least one component of a basic modulation wavevector $\mathbf{q}_j$ with respect to the lattice of main reflections is irrational. As argued later, even in the case of a commensurate modulation, *i.e.* when all components of these modulation wavevectors are rational, it is sometimes convenient to adopt the description of equation (9.8.1.1) and to apply the formalism developed for the incommensurate crystal case.

The modulated crystal case presented above is only the simplest one giving rise to incommensurate crystal structures. Another class is represented by the so-called *composite* or *intergrowth crystal structures*. Generally, the two (or more) subsystems do not exist as such separately, but only in the given combination. The basic lattices are incommensurate, and the interaction between the subsystems gives rise to a modulation of these. These crystals are different from the previous ones, in the sense that they show more than one set of main reflections. In the case of an intergrowth crystal, the Bragg reflections can be labelled by a finite set of integral indices as well and the Fourier wavevectors form a Fourier module as defined above. The difference from the previous case is that the basic structure itself is incommensurate, even if one disregards the modulation.

A third class of incommensurate crystals is represented by the *quasicrystals* (examples of which are the icosahedral and decagonal phases). In that case also, the basic structure is incommensurate, the difference from the previous cases being that the splitting in subsystems of main reflections and/or in main reflections and satellites is not a natural one, even in the lowest approximation.

It is justified to assume that crystal phases allow for an even wider range of ordered structures than mentioned above. Nevertheless, all the cases studied so far allow a

common approach based on higher-dimensional crystallography, *i.e.* on crystallographic properties one obtains after embedding the crystal structure in a higher-dimensional Euclidean space.

To present that approach in its full generality would require a too abstract language. On the other hand, restriction to the simplest case of a modulated crystal would give rise to misleading views. In what follows, the basic ideas are formulated as simply as possible, but still within a general point of view. Their application and the illustrative examples are mainly restricted to the modulated crystal case. The tables presented here cover essentially the one-dimensional modulated case [$d = 1$ in equation (9.8.1.1)]. However, to illustrate the more general cases, also tables for modulated crystals with a higher-dimensional modulation, and for other types of aperiodic crystals, like quasicrystals, will be given. In these cases, however, completeness is not possible in the present article.

9.8.1.2. The basic ideas of higher-dimensional crystallography

Incommensurate modulated crystals are systems that do not obey the classical lattice periodicity requirements for crystals. Nevertheless, their long-range order is as perfect as that of conventional crystals. In the diffraction pattern they also show sharp, well separated spots, and in the morphology flat faces. Dendritic and flat face crystallization with typical point-group symmetry is observed in both commensurate and incommensurate materials. Therefore, we shall consider both as crystalline phases and generalize for that reason the concept of a crystal. The positions of the Bragg diffraction peaks given in (9.8.1.1) are a special case. In general, they are elements of a vector module M^* and can be written as

$$\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}_i^*, \quad \text{integers} \quad h_i. \tag{9.8.1.2}$$

This leads to the following *definition of crystal*.

An *ideal crystal* is considered to be a matter distribution having Fourier wavevectors expressible as integral linear combinations of a finite number (say n) of them and such that its diffraction pattern is characterized by a discrete set of resolved Bragg peaks, which can be indexed accordingly by a set of n integers $h_1, h_2, \ldots, h_n$.

Implicit in this definition is the possibility of neglecting diffraction intensities below a given threshold, allowing one to identify and to label individual Bragg peaks even when n is larger than the dimension m of the crystal, which is usually three. Actually, for incommensurate crystals, the unresolved Bragg peaks of arbitrarily small intensities form a dense set, because they may come arbitrarily close to each other.

Here some typical examples are indicated. In the *ordinary crystal* case, $n = m = 3$ and $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ are conventionally denoted by $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ and the indices h_1, h_2, h_3 by h, k, ℓ.

In the case of a one-dimensionally *modulated crystal*, which can be described as a periodic plane wave deformation of a lattice periodic crystal (defining the basic structure), one has $n = 4$. Conventionally, $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, $\mathbf{a}_3^*$ are chosen to be $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ generating the positions of the main reflections, whereas $\mathbf{a}_4^* = \mathbf{q}$ is the wavevector of the modulation. The corresponding indices are usually denoted by h, k, ℓ, and m. Also, crystals having two-

and three-dimensional modulation (rank 5 and 6, respectively) are known.

In the case of a *composite crystal*, one can identify two or more subsystems, each with its own basic structure. As an example, consider the case where two subsystems share $\mathbf{a}^*$ and $\mathbf{b}^*$ of their reciprocal-lattice basis, whereas they differ in periodicity along the c axis and have, respectively, $\mathbf{c}_1^*$ and $\mathbf{c}_2^*$ as third basis vector. Then again, $n = 4$, and $\mathbf{a}_1^*, \ldots \mathbf{a}_4^*$ can be chosen as $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}_1^*$, and $\mathbf{c}_2^*$. The indices can be noted by h, k, ℓ_1, ℓ_2. In general, the subsystems interact, giving rise to modulations and possibly (but not necessarily) to a larger value of n. In addition to the main reflections from the undistorted subsystems, satellites then occur. One may distinguish common reflections ($\ell_1 = \ell_2 = 0$), main reflections for system 1 (ℓ_2=0), those for system 2 ($\ell_1 = 0$) and sum reflections (both ℓ_1 and ℓ_2 different from zero).

In the case of a *quasicrystal*, the Bragg reflections require more than three indices, but they do not arise from structurally different subsystems having lattice periodicity. So, for the icosahedral phase of AlMnPd alloy, $n = 6$, and one may take as basis six vectors, one from each pair of vectors pointing to parallel faces of a dodecahedron.

The *Laue point group* P_L of a crystal is the point symmetry group of its diffraction pattern. This subgroup of the orthogonal group $O(3)$ is of finite order. The finite order of the group follows from the discreteness of the (resolved) Bragg peak positions, implying a finite number only of peaks of the same intensity lying at a given distance from the origin.

Under a symmetry rotation R, the indices of each reflection are transformed into those of the reflection at the rotated position. Therefore, a symmetry rotation is represented by an $n \times n$ non-singular matrix $\Gamma(R)$ with integral entries. Accordingly, a Laue point group P_L admits an n-dimensional faithful integral representation $\Gamma(P_L)$. Because any finite group of matrices is equivalent with a group of orthogonal matrices of the same dimension, it follows that:
(1) P_L is isomorphic to an n-dimensional crystallographic point group;
(2) there exists a lattice basis $a_{s1}^*, \ldots, a_{sn}^*$ of a Euclidean n-dimensional (reciprocal) space, which projects on the Fourier wavevectors $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$;
(3) the three-dimensional Fourier components $\hat{\rho}(h_1, \ldots, h_n)$ of the crystal density function $\rho(\mathbf{r})$ can be attached to corresponding points of an n-dimensional reciprocal lattice and considered as the Fourier components of a density function $\rho_s(r_s)$ having lattice periodicity in that higher-dimensional space (r_s is an n-dimensional position vector).

Such a procedure is called the *superspace embedding* of the crystal.

Notice that this procedure only involves a reinterpretation of the structural data (expressed in terms of Fourier coefficients): the structural information in the n-dimensional space is exactly the same as that in the three-dimensional description.

The *symmetry group* of a crystal is then defined as the Euclidean symmetry group of the crystal structure embedded in the superspace.

Accordingly, the symmetry of a crystal whose diffraction pattern is labelled by n integral indices is an n-dimensional space group.

The *equivalence relation* of these symmetry groups follows from the requirement of invariance of the equivalence class with respect to the various possible choices of bases

and embeddings. Because of that, the equivalence relation is not simply the one valid for n-dimensional crystallography.

In the case of modulated crystals, such an equivalence relation has been worked out explicitly, giving rise to the concept of (3+d)-dimensional *superspace group* type.

The concepts of point group, lattice holohedry, Bravais class, system of non-primitive translations (or vector system), and so on, then follow from the general properties of n-dimensional space groups together with the (appropriate) equivalence relations.

A glossary of symbols is given in Appendix A and a list of definitions in Appendix B.

9.8.1.3. The simple case of a displacively modulated crystal

9.8.1.3.1. The diffraction pattern

To introduce what follows, the simple case of a displacively modulated crystal structure is considered. The point-atom approximation is adopted and the modulation is supposed to be a sinusoidal plane wave. This means that the structure can be described in terms of atomic positions of a *basic structure* with three-dimensional space group symmetry, periodically (in space) displaced according to the modulation wave. Writing for the position of the jth particle in the unit cell of the basic structure given by the lattice vector $\mathbf{n}$:

$$\mathbf{r}_0(\mathbf{n}, j) = \mathbf{n} + \mathbf{r}_j, \tag{9.8.1.3}$$

the position of the same particle in the modulated structure is given by

$$\mathbf{r}(\mathbf{n}, j) = \mathbf{n} + \mathbf{r}_j + \mathbf{U}_j \sin[2\pi\mathbf{q}.(\mathbf{n} + \mathbf{r}_j) + \phi_j], \tag{9.8.1.4}$$

where $\mathbf{q}$ is the wavevector of the modulation and $\mathbf{U}_j$ is the polarization vector for the jth particle's modulation. (This is not the most general sinusoidal modulation, because different components $U_{j\alpha}$ may have different phases $\phi_{j\alpha}$ ($\alpha = 1, 2, 3$)). In general, the symmetry of the modulated structure is different from that of the basic structure and the only translations that leave the modulated structure invariant are those lattice translations $\mathbf{m}$ of the basic structure satisfying the condition $\mathbf{q}.\mathbf{m}$=integer. If the components α, β, and γ of the wave vector $\mathbf{q}$ with respect to the basis $\mathbf{a}^*$,$\mathbf{b}^*$, $\mathbf{c}^*$ are all rational numbers, there is a full lattice of such translations, the structure then is a *superstructure* of the original one and has three-dimensional space group symmetry. If at least one of the components of $\mathbf{q}$ is irrational, the structure does not have three-dimensional lattice translation symmetry. Nevertheless, the crystal structure is by no means disordered: it is fully determined by the basic structure and the modulation wave(s).

The crystalline order is seen in the structure factor, which is given by the expression

$$\begin{aligned} S_{\mathbf{H}} &= \sum_{\mathbf{n},j} f_j \exp[2\pi i \mathbf{H}.\mathbf{r}(\mathbf{n}, j)] \qquad (9.8.1.5) \\ &= \sum_{\mathbf{n},j} f_j \exp[2\pi i \mathbf{H}.(\mathbf{n} + \mathbf{r}_j)] \\ &\quad \times \exp 2\pi i \mathbf{H}.\mathbf{U}_j \sin[2\pi\mathbf{q}.(\mathbf{n} + \mathbf{r}_j) + \phi_j] \end{aligned}$$

where f_j is the atomic scattering factor (which still, in general, depends on $\mathbf{H}$). Using the Jacobi-Anger relation, one can rewrite this as

$$\begin{aligned} S_{\mathbf{H}} &= \sum_{\mathbf{n},j} \sum_{m=-\infty}^{\infty} \exp[2\pi i(\mathbf{H} - m\mathbf{q}).(\mathbf{n} + \mathbf{r}_j)] \\ &\quad \times f_j \exp(-im\phi_j) J_{-m}(2\pi \mathbf{H}.\mathbf{U}_j), \end{aligned} \tag{9.8.1.6}$$

where $J_m(x)$ is the mth order Bessel function. The summation over $\mathbf{n}$ results in a sum of δ functions on the positions of the reciprocal lattice spanned by $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$:

$$\Delta(\mathbf{H} - m\mathbf{q}) = \sum_{h,k,\ell} \delta(\mathbf{H} - m\mathbf{q} - h\mathbf{a}^* - k\mathbf{b}^* - \ell\mathbf{c}^*).$$

Consequently, the structure factor $S_{\mathbf{H}}$ vanishes unless there are integers h, k, ℓ and m such that

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}. \tag{9.8.1.7}$$

If $\mathbf{q}$ is incommensurate, *i.e.* if there is no integer N such that $N\mathbf{q}$ belongs to the reciprocal lattice spanned by $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$, one needs more than three integers (in the present case four) for indexing $\mathbf{H}$. This is characteristic for incommensurate crystal phases.

In the diffraction pattern of such a modulated phase, one distinguishes between main reflections (for which m=0) and satellites (for which $m \neq 0$). The intensities of the satellites fall off rapidly for large m so that the diffraction spots remain separated, although the vectors of the Fourier module (9.8.1.7) may come arbitrarily close to each other.

In the commensurate case also, there are main reflections and satellites, but, since here there is an integer N such that $N\mathbf{q}$ belongs to the reciprocal lattice, one may restrict the values of m to the range from 0 to $N - 1$.

9.8.1.3.2. The symmetry

There is more than one way for expressing the long-range order present in an incommensurate crystal in terms of symmetry. One natural way is to adopt the point of view that the measuring process limits the precision in the determination of the modulation wavevector. Accordingly, one can try an *approximation* of the modulation wavevector $\mathbf{q}$ *by a commensurate one*: an irrational number can be approximated arbitrarily well by a rational one.

There are two main disadvantages in this approach. Firstly, a good approximation requires, in general, a large unit cell for the corresponding superstructure, which involves a large number of position parameters. Secondly, the space group one finds may depend essentially on the rational approximation adopted. Consider, for example, an orthorhombic basic structure with space group $Pcm2_1$ and modulation wavevector $\mathbf{q}$=$\gamma\mathbf{c}^*$, polarization along the b direction and positions of the particles given by

$$\mathbf{r}(\mathbf{n}, j) = \mathbf{n} + \mathbf{r}_i + \mathbf{U} \sin[2\pi(\mathbf{q}.\mathbf{n} + \mathbf{r}_j)], \tag{9.8.1.8}$$

where for convenience the polarization has been taken as independent of j. Under the glide reflection $\{m_x|(m+\frac{1}{2})\mathbf{c}\}$ (with integer m) present in the basic structure, the transformed positions are

$$\mathbf{r}'(\mathbf{n},j) = \mathbf{r} + \mathbf{U}\sin 2\pi[\mathbf{q}.\mathbf{r} - \gamma(m+\frac{1}{2})], \quad \text{with} \quad \mathbf{r} = \mathbf{n} + \mathbf{r}_j. \tag{9.8.1.9}$$

Consider the rational approximation P/Q of γ, with P and Q relatively prime integers. Then such a glide transformation as given above is (for certain values of m) a symmetry of the modulated structure only if P is even and Q is odd, because only in that case the equation $P(m+\frac{1}{2}) = \ell Q$ has a solution with integers ℓ and m. Analogously, the mirror in the y direction only occurs as a glide plane if P/Q is odd/even, whereas the screw axis along z requires the case odd/odd. Hence, if, for example, one approximates the same irrational number successively by 5/12, 7/17 and 8/19, one finds different symmetry groups. Furthermore, in all the cases the point group is monoclinic and the information contained in the orthorhombic point-group symmetry of the main reflections is lost. The symmetry would depend on the approximation.

These difficulties are avoided if one embeds the modulated crystal according to the basic ideas expressed in the previous section. Conceptually, it corresponds (de Wolff, 1974, 1977; 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 intersection of the periodic structure with the physical space, but there the distances are not preserved. To illustrate this, consider the effect of a lattice translation on the structure in physical space. It is, generally, a combination of a lattice translation of the basic structure and a compensating phase shift. The former is a Euclidean transformation, the latter is not. Changing the phase changes the distances between the atoms. Therefore, the transformation of the physical structure is non-Euclidean.

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 $\phi = 2\pi r_I$ of the modulation or the 'internal coordinate' r_I. The positions in three dimensions are then the intersection of the lines of the atomic positions (parametrized by ϕ) with the hyperplane $\phi = 0$. For the modulated structure of equation (9.8.1.4), the lines are given, for respectively a sinusoidal and a general modulation, by

$$\begin{aligned} &a) \quad (\mathbf{n} + \mathbf{r}_j + \mathbf{U}_j \sin\{2\pi[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j) + r_I] + \phi_j\}, r_I), \quad \text{any real } \phi, \\ &b) \quad (\mathbf{n} + \mathbf{r}_j + \mathbf{u}_j(\mathbf{q}.[\mathbf{n}+\mathbf{r}_j] + r_I), r_I), \end{aligned} \tag{9.8.1.10}$$

where $\mathbf{u}_j(x)$ is a periodic function: $\mathbf{u}_j(x+1) = \mathbf{u}_j(x)$. A general point in four-dimensional space is r_s=($\mathbf{r}$,ϕ) 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 r_I as a parameter in the three-dimensional 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 notations are considered to be equivalent:

$$r_s = (\mathbf{r}, \mathbf{r}_I) = \mathbf{r} + r_I\mathbf{d} = (\mathbf{r}, r_I).$$

The index I in r_I means 'internal', the additional space being considered as an internal space, in contradistinction to the physical space of the crystal called 'external space'. The sum of the internal and external space is called *superspace*. Other authors have introduced the terms parallel and perpendicular space, respectively.

The pattern of lines (9.8.1.10) has lattice periodicity. Indeed, it is invariant under the shift $r_I \rightarrow r_I + 1$ 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 $r_I \rightarrow r_I - \mathbf{q}.\mathbf{n}$. Therefore, (9.8.1.10) is invariant under translations from a four-dimensional lattice with basis

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

In accordance with the descriptions given for r_s, equivalent descriptions for a_{s4} are ($\mathbf{0}$,1) and (0,$\mathbf{d}$) with dual basis vector a^*_{s4}=($\mathbf{q}$,1)=($\mathbf{q}$,$\mathbf{d}^*$), where $\mathbf{d}^*$ is the 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

$$\mathbf{r} = x_1\mathbf{a} + x_2\mathbf{b} + x_3\mathbf{c}, \quad \text{and} \;\; r_I = x_4 - \mathbf{q}.\mathbf{r}. \tag{9.8.1.12}$$

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 $\epsilon = \pm 1$, then the point ($\mathbf{r}$,r_I) is transformed to $\{R\mathbf{r}+\mathbf{v}, \epsilon r_I + \Delta)$. The pattern (9.8.1.10) is left invariant by ($\{R|\mathbf{v}\}$,$\{\epsilon|\Delta\}$) if

$$\begin{aligned} (R\mathbf{n} + R\mathbf{r}_j + \mathbf{v} \;&+\; R\mathbf{u}_j[\mathbf{q}.(\mathbf{n} + \mathbf{r}_j) + \epsilon r_I - \epsilon\Delta], r_I) \\ &= (\mathbf{n}' + \mathbf{r}_{j'} + \mathbf{u}_{j'}[\mathbf{q}.(\mathbf{n}' + \mathbf{r}_{j'})) + r_I], r_I). \end{aligned} \tag{9.8.1.13}$$

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 operations all the elements ($\{R|\mathbf{v}\}$,$\{\epsilon|\Delta\}$) satisfying (9.8.1.13). These form a space group in four dimensions.

The reciprocal to the basis (9.8.1.11) is

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

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 on the physical space is of the form (9.8.1.7), as it should be.

The superspace approach may also be used for densities, *i.e.* beyond the point-atom approximation. Suppose the quasiperiodic structure is given by a density function $\rho(\mathbf{r})$. If this is the density for a crystal with a one-dimensional modulation, its Fourier decomposition is given by

$$\rho(\mathbf{r}) \;=\; \sum_{\mathbf{k}\in M^*} \hat{\rho}(\mathbf{k}) \exp(2\pi i \mathbf{k}.\mathbf{r}), \tag{9.8.1.15}$$

where the Fourier module M^* consists of the vectors (9.8.1.7). This density ρ is not invariant under a three-dimensional space group, but one may construct a corresponding density function in four dimensions as follows. Each vector of M^* is the projection of a reciprocal-lattice vector in four dimensions. If Σ^* is the reciprocal lattice in four dimensions, and $\mathbf{k}$ the projection of k_s=($\mathbf{k}$,k_I), one may define

$$\rho_s(r_s) = \rho_s(\mathbf{r}, r_I) \;=\; \sum_{k_s\in\Sigma^*} \hat{\rho}(\mathbf{k}) \exp(2\pi i(\mathbf{k}.\mathbf{r} + k_I.r_I)). \tag{9.8.1.16}$$

By construction, this density is invariant under the translations spanned by the vectors (9.8.1.11). Therefore, ρ_s has as symmetry group a four-dimensional space group. Notice that the restriction of ρ_s to the physical space $r_I = 0$ gives the physical density:

$$\rho_s(\mathbf{r}, 0) \;=\; \rho(\mathbf{r}) \;=\; \sum_{\mathbf{k}\in M^*} \hat{\rho}(\mathbf{k}) \exp(2\pi i \mathbf{k}.\mathbf{r}).$$

The invariance of ρ_s is formulated as follows. For an element of the four-dimensional space group

$$g \;=\; (\{R|\mathbf{v}\}, \{\epsilon|\Delta\}),$$

the function ρ_s is invariant if

$$\rho_s(r_s) = \rho_s(gr_s) \leftrightarrow \rho_s(\mathbf{r}, r_I) = \rho_s(R\mathbf{r} + \mathbf{v}, \epsilon r_I + \Delta). \tag{9.8.1.17}$$

The group of all elements satisfying this condition is the superspace group of the incommensurate structure. Notice that this more general description is not limited to incommensurate modulated structures.

The symmetry condition (9.8.1.17) is an expression for the embedded structure in direct space. It has its equivalent expression in reciprocal space. This is a condition on the Fourier components $\hat{\rho}_s(k_s)$ which is identical, by construction, with $\hat{\rho}(\mathbf{k})$. A four-dimensional transformation $(\{R|\mathbf{v}\}, \{\epsilon|\Delta\})$ is a symmetry operation of $\rho(\mathbf{r})$ if

$$\hat{\rho}(\mathbf{k}) \;=\; \hat{\rho}(R^{-1}\mathbf{k}) \exp(-2\pi i \mathbf{k}.\mathbf{v}) \;\exp(-2\pi i k_I.\Delta). \tag{9.8.1.18}$$

As one sees, this is an expression for the three-dimensional function $\hat{\rho}$. For a three-dimensional lattice periodic structure, the expression is the well known condition

$$\hat{\rho}(\mathbf{k}) \;=\; \hat{\rho}(R^{-1}\mathbf{k})\exp(-2\pi i\mathbf{k}.\mathbf{v}).$$

The extra phase shift for an incommensurate phase is a kind of gauge transformation associated with the three-dimensional Euclidean transformation $\{R|\ \mathbf{v}\}$, and is a phase shift in internal space. The formulation in reciprocal space is not so well suited for describing the structure, but it gives a dual view on the structure determination problem. From equation (9.8.1.18) it is seen that for the case that a vector from the Fourier module is invariant under the orthogonal transformation R, the component must be zero if the sum of the two exponents is not equal to an integer. This leads directly to extinction rules.

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 the condensation of a soft mode. The irreducible representation of the space group of the basic structure that characterizes the soft mode gives information on the modulation function as well. (See Janssen & Janner 1984.) Heine & McConnell have treated the symmetry with a method related to the Landau theory of phase transitions, and this is close to the representation theory (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 called the internal coordinates (Perez-Mato, Madariaga & Tello, 1984, 1986; Perez-Mato, Madariaga, Zuñiga & Garcia Arribas, 1987). This method is related to the one advocated by Mermin *et al.* who use an approach equivalent to the reciprocal space formulation explained above (Rokhsar, Wright & Mermin, 1988; Lifshitz, 1996). Alternative treatments of the problem were given by Koptsik (1978) and by de Wolff (1984).

9.8.1.4. Basic symmetry considerations

9.8.1.4.1. Bravais classes of Fourier modules

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

$$\mathbf{H} = \sum_{i=1}^{3} h_i\mathbf{a}_i^* + m\mathbf{q}. \qquad (9.8.1.19)$$

This set of vectors is the Fourier module M^*. The vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3)$ 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.

The Fourier 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 reciprocal lattice Λ^* 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 main reflections are 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 from Λ^*).

An element R of K then transforms the basic vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3)$ and $\mathbf{q}$ into vectors of M^*. Denoting $\mathbf{q}$ by $\mathbf{a}_4^*$ this implies

$$R\mathbf{a}_i^* \;=\; \sum_{j=1}^{4} \Gamma^*(R)_{ji}\mathbf{a}_j^*, \quad i = 1, \ldots, 4, \tag{9.8.1.20}$$

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

$$\Gamma^*(R) = \begin{pmatrix} \Gamma_E^*(R) & \Gamma_M^*(R) \\ 0 & \epsilon(R) \end{pmatrix}, \text{ where } \epsilon(R) = \pm 1. \tag{9.8.1.21}$$

This matrix represents the orthogonal transformation R when referred to the basis vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3, 4)$ of the Fourier module M^*. As in the case of lattices, two Fourier 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 Fourier modules. Equivalent Fourier 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 (9.8.1.19). Within such a larger vector module, the actual diffraction peaks then obey *centring conditions*. For a Fourier module of 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 index the diffraction peaks with respect to the non-primitive lattice basis $\mathbf{a}_1^*$, $\frac{1}{2}\mathbf{a}_2^*$, $\mathbf{a}_3^*$ and the wavevector $\alpha\mathbf{a}_1^*$. When the indices with respect to this basis are H_1, H_2, H_3 and H_4, the centring condition is $H_2 + H_4$=even.

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 (9.8.1.19) as *projections* of four-dimensional lattice vectors H_s=($\mathbf{H}$,H_I), which can be written as

$$H_s \;=\; \sum_{i=1}^{4} h_i a_{si}^*, \tag{9.8.1.22}$$

where m in Eq. (9.8.1.19) has now been replaced by h_4 and

$$a^*_{si} \;=\; (\mathbf{a}^*_i, 0), \quad i = 1, 2, 3; \quad a^*_{s4} \;=\; (\mathbf{q}, 1). \tag{9.8.1.23}$$

As will be explained in Section 9.8.4.1, these vectors span the four-dimensional reciprocal lattice for a periodic structure having as three-dimensional intersection (defined by the hyperplane $r_I = 0$ the modulated crystal (a specific example has been given in Subsection 9.8.1.3, see also (9.8.1.16)). 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

$$R_s a_{si} \;=\; \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj} \quad (i = 1, 2, 3, 4), \tag{9.8.1.24}$$

where $\Gamma(R)$ is the transpose of the matrix $\Gamma^*(R^{-1})$, appearing in (9.8.1.21) and therefore for incommensurate one-dimensionally modulated structures it has the form

$$\Gamma(R) \;=\; \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \epsilon(R) \end{pmatrix}. \tag{9.8.1.25}$$

9.8.1.4.3. Four-dimensional crystallography

Let us summarize the results obtained in the previous subsection. 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 (or 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 $\epsilon = \pm 1$ and act on the four-dimensional lattice basis as

$$(R, \epsilon) a_{si} \;=\; \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj}, \quad i = 1, \ldots, 4, \tag{9.8.1.26}$$

where ϵ stands for $\epsilon(R)$ as in (9.8.1.4.2). So the point-group symmetry operations are crystallographic and given by pairs of a three-dimensional and a one-dimensional point-group transformation. The case $\epsilon = -1$ corresponds to an inversion of the phase of the modulation.

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

Two point groups K_s and K'_s belong to the same *geometric crystal class* if their three-dimensional parts (K_E and K'_E, respectively) are in the same three-dimensional

crystal class [*i.e.* are conjugated subgroups of $O(3)$] and the internal parts of corresponding elements are equal. (This is a stronger condition than simple geometric equivalence in four dimensions, which is the condition of conjugation in $O(4)$.)

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 mentioned in that symbol.

Also the notion of *arithmetic equivalence* can be generalized to these four-dimensional point groups, as they admit the same faithful representation $\Gamma(K)$ given above. This means that two such groups are arithmetically equivalent if there is a basis transformation for the Fourier module which transforms main reflections into main reflections and satellites into satellites and which transforms the matrix groups into each other. The arithmetic crystal classes are determined by the arithmetic equivalence class of $\Gamma_E(K)$ and by the condition

$$R\mathbf{q} \equiv \epsilon(R)\mathbf{q} \ \text{ modulo } \Lambda^*, \tag{9.8.1.27}$$

where Λ^* is the reciprocal lattice for the basic structure. Also here the arithmetic equivalence for incommensurate structures is not the same as that for four-dimensional groups of integer matrices, as the relation between the spaces V_s and V_E 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 special role played by the three-dimensional subspace V_E. 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

$$g_s r_s \ = \ \{(R,\epsilon)|(\mathbf{v},\Delta)\}(\mathbf{r}, r_I) \ = \ (R\mathbf{r}+\mathbf{v}, \epsilon r_I + \Delta) \tag{9.8.1.28}$$

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 equation (9.8.1.28), one obtains the following relations [*cf.* (9.8.1.13)]

$$\mathbf{u}_{j'}[\mathbf{q}.(\mathbf{n}'+\mathbf{r}_{j'})] = R\mathbf{u}_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j) - \epsilon\Delta], \tag{9.8.1.29}$$

with

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

These are purely three-dimensional symmetry relations, but generally not Euclidean.

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

$$\begin{pmatrix} \cos\phi & -\sin\phi & 0 & 0 \\ \sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & \epsilon \end{pmatrix}; \quad \epsilon, \delta = \pm 1. \tag{9.8.1.30}$$

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_E in combination with $\epsilon = -1$ or with $\epsilon = +1$ possibly in combination with a shift Δ. (If $\epsilon = -1$ the intrinsic part in V_I is zero.) In Section 9.8.3.3 it will be shown that the intrinsic value of Δ is one of the following:

$$0, \frac{1}{2}, \pm\frac{1}{3}, \pm\frac{1}{4}, \pm\frac{1}{6} \tag{9.8.1.31}$$

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

9.8.1.4.4. Generalized nomenclature

In Section 9.8.4 the theory will be 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 expressions 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)-dimensional point groups. All these tables use a simple numbering system. A workgroup of the IUCr has developed a proposal for the notation of higher-dimensional crystallographic groups. In that proposal, superspace groups appear as special case (Janssen, Birman, Koptsik, Senechal, Yamamoto, Abrahams & Hahn , 1999; Janssen, Birman, Denoyer, Koptsik, Verger-Gaugry, Weigel, Yamamoto, Abrahams, & Kopsky, 2002).

The difference in the listing of four-dimensional crystallographic groups one finds in Brown *et al.* and in Fast & Janssen 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 occur as symmetry groups of quasiperiodic structures in three dimensions. In particular those for incommensurate one-dimensionally modulated crystals (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 non-equivalent 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 will be 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 list by Fast & Janssen (1969) (and of course in the book by Brown *et al.*) and have been considered again by van Smaalen (1987), who applied them to structure determination. The Bravais classes for the commensurate (3+1)-dimensional case are presented here as well (Section 9.8.3.1).

The relation between modulated crystals and superspace groups has been treated in a textbook by Opechowski (1986).

Note that no new names have been introduced for the underlying crystallographic concepts, like Bravais classes, arithmetic and geometric 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 atom A at site $\mathbf{n}$+$\mathbf{r}_j$ is

$$P_A(\mathbf{n}+\mathbf{r}_j) = p_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j)], \tag{9.8.1.32}$$

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

$$\begin{aligned} S_{\mathbf{H}} &= \sum_{\mathbf{n},j} \left[f_A p_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j)] + f_B\left(1 - p_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j)]\right)\right] \\ &\quad \times \exp[2\pi i \mathbf{H}.(\mathbf{n}+\mathbf{r}_j)], \end{aligned} \tag{9.8.1.33}$$

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

$$p_j(x) = \sum_m w_{jm} \exp(2\pi i m x). \tag{9.8.1.34}$$

Hence,

$$S_{\mathbf{H}} = \sum_j \Bigg(f_B \Delta(\mathbf{H}) \exp(2\pi i \mathbf{H}.\mathbf{r}_j) + (f_A - f_B) \sum_m \Delta(\mathbf{H} + m\mathbf{q}) w_{jm} \times \exp[2\pi i (\mathbf{H} + m\mathbf{q}).\mathbf{r}_j] \Bigg), \quad (9.8.1.35)$$

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

$$\Delta(\mathbf{H}) = \sum_{h_1,h_2,h_3} \delta(\mathbf{H} - \sum_{i=1}^{3} h_i \mathbf{a}_i^*).$$

Consequently, the diffraction peaks occur at positions $h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}$. For a simple sinusoidal function ($m = \pm 1$ in equation 9.8.1.34), there are only main reflections and first-order satellites ($m = \pm 1$). One may introduce an additional coordinate r_I and generalize equation 9.8.1.32 to

$$P_A(\mathbf{n} + \mathbf{r}_j, r_I) = p_j[\mathbf{q}.(\mathbf{n} + \mathbf{r}_j) + r_I], \quad (9.8.1.36)$$

which has a (3+1)-dimensional superspace-group symmetry. Generalization to more complex modulation cases is then straight-forward.

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-dimensionally modulated case, *i.e.* to the n=4 case. Extension to the more general 3+d case is conceptually not difficult and does not modify the 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. [Except for deviations from Friedel's law caused by dispersion: see *ITB* (1993, p.241, Subsection 2.3.4.1).]

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 point 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 *ITA* 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 $n = 4$ case.

The main reflections are indexed by $hk\ell 0$ and the satellite reflections by $hklm$ ($m \neq 0$). The Fourier wavevector of a general reflection $hk\ell m$ is given by

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}. \qquad (9.8.2.1)$$

Note that this step involves a choice because the system of satellite reflections is only defined modulo the reciprocal lattice of the main reflections. When the 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. 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 the Fourier transform of the function $\hat{\rho}(\mathbf{k})$ restricted to the wavevectors $\mathbf{k}$ in the reciprocal lattice of the main reflections. Therefore, it is a periodic structure. It is unique, but possibly involves split atoms. The space group of the average structure is often the symmetry 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 incommensurate 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

$$\alpha = \mathbf{q}.\mathbf{a}, \quad \beta = \mathbf{q}.\mathbf{b}, \quad \gamma = \mathbf{q}.\mathbf{c}. \qquad (9.8.2.2)$$

The (3+1)-dimensional Bravais class is fixed by the three-dimensional Bravais (of Λ) 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 vector $\mathbf{q}$ must be considered. The vector $\mathbf{q}$ can be split into an invariant (or irrational) and a rational component according to

$$\mathbf{q} \;=\; \mathbf{q}^i + \mathbf{q}^r, \quad \text{with} \quad \mathbf{q}^i = \frac{1}{N}\sum_R \epsilon(R)\; R\mathbf{q}, \qquad (9.8.2.3)$$

where the summation is over the elements R of the Laue group P_L, N is the order of P_L, and $\epsilon = \pm 1$ follows from the property

$$R\mathbf{q} \;=\; \epsilon(R)\mathbf{q} \;\; \text{(modulo main reflection vectors)}.$$

If the splitting (9.8.2.3) results in $\mathbf{q}^r$=0, there is no problem. For $\mathbf{q}^r \neq 0$ we choose $\mathbf{q}^i$ as the new modulation wavevector. This may cause satellites to be assigned to extinct main reflections, or even to 'main reflections' with non-integer indices. In this case, it is desirable to choose a new basis $\mathbf{a}_c^*$,$\mathbf{b}_c^*$,$\mathbf{c}_c^*$ such that all reflections can be written as

$$H\mathbf{a}_c^* + K\mathbf{b}_c^* + L\mathbf{c}_c^* + m\mathbf{q}^i \tag{9.8.2.4}$$

with H, K, L and m integers. The new basis is the conventional basis for the M^* module and corresponds to the choice of a conventional cell for the (3+1)-dimensional Bravais lattice.

Observed (possible) centring conditions for the reflections can be applied to determine the (3+1)-dimensional Bravais class.

Example 1. As an example, consider a C-centred orthorhombic lattice with modulation wavevector $\mathbf{q}$=($\alpha 0\frac{1}{2}$), or $\mathbf{q}^i$=(α00) and $\mathbf{q}^r$=(00$\frac{1}{2}$). The general reflection condition is: for $hk\ell 0$: $h + k$ = even. A reflection

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m(\alpha\mathbf{a}^* + \frac{1}{2}\mathbf{c}^*) \tag{9.8.2.5}$$

can be described on the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\frac{1}{2}\mathbf{c}^*$ and $\mathbf{q}^i$ as

$$\mathbf{H} = H\mathbf{a}_c^* + K\mathbf{b}_c^* + L\mathbf{c}_c^* + m\mathbf{q}^i. \tag{9.8.2.6}$$

Because $H = h$, $K = k$, $L = 2\ell+m$, and h, k, and ℓ are integers, with $h+k$ =even because of the C-centring, one has the conditions $H + K$=even and $L + m$=even. The adopted conventional basis has centring ($\frac{1}{2}\frac{1}{2}00, 00\frac{1}{2}\frac{1}{2}, \frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}$). After interchange of H and L, one gets $K+L$=even and $H+m$=even, which according to Table (9.8.3.6) gives $mmmA(\frac{1}{2}0\gamma)$ Changing back to the original setting gives the Bravais class $mmmC(\alpha 0\frac{1}{2})$.

Example 2. As a second example, consider a C-centred orthorhombic lattice of main reflections. Suppose that an arbitrary reflection is given by

$$H\mathbf{a}_c^* + K\mathbf{b}_c^* + L\mathbf{c}_c^* + m\gamma\mathbf{c}^* \tag{9.8.2.7}$$

with respect to the conventional basis of the C-centred lattice and that the general reflection condition is

$$H + K + m = \text{even}. \tag{9.8.2.8}$$

This is in agreement with the C-centring condition $H + K$=even for the main reflections. Equation (9.8.2.8) implies a centring ($\frac{1}{2}\frac{1}{2}0\frac{1}{2}$) of the (3+1)-dimensional lattice Σ. Its conventional basis corresponding to (9.8.2.7) is

$$(\mathbf{a}, 0),\ (\mathbf{b}, 0),\ (\mathbf{c}, -\gamma),\ (0, 1). \tag{9.8.2.9}$$

Because of the centring translation [(**a**+**b**)/2,1/2], a primitive basis of Σ is

$$\left(\frac{\mathbf{a}+\mathbf{b}}{2}, -\frac{1}{2}\right), \left(\frac{\mathbf{a}-\mathbf{b}}{2}, -\frac{1}{2}\right), (\mathbf{c}, -\gamma), (0, 1), \tag{9.8.2.10}$$

which corresponds, according to (9.8.1.11), to a choice $\mathbf{q}=\mathbf{a}^*+\gamma\mathbf{c}^*$. In terms of this modulation wavevector, an arbitrary reflection can be described as

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m(\mathbf{a}^* + \gamma\mathbf{c}^*). \tag{9.8.2.11}$$

Because $H = h + m$, $K = k$, and $L = \ell$, the reflection condition (9.8.2.8) now becomes $h + k$=even, again in agreement with the fact that the lattice of main reflections is C-centred.

(5) *Step five*: one lists all point groups (more precisely, the arithmetic crystal classes) compatible with the external Bravais class (*i.e.* the three-dimensional one), the components of the modulation wavevector $\mathbf{q}$ with respect to the conventional basis of this class, and the observed general extinctions. These groups are listed in Table 9.8.3.6.

The external part of the (3+1)-dimensional point group does not need to be the same as the point group of the average structure: it can never be larger, but is possibly a subgroup only.

(6) *Step six* consists of finding the superspace groups compatible with the previously derived results and with the special extinctions observed in the diffraction pattern.

For each arithmetic point group, the non-equivalent superspace groups are listed in the Tables. For (3+1)-dimensional superspace groups this is Table 9.8.3.9.

Example 3. Continue with example 2 of step 4. The external Bravais class of the modulated crystal is $mmmC$ and $\mathbf{q}=(10\gamma)$. Consider the two cases of special reflection conditions.

(1) The observed condition is $00Lm$: $m = 2n$. Then there is only one superspace group that obeys this condition: No. 21.4 with symbol $C222(10\gamma)00s$ in Table 9.8.3.9. [See Subsection 9.8.3.3 for explanation of the symbols; note that $C222$ denotes the external part of the (3+1)-dimensional space group.]

(2) There is no special reflection condition. Possible superspace groups are:

$C222(10\gamma)$	No. 21.3,	$Cmm2(10\gamma)$,	No. 35.4,
$C2mm(10\gamma)$	No. 38.3,	$Cmmm(10\gamma)$,	No. 65.4

In this second case, there are thus four possible superspace groups, three without and one with inversion symmetry. The difficulty stems from the fact that, in the absence of anomalous dispersion, the Laue group always has an inversion centre. Just as in three-dimensional crystallography, the ambiguity can only be solved by a complete determination of the structure, or by non-diffraction methods.

In the determination of modulated structures, one generally starts with the assumption that the external part of the (3+1)-dimensional point group is equal to the point group of the basic structure. This is, however, not necessarily true. The former may be a subgroup of the latter. Especially, when the basic structure contains atoms at special positions, the point-group symmetry may be lowered by the modulation.

(7) *Step seven* concerns the restrictions imposed on/by the displacive or occupation modulation waves. For each occupied special Wyckoff position of the basic structure, one has to verify the validity of the restrictions imposed by the elements of the superspace group on the modulation as expressed in equation (9.8.1.29).

During the structure determination, one should check for each Wyckoff position which is occupied by an atom of the basic structure, whether the assumed displacive or occupation modulations obey the site symmetry of the Wyckoff position considered. An atom at a special position transforms into itself by the site symmetry of the position. For such a symmetry transformation, $j' = j$, $\mathbf{v}$=0. Moreover, if ϵ= -1, then Δ may be chosen to be zero (by an origin shift). Then according to (9.8.1.29), one has for a displacive modulation

$$\begin{aligned} \mathbf{u}_j(\mathbf{q}.\mathbf{r}) &= R\mathbf{u}_j(\mathbf{q}.\mathbf{r}-\Delta) \qquad \text{for } \epsilon = 1, \\ \mathbf{u}_j(\mathbf{q}.\mathbf{r}) &= R\mathbf{u}_j(\mathbf{q}.\mathbf{r}) \qquad \text{for } \epsilon = -1, \end{aligned} \tag{9.8.2.12}$$

and, for occupation modulation

$$\begin{aligned} p_j(\mathbf{q}.\mathbf{r}) &= p_j(\mathbf{q}.\mathbf{r}-\Delta) \qquad \text{for } \epsilon = 1, \\ p_j(\mathbf{q}.\mathbf{r}) &= p_j(\mathbf{q}.\mathbf{r}) \qquad \text{for } \epsilon = -1, \end{aligned} \tag{9.8.2.13}$$

Example 4. Assume, as for the case discussed above, that the basic structure has the space group $Cmmm$. Can the superspace group be $Cmmm(10\gamma)$? In this superspace group Δ=0 for all symmetry operations with ϵ=1. Displacive modulations at special positions must thus obey $\mathbf{u}_j(\mathbf{q}.\mathbf{r})$=$R\mathbf{u}_j(\mathbf{q}.\mathbf{r})$ for the superspace group to be correct. For an atom at a special position with site symmetry mmm, this is not possible for all site-symmetry operations unless $\mathbf{u}_j$=0. Suppose that the structure model contains a displacive modulation polarized along $\mathbf{a}$ for that atom. The allowed site symmetry is then lowered to $2mm$, and as a consequence the superspace group is $C2mm(10\gamma)$ rather than $Cmmm(10\gamma)$.

9.8.3. Introduction to the tables

In what follows, the tables dealing with the (3+1)-dimensional case will be presented. In addition a number of (2+1,)-, (2+2)-, (3+2)-, and (3+3)-dimensional cases will illustrate the more general case. Tables for other quasiperiodic cases than modulated structures, such as quasicrystals, are exemplified in Section 9.8.5

9.8.3.1. Tables of Bravais classes

The (3+1)-dimensional lattice Σ^* is determined by the three-dimensional vectors $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ and the modulation wavevector $\mathbf{q}$. The former three vectors give by duality $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$, the external components of lattice basis vectors, and the products -$\mathbf{q}$.$\mathbf{a}$=-α,

-$\mathbf{q}.\mathbf{b}$=-β, and -$\mathbf{q}.\mathbf{c}$=-γ the corresponding internal components. Therefore, it is sufficient to give the arithmetic crystal class of the group $\Gamma_E(K)$ and the components σ_j ($\sigma_1 = \alpha, \sigma_2 = \beta, \sigma_3 = \gamma$) of the modulation vector $\mathbf{q}$ with respect to a conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$. The arithmetic crystal class is denoted by a modification of the symbol for the three-dimensional symmorphic space group of this class plus an indication for the row matrix σ (having entries σ_j). In this way, one obtains the so-called one-line symbols used in Tables 9.8.3.2-9.8.3.5.

As an example, the symbol $2/mB(0\frac{1}{2}\gamma)$ denotes a Bravais class for which the main reflections belong to a B-centred monoclinic lattice (unique axis $\mathbf{c}$) and the satellite positions are generated by the point-group transforms of $\frac{1}{2}\mathbf{b}^* + \gamma\mathbf{c}^*$. Then the matrix σ becomes $(0\frac{1}{2}\gamma)$. It has as irrational part $\sigma^i = (00\gamma)$ and as rational part $\sigma^r = (0\frac{1}{2}0)$. The external part of the (3+1)-dimensional point group of the Bravais lattice is $2/m$. By use of the relation [*cf.* 9.8.2]

$$R\mathbf{q}^i \;=\; \epsilon\mathbf{q}^i, \qquad R\mathbf{q}^r \equiv \epsilon\mathbf{q}^r \text{ (modulo } \mathbf{b}^*), \tag{9.8.3.1}$$

we see that the operations 2 and m are associated with the internal space transformations $\epsilon = 1$ and $\epsilon = -1$, respectively. This is denoted by the one-line symbol $(2/m, 1\bar{1})$ for the (3+1)-dimensional point group of the Bravais lattice. In direct space, the symmetry operation $(R, \epsilon(R))$ is represented by the matrix $\Gamma(R)$ which transforms the components $v_j,\ j = 1, \ldots, 4$, of a vector v_s to:

$$v'_j \;=\; \sum_{k=1}^{4} \Gamma(R)_{jk} v_k.$$

The operations (2,1) and $(m, \bar{1})$ are represented by the matrices:

$$\Gamma(2) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix};\ \Gamma(m) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}. \tag{9.8.3.2}$$

The 3×3 part $\Gamma_E(R)$ of each matrix is obtained by considering the action of R on the external part $\mathbf{v}$ of v_s. The 1×1 part $\Gamma_I(R)$ is the value of the ϵ associated with R and the remaining part $\Gamma_M(R)$ follows from the relation

$$\Gamma_M(R) \;=\; -\Gamma_I(R)\sigma^r + \sigma^r\Gamma_E(R), \tag{9.8.3.3}$$

where $\Gamma_M(R)$, $\Gamma_E(R)$, and $\Gamma_I(R) = \epsilon(R)$ are defined as in Eq. (9.8.1.25).

Bravais classes can be denoted in an alternative way by two-line symbols. In the two-line symbol, the Bravais class is given by specifying the arithmetic crystal class of the external symmetry, the associated elements $\Gamma_I(R) = \epsilon$ by putting their symbol under the corresponding symbols of $\Gamma_E(R)$, and by the rational part σ^r indicated by a prefix. In Table 9.8.3.1, this prefix is given for the components of $\mathbf{q}^r$ that play a role in the classification.

Table 9.8.3.1: *Centring symbols for (3+1)D lattices.* The vectors $\mathbf{q}^{\mathrm{r}}$ correspond to centerings in superspace.

P	(000)	R	$(\frac{1}{3},\frac{1}{3},0)$		
A	$(\frac{1}{2},0,0)$	B	$(0,\frac{1}{2},0)$	C	$(0,0,\frac{1}{2})$
L	(1,0,0)	M	(0,1,0)	N	(0,0,1)
U	$(0,\frac{1}{2},\frac{1}{2})$	V	$(\frac{1}{2},0\frac{1}{2})$	W	$(\frac{1}{2},\frac{1}{2},0)$

Note that the integers appearing here are not equivalent to zero because they express components with respect to a conventional lattice basis (and not a primitive one). For the Bravais class mentioned above, the two-line symbol is $B_{1\ \bar{1}}^{2/mB}$. $2/mB$ is the arithmetic crystal class of the external part, that of the internal part is $1\bar{1}p$, but p is omitted because there is only one possibility in one dimension. This two-line symbol has the advantage that the internal transformation (the value of ϵ) is explicitly given for the corresponding generators. It has however, certain typographical drawbacks. It is difficult for the printer to put the symbol together in the right way.

In the Tables 9.8.3.2-5, the symbols are given in the one-line form. It is, however, easy to derive from each one-line symbol the corresponding two-line symbol because the bottom line for the two-line symbol appears in the tables as the internal part of the point-group symbol.

The number of symbols in the bottom line of the two-line symbol should be equal to that of the generators given in the top line. A symbol '1' is used in the bottom line if the corresponding R_I is the unit transformation. If necessary, a mirror perpendicular to a crystal axis is indicated by $\dot{m}$ and one that is not by $\ddot{m}$. This situation occurs for $d \geq 2$. So the (2+2)-dimensional class P_{4m}^{4mp} is actually $P_{4\dot{m}}^{4\dot{m}p}$ and this is different from the class $P_{4\ddot{m}}^{4\dot{m}p}$. In a one-line symbol, their difference is apparent, the first corresponding to $4mp(\alpha 0)$, whereas the second is $4mp(\alpha\alpha)$.

9.8.3.2. Tables for geometric and arithmetic crystal classes

In Table 9.8.3.6, the geometric and arithmetic crystal classes of the (3+1)-dimensional superspace are given.

The symbols for *geometric crystal classes* indicate the pairs $[R, \epsilon(R)]$ of the generators of the point group. This is done by giving the geometric crystal class for the point group K_E and the symbols for the corresponding elements of K_I. So, for example, the geometric crystal class belonging to the holohedral point group of the Bravais class $2/mB(0\frac{1}{2}\gamma)$, mentioned above, is $(2/m, 1\bar{1})$.

The notation for the *arithmetic crystal classes* is similar to that of the Bravais classes. In the tables, their one-line symbols are given. They consist of the (modified) symbol of the three-dimensional symmorphic space group and, in parentheses, the appropriate components of the modulation wave vector. The three arithmetic crystal classes

implying a lattice belonging to the Bravais class $2/mB(0\frac{1}{2}\gamma)$ are $2B(0\frac{1}{2}\gamma)$, $mB(0\frac{1}{2}\gamma)$, and $2/mB(0\frac{1}{2}\gamma)$. The corresponding geometric crystal classes are $(2,1)$, $(m,\bar{1})$, and $(2/m,1\bar{1})$.

9.8.3.3. Tables of superspace groups

9.8.3.3.1. Symmetry elements

The transformation g_s belonging to a (3+1)-dimensional superspace group consists of a point-group transformation R_s given by the integral matrix $\Gamma(R)$ and of the associated translation. So the superspace group is determined by the arithmetic crystal class of its point group and the corresponding translational components. The symbol for the arithmetic crystal class has been discussed in Subsection 9.8.3.2. Given a point-group transformation R_s, the associated translation is determined up to a lattice translation. As in three dimensions, the translational part generally depends on the choice of the origin. To avoid this arbitrariness, one decomposes that translation into a component (called intrinsic) independent of the origin, and a remainder. The (3+1)-dimensional translation v_s associated with the point-group transformation R_s is given by

$$v_s \;=\; \sum_{i=1}^{3+1} v_i a_{si}. \tag{9.8.3.4}$$

Its origin-independent part v_s^0 is given by

$$v_s^0 = \sum_{j=1}^{4} v_j^0 a_{si} \quad \text{with} \quad v_j^0 = \frac{1}{n}\sum_{m=1}^{n}\sum_{k=1}^{4}\Gamma(R^m)_{jk} v_k, \tag{9.8.3.5}$$

where n is now the order of the point-group transformation R (so that R^n is the identity). As customary also in three-dimensional crystallography, one indicates in the space-group symbol the invariant components v_j^0. Notice that this means that there is an origin for R_s in (3+1)-dimensional superspace such that the translation associated with R_s has these components. This origin, however, may not be the same for different transformations R_s, as is known already in three-dimensional crystallography.

Written in components, the non-primitive translation v_s associated with the point-group element (R, R_I) is $(\mathbf{v},v_I)$, where v_I can be written as δ-$\mathbf{q}.\mathbf{v}$. In accordance with (9.8.1.12), δ is defined as v_4. The origin-independent part v_s^0 of v_s is

$$v_s^0 = (\mathbf{v}^0, v_I^0) = \frac{1}{n}\sum_{m=1}^{n}(R^m\mathbf{v}, R_I^m v_I) = (\mathbf{v}^0, \phi - \mathbf{q}.\mathbf{v}^0), \tag{9.8.3.6}$$

where

$$v_4^0 \;=\; v_I^0 + \mathbf{q}.\mathbf{v}^0.$$

The internal transformation $R_I(R) = \epsilon(R)$ is either +1 or -1. When ϵ= -1 it follows from (9.8.3.6) that $v_I^0 = 0$. For $\epsilon = +1$, one has $v_I^0 = v_I$. Because in that case

$$\mathbf{q}.\mathbf{v}^0 = \frac{1}{n}\sum_{m=1}^{n}\mathbf{q}.R^m\mathbf{v} = \mathbf{q}^i.\mathbf{v}, \tag{9.8.3.7}$$

it follows that

$$v_4^0 = v_I + \mathbf{q}.\mathbf{v}^0 = \delta - \mathbf{q}.\mathbf{v} + \mathbf{q}.\mathbf{v}^0 = \delta - \mathbf{q}^r.\mathbf{v}. \qquad (9.8.3.8)$$

For R_s of order n, R_s^n is the identity and the associated translation is a lattice translation. The ensuing values for v_4^0 are 0, $\frac{1}{2}$, $\pm\frac{1}{3}$, $\pm\frac{1}{4}$ or $\pm\frac{1}{6}$ (modulo integers). This remains true in the case of a centred basis. The symbol for the (3+1)-dimensional space-group element is determined by the intrinsic part of its three-dimensional translation and v_4^0. Again, that information can be given in terms of either a one-line or a two-line symbol.

In the one-line symbol, one finds: the symbol according to *International Tables for Crystallography*, Volume A, for the space group generated by the elements $\{R|\mathbf{v}\}$, in parentheses the components of the modulation vector $\mathbf{q}$ followed by the values v_4^0, one for each generator appearing in the three-dimensional space group symbol. A letter symbolizes the value of v_4^0 according to

v_4^0	0	$\frac{1}{2}$	$\pm\frac{1}{3}$	$\pm\frac{1}{4}$	$\pm\frac{1}{6}$
symbol	0	s	t	q	h

. (9.8.3.9)

As an example, consider the superspace group

$$P2_1/m(\alpha\beta 0)0s.$$

The external components $\{R|\mathbf{v}\}$ of the elements of this group form the three-dimensional space group $P2_1/m$. The modulation wavevector is $\alpha\mathbf{a}^* + \beta\mathbf{b}^*$ with respect to a conventional basis of the monoclinic lattice with unique axis $\mathbf{c}$. Therefore, the four-dimensional point group is $(2/m, \bar{1}1)$. The point-group element $(2,\bar{1})$ is associated with a non-primitive translation with intrinsic part $(\frac{1}{2}\mathbf{c},0)$=$(00\frac{1}{2}0)$, and the point-group generator $(m,1)$ one with $(\mathbf{0},\frac{1}{2})$=$(000\frac{1}{2})$.

In the two-line symbol, one finds in the upper line the symbol for the three-dimensional space group, in the bottom line the value of v_4^0 for the case $\epsilon = 1$ and the symbol '$\bar{1}$' when $\epsilon = -1$. The rational part of $\mathbf{q}$ is indicated by means of the appropriate prefix (Table 9.8.3.1). In the case considered, $\mathbf{q}^r$=000. So the prefix is P and the superspace group is denoted by the two-line symbol

$$P^{P2_1/m}_{\bar{1}\quad s}.$$

In Table 9.8.3.9, the (3+1)-dimensional superspace groups are given by one-line symbols. It is an adapted version of the tables given by de Wolff, Janssen & Janner (1981) and corrected by Yamamoto, Janssen, Janner & de Wolff (1985).The given symbols are short symbols. Sometimes, a more extensive symbol is required. Then, for the example given above one has $P112_1/m(\alpha\beta 0)000s$ for the one-line symbol. Note that in the short one-line symbol for superspace groups with $v_4^0 = 0$ (where the non-primitive translations can be transformed to zero by a choice of origin) the zeros for the translational part are omitted. Not so, of course, in the full symbol. For example, short symbol $P2_1/m(\alpha\beta 0)$ and full symbol $P112_1/m(\alpha\beta 0)0000$.

9.8.3.3.2. Reflection conditions

The indexing of diffraction vectors is a matter of choice of basis. When the basis chosen is not a primitive one, the indices have to satisfy certain conditions known as *centring conditions*. This holds for the main reflections (centring in physical space) as well as for satellites (centring in superspace). These centring conditions have been discussed in Subsection 9.8.2

In addition to these general reflection conditions, there may be special reflection conditions related to the existence of non-trivial non-primitive translations in the (3+1)-dimensional superspace group, just as is the case for glide planes and screw axes in three dimensions.

Special reflection conditions can be derived from transformation properties of the structure factor under symmetry operations. Transforming the geometric structure factor by an element $g_s = (\{R|\mathbf{v}\}, \{R_I|v_I\})$, one obtains

$$S_{\mathbf{H}} \;=\; S_{R^{-1}\mathbf{H}} \exp[-2\pi i(\mathbf{H}.\mathbf{v} + H_I.v_I)]. \tag{9.8.3.10}$$

Therefore, if $R\mathbf{H}$=$\mathbf{H}$, the corresponding structure vanishes unless $\mathbf{H}.\mathbf{v} + H_I.v_I$ is an integer.

The form of such a reflection condition in terms of allowed or forbidden sets of indices depends on the basis chosen. When a lattice basis is chosen, one has

$$H_s \;=\; (\mathbf{H}, H_I) \;=\; \sum_{i=1}^{4} h_i a^*_{si}, \tag{9.8.3.11}$$

$$v_s \;=\; (\mathbf{v}, v_I) \;=\; \sum_{i=1}^{4} v_i a_{si}. \tag{9.8.3.12}$$

Then the reflection condition becomes

$$H_s.v_s = \sum_{i=1}^{4} h_i v_i \;=\; \text{integer} \quad \text{for } R\mathbf{H} = \mathbf{H}. \tag{9.8.3.13}$$

In terms of external and internal shift components, the reflection condition can be written as

$$H_s.v_s \;=\; \mathbf{H}.\mathbf{v} + H_I.v_I = \mathbf{H}.\mathbf{v} + mv_I = \text{integer} \;\; \text{for } R\mathbf{H} = \mathbf{H}. \tag{9.8.3.14}$$

With $\mathbf{H}$=$\mathbf{K}$+$m\mathbf{q}$ and $v_I = \delta - \mathbf{q}.\mathbf{v}$, this gives

$$\mathbf{K}.\mathbf{v} + m\delta = \text{integer for } R\mathbf{H} = \mathbf{H}. \tag{9.8.3.15}$$

For $\mathbf{v}$=$v_1\mathbf{a} + v_2\mathbf{b} + v_3\mathbf{c}$ and $\mathbf{K}$=$h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*$ one gets the expression

$$hv_1 + kv_2 + \ell v_3 + m\delta \;=\; \text{integer for } R\mathbf{H} = \mathbf{H}. \tag{9.8.3.16}$$

When the modulation wavevector has a rational part, one can choose another basis (a conventional basis) such that $\mathbf{K}$'=$\mathbf{K}$+$m\mathbf{q}^r$ has integer coefficients:

$$\mathbf{H} = \mathbf{K}' + m\mathbf{q}^i = H\mathbf{a}^*_c + K\mathbf{b}^*_c + L\mathbf{c}^*_c + m\mathbf{q}^i. \tag{9.8.3.17}$$

Then, (9.8.3.15) with $v_4^0 = \delta - \mathbf{q}^r.\mathbf{v}$ becomes:

$$\mathbf{K}'.\mathbf{v} + mv_4^0 \;=\; \text{integer for } R\mathbf{H} = \mathbf{H} \tag{9.8.3.18}$$

and (9.8.3.16) transforms into

$$Hv_1' + Kv_2' + Lv_3' + mv_4^0 \;=\; \text{integer for } R\mathbf{H} = \mathbf{H}, \tag{9.8.3.19}$$

in which v_i' are the components of $\mathbf{v}$ with respect to the (conventional) basis $\mathbf{a}_c$, $\mathbf{b}_c$, and $\mathbf{c}_c$.

As an example, we consider a (3+1)-dimensional space-group transformation with R a mirror perpendicular to the x-axis, $\epsilon = 1$, $\mathbf{v}=\frac{1}{2}\mathbf{b}$, and $v_4^0 = \frac{1}{4}$ with $\mathbf{b}$ orthogonal to $\mathbf{a}$. The modulation wavevector is supposed to be $(\frac{1}{2}\frac{1}{2}\gamma)$. Then $\delta = \frac{1}{4} + \mathbf{q}^r.\mathbf{v} = \frac{1}{2}$. The vectors $\mathbf{H}$ left invariant by R satisfy the relation $2h + m = 0$. For such a vector, the reflection condition becomes

$$\mathbf{K}.\mathbf{v} + m\delta = \frac{1}{2}\mathbf{K}.\mathbf{b} + \frac{1}{2}m = \frac{k+m}{2} = \text{integer, or } k + m = 2n.$$

For the basis $\frac{1}{2}(\mathbf{a}^* + \mathbf{b}^*)$, $\frac{1}{2}(\mathbf{a}^* - \mathbf{b}^*)$, $\mathbf{c}^*$, the rational part of the wavevector vanishes. The indices with respect to this basis are $H = h + k + m$, $K = h - k$, $L = \ell$ and m. The condition now becomes

$$\mathbf{K}'.\mathbf{v} + mv_4^0 \;=\; \frac{H - K + m}{4} \;=\; \text{integer},$$

$$\text{or } H - K + m = 4n, \text{ for } K = -H.$$

Of course, both calculations give the same result: $k + m = 2n$ for $h, k, \ell, -2h$ and $H - K + m = 4n$ for $H, -H, L, m$.

The special reflection conditions for the elements occurring in (3+1)-dimensional superspace groups are given in Table 9.8.3.9.

9.8.3.4. Guide to the use of the Tables

In the tables, Bravais classes, point groups, and superspace groups are given for three-dimensional incommensurate modulated crystals with a modulation of dimension one and for two-dimensional crystals (*e.g.* surfaces) with one- and two-dimensional modulation (Janssen, Janner & de Wolff, 1980). In the following, we discuss briefly the information given and its organization. Examples of their use can be found in Subsection 9.8.3.5.

To determine the symmetry of the modulated phase, one first determines its average structure, which is obtained from the main reflections. Since this structure has three-dimensional space-group symmetry, this analysis is performed in the usual way.

The diffraction pattern of the three-dimensional modulated phase can be indexed by 3+1 integers. The Bravais class is determined by the symmetry of the vector module spanned by the 3+1 basis vectors. The crystallographic system of the pattern is equal to or lower than that implied by the main reflections. One chooses a conventional basis

($\mathbf{q}^r$=0) for the vector module, and finds the Bravais class from the general reflection conditions using Table 9.8.3.10. The relation between indices $hk\ell m$ with respect to the basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, and $\mathbf{q}$ and $HKLm$ with respect to the conventional basis $\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{c}_c^*$, and $\mathbf{q}^i$ is also given there.

Tables 9.8.3.4-5 give the number labelling the (3+1)-dimensional Bravais class, its symbol, its external and internal point group, and the modulation wavevector. Moreover, the superspace conventional basis (for which the rational part $\mathbf{q}^r$ vanishes) and the corresponding (3+1)-dimensional centring are given. Because the four-dimensional lattices belong to Euclidean Bravais classes, the corresponding class is also given in the notation of Janssen (1969) and Brown *et al*. (1978). The corresponding (2+1)- and (2+2)-dimensional cases are given in Tables 9.8.3.2 and 9.9.3.3, respectively.

The point group of the modulated structure is a subgroup of the holohedry of its lattice Λ. In Table 9.8.3.6, for each system the (3+1)-dimensional point groups are given. Each system contains one or more Bravais classes. Each geometric crystal class contains one or more arithmetic crystal classes. The (3+1)-dimensional arithmetic classes belonging to a given geometric crystal class are also listed in Table 9.8.3.6.

Starting from the space group of the average structure, one can determine the (3+1)-dimensional superspace group. In Table 9.8.3.9, the full list of these (3+1)-dimensional superspace groups is given for the incommensurate case and are ordered according to their basic space group. They have a number $n.m$ where n is the number of the basic space group one finds in *International Tables for Crystallography*, Volume A. The various (3+1)-dimensional superspace groups for each basic group n are distinguished by the number m. Furthermore, the symbol of the basic space group, the point group and the symbol for the corresponding superspace group are given. In the last column, the special reflection conditions are listed for typical symmetry elements. These may help in the structure analysis. The (2+d)-dimensional superspace groups, relevant for modulated surface and interface structures, are given in Tables 9.8.3.7 and 9.8.3.8, for d=1 and d = 2, respectively.

9.8.3.5. Examples

(A) Na_2CO_3.

Na_2CO_3 has a phase transition at about 753K from the hexagonal to the monoclinic phase. At about 633K, one vibration mode becomes unstable and below the transition temperature T_i=633K there is a modulated γ-phase (de Wolff & Tuinstra, 1986). At low temperature (128K), a transition to a commensurate phase has been reported.

The main reflections in the modulated phase belong to a monoclinic lattice, and the satellites to a modulation with wavevector $\mathbf{q}$=$\alpha\mathbf{a}^*$+$\gamma\mathbf{c}^*$ (unique axis $\mathbf{b}$). The dimension of the modulation is one. The main reflections satisfy the condition

$$hk\ell 0,\ h+k\ =\ \text{even}.$$

Therefore, the lattice of the average structure is C-centred monoclinic. For satellites, the same general condition holds ($hk\ell m,\ h+k$ =even). From Table 9.8.3.10, one sees after a

change of axes that the Bravais class of the modulated structure is

$$\text{No. } 4 : 2/mC(\alpha 0\gamma).$$

Table 9.8.3.4 shows that the point group of the Fourier module is $2/m(\bar{1}1)$. The point group of the modulated structure is is equal to or a subgroup of this one.

The space group of the average structure determined from the main reflections is $C2/m$ (No. 12 in *International Tables for Crystallography*, Volume A). The superspace group may then be determined from the special reflection condition

$$h0\ell m, \quad m = \text{even}$$

using Table 9.8.3.9. There are five superspace groups with basic group No. 12. Among them there are two in Bravais class 4. The reflection condition mentioned leads to the group

$$\text{No. } 12.2 \;=\; C2/m(\alpha 0\gamma)0s \;=\; P^{C2/m}_{\bar{1}\;s}.$$

In principle, the superspace group could be a subgroup of this, but, since the transition unmodulated-modulated is of second order, Landau theory predicts that the basic space group is the symmetry group of the unmodulated monoclinic phase, which is $C2/m$.

(B) $ThBr_4$.

Thorium tetrabromide has an incommensurately modulated phase below T_i=95K (Currat, Bernard & Delamoye, 1986). Above that temperature, the structure has space group $I4_1/amd$ (No. 141 in *International Tables for Crystallography*, Volume A). At T_i, a mode becomes unstable and a modulated β-phase sets in with modulation wavevector $\gamma\mathbf{c}^*$. The dimension of the modulation is one, consequently.

The main reflections belong to a tetragonal lattice. The general reflection condition is

$$hk\ell m, \; h + k + \ell \;=\; \text{even}.$$

Looking at Table 9.8.3.10, one finds the Bravais class to be No. 21 $=4/mmmI(00\gamma)$. Table 9.8.3.4 gives $4/mmm(1\bar{1}11)$ for the point group of the Fourier module.

For the determination of the symmetry group of the modulated structure, one has the special reflection conditions:

$$hk00, h \text{ even}; \quad hh\ell 0, \; 2h + \ell = 4n; \quad 00\ell 0, \; \ell = 4n;$$

$$0k\ell m \text{ and } h0\ell m, \text{ absent for } m = 1$$

Higher-order satellites have not been observed. The main reflections lead to the basic group $I4_1/amd$. If one generalizes the reflection condition observed for $(0k\ell m)$ to: $0k\ell m$, m = even, the superspace group is found from Table 9.8.3.9 under the groups $141.m$ as

$$\text{No. } 141.2 = I4_1/amd(00\gamma)s0s0 = P^{I4_1/amd}_{s\;\;\bar{1}s1}.$$

(C) PAMC

Bis(n-propylammonium) tetrachloromanganate (PAMC) has several phase transitions.

Above about 395K, it is orthorhombic with space group *Abma*. At T_i, this β-phase goes over into the incommensurately modulated γ-phase (Depmeier, 1986; Kind & Muralt, 1986). The wavevector of the modulation is $\alpha\mathbf{a}^* + \mathbf{c}^*$. Therefore, the dimension of the modulation is one. Interchanging the a- and c-axes, one sees from Table 9.8.3.4 that the Bravais class is No. $14 = mmmC(10\gamma)$. In this new setting, the conventional basis of the Fourier module is $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, and $\gamma\mathbf{c}^*$, and the general reflection condition becomes

$$HKLm,\ H + K + m = \text{even}.$$

Therefore, if one considers the Fourier module as the projection of a four-dimensional lattice, the reflection condition corresponds to a $(\frac{1}{2}\frac{1}{2}0\frac{1}{2})$ centring in four dimensions.

The point group of the Fourier module is $mmm(11\bar{1})$ The basic space group being *Abma* (or *Ccmb* in the new setting), the superspace group follows from Table 9.8.3.9 as

$$\text{No. } 64.3 = Ccmb(10\gamma) = L^{Ccmb}_{11\bar{1}}$$

or, in the original settings,

$$\text{No. } 64.3 = Abma(\alpha 01) = N^{Abma}_{\bar{1}11}.$$

Number 64.4 can be excluded because the reflections do not show the special condition $0KLm,\ m = \text{even}$.

9.8.3.6. Ambiguities in the notation

The intrinsic part v_s^0 of the translation part v_s of a (3+1)-dimensional superspace-group element is uniquely determined by (9.8.3.5). This does not imply that, for each element of the point group, the intrinsic part of the translation associated with it is unique modulo lattice vectors. The reason is that, for a given element R of the point group and given origin, the translation part may be changed by a lattice vector. This situation is well known in three-dimensional crystallography. For example, the two-fold rotation $(x, y, z) \rightarrow (-x, z, y)$ in the space group $P4_132$ has according to Volume A of *International Tables of Crystallography* a translation part $(\frac{1}{4}, \frac{3}{4}, \frac{1}{4})$. Its intrinsic part is $(0, \frac{1}{2}, \frac{1}{2})$ according to (9.8.3.5). However, when the translation part is equivalently taken as $(\frac{1}{4}, \frac{3}{4}, -\frac{3}{4})$, the intrinsic part vanishes. Therefore, in the symbol for that space group, the third generator is the rotation '2', and not the screw axis '2_1'.

The same situation may occur in (3+1) dimensions. This can be seen very clearly from the definition of v_4^0 in (9.8.3.8). Since $\mathbf{v}$ is only determined modulo a lattice vector, one may add to it a lattice vector that has a non-vanishing product with $\mathbf{q}^r$. This results in a change of v_4^0. For example, the (3+1)-dimensional space group $Pmmm(\frac{1}{2}0\gamma)000$ has a mirror perpendicular to the $\mathbf{a}$ axis with associated value $v_4^0 = 0$. the parallel mirror at a distance $a/2$ has $\mathbf{v}$=$\mathbf{a}$ and consequently v_4^0=$\frac{1}{2}$. Hence, the symbols $Pmmm(\frac{1}{2}0\gamma)000$ and $Pmmm(\frac{1}{2}0\gamma)s00$ indicate the same group. This non-uniqueness in the symbol, however, does not have serious practical consequences.

Table 9.8.3.2: *(2+1)-dimensional Bravais classes for incommensurate structures.* The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + m\mathbf{q}$, where $\mathbf{q}$ is the modulation wavevector. If the rational part $\mathbf{q}^r$, as defined in Eq. (9.8.2.3), is not zero, there is a corresponding centring translation in three-dimensional space. The conventional basis ($\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{q}^i$) given for the vector module M^* is shown such that $\mathbf{q}^r$=0. The basis vectors are given by components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$ of the lattice Λ^* of main reflections.

No.	Symbol	K_E	K_I	$\mathbf{q}$	Conventional basis	Centring
Oblique						
1	$2p(\alpha\beta)$	2	$\bar{1}$	$(\alpha\beta)$	(10),(01),$(\alpha\beta)$	

This is the beginning of Table 9.8.3.1(a) in ITCC 1999

Another source of ambiguity is the fact that the assignment of a satellite to a main reflection is not unique. For example, the reflection conditions for the group $I2cb(00\gamma)0s0$ are $h + k + \ell$ = even because of the centring and $l + m$ = even and $h + m$ = even for $h0\ell m$ because of the two glide planes perpendicular to the b axis. When one takes for the modulation vector $\mathbf{q}$=$\gamma'\mathbf{c}^*$ = (1-γ)$\mathbf{c}^*$, the new indices are h, k, ℓ' and m' with $\ell' = l + m$ and $m' = -m$. Then the reflection conditions become ℓ' = even and $h + m'$ = even for $h0\ell'm'$. The first of these conditions implies a symbol $I2cb(00\gamma)000$ for the group considered. This, however, is the symbol for the non-equivalent group with condition h = even for $h0\ell m$, This difficulty may be avoided by using sometimes a non-standard setting of the three-dimensional space group (see Yamamoto *et al.*, 1985). In this case, the setting $I2ab$ instead of $I2cb$ avoids the problem.

9.8.4. Theoretical foundation

9.8.4.1. Lattices and metric

A (lattice) periodic crystal structure is defined in a three-dimensional Euclidean space V and is invariant under translations $\mathbf{n}$ which are integral linear combinations of three fundamental ones $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$:

$$\mathbf{n} = \sum_{i=1}^{3} n_i \mathbf{a}_i, \quad n_i \text{ integers.} \tag{9.8.4.1}$$

These three translations are linearly independent and span a lattice Λ. The *dimension* of Λ is the dimension of the vector space spanned by $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, and the *rank* is the (smallest) number of free generators of those linear combinations. In the present case,

Table 9.8.3.3: *(2+2)-dimensional Bravais classes for incommensurate structures.* The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The basis of the vector module M^* contains two modulation wavevectors and the reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + m_1\mathbf{q}_1 + m_2\mathbf{q}_2$. If $\mathbf{q}_1^r$ or $\mathbf{q}_2^r$ are not zero, there are corresponding centring translations in four-dimensional space. The conventional basis ($\mathbf{a}_c^*$, $\mathbf{b}_c^r$, $\mathbf{q}_1^i$, $\mathbf{q}_2^i$) for the vector module M^* is chosen such that $\mathbf{q}_1^r = \mathbf{q}_2^r = 0$. The basis vectors are indicated by their components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$ of the lattice Λ^* of main reflections.

No.	Symbol	K_E	K_I	$\mathbf{q}_1$	$\mathbf{q}_2$	Conventional basis	Centring
Oblique							
1	$2p(\alpha\beta,\lambda\mu)$	2	2	$(\alpha\beta)$	$(\lambda\mu)$	(10),(01),$(\alpha\beta)$,(λ,μ)	

This is the beginning of Table 9.8.3.1(b) in ITCC 1999

Table 9.8.3.4: *(3+1)-dimensional Bravais classes for incommensurate structures.* The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}$. If $\mathbf{q}^r$ is not zero, there is a corresponding centring translation in four-dimensional space. The conventional basis ($\mathbf{a}_c^*$, $\mathbf{b}_c^r$, $\mathbf{c}_c^*$, $\mathbf{q}^i$) for the vector module M^* is chosen such that $\mathbf{q}^r = 0$. The basis vectors are indicated by their components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ of the lattice Λ^* of main reflections. The Bravais classes can also be found in Janssen (1969) and Brown *et al.* (1978). The notation of the Bravais classes there is here given in the columns Ref.a and Ref. b, respectively

.

No.	Symbol	K_E	K_I	$\mathbf{q}$	Conventional basis	Centring translation(s)	Ref. a	Ref. b
Triclinic								
1	$\bar{1}P(\alpha\beta\gamma)$	$\bar{1}$	$\bar{1}$	$(\alpha\beta\gamma)$	(100),(010),(001),$(\alpha\beta\gamma)$		I P	I/I

This is the beginning of Table 9.8.3.2(a) in ITCC 1999

Table 9.8.3.5: *(3+1)-dimensional Bravais classes for commensurate structures.* The holohedral point group K_s is given in terms of its external and internal parts, K_E and K_I, respectively. The reflections are given by $h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}$. The wavevector $\mathbf{q}$ has rational components with respect to $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$. The rank of the vector module is three. Therefore, there are three basis vectors for M^*. They are given by their components with respect to the conventional basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ of the lattice Λ^* of main reflections. If they do not coincide with the primitive basis vectors of the lattice Λ^*, there is a centring in four dimensions. The notation in Janssen (1969) is here given in the column 'Ref.a' Notice that for a commensurate one-dimensional modulation cubic symmetry is also possible.

No.	Symbol	K_E	K_I	$\mathbf{q}$	Conventional basis	Centring translation(s)	Ref.a II P
Triclinic							
1	$\bar{1}P(000)$	$\bar{1}1$	$1\bar{1}$	(000)	(100),(010),(001)		

This is the beginning of Table 9.8.3.2(b) in ITCC 1999

Table 9.8.3.6: *(3+1)-dimensional point groups and arithmetic crystal classes.* The four-dimensional point group K_s has external part K_E, which belongs to a three-dimensional system. Depending on the Bravais class of the four-dimensional lattice left invariant by K_s, this point group gives rise to an integral 4×4 matrix group $\Gamma(K)$ which belongs to one of the arithmetic crystal classes given in the last column.

System	Point group		External	Arithmetic
	K_E	K_s	Bravais class	crystal class(es)
Triclinic	1	(1,1)	$\bar{1}P$	$1P(\alpha\beta\gamma)$
	$\bar{1}$	$(\bar{1},\bar{1})$	$\bar{1}P$	$\bar{1}P(\alpha\beta\gamma)$

This is the beginning of Table 9.8.3.3 in ITCC 1999

Table 9.8.3.7: *(2+1)-dimensional superspace groups.* The number labelling the superspace group is denoted by $n.m$, where n is the number attached to the two-dimensional basic space group and m numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the three-dimensional point group K_s, the number of the three-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.2) and the superspace-group symbol are also given.

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol
Oblique				
1.1	$p1$	(1,1)	1	$p1(\alpha\beta)$

This is the beginning of Table 9.8.3.4(a) in ITCC 1999

Table 9.8.3.8: *(2+2)-dimensional superspace groups.* The number labelling the superspace group is denoted by $n.m$, where n is the number attached to the two-dimensional basic space group and m numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the four-dimensional point group K_s, the number of the four-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.3) and the superspace-group symbol are also given.

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol
Oblique				
1.1	$p1$	(1,1)	1	$p1(\alpha\beta,\lambda\mu)$
2.1	$p2$	(2,2)	1	$p2(\alpha\beta,\lambda\mu)$

This is the beginning of Table 9.8.3.4(b) in ITCC 1999

Table 9.8.3.9: *(3+1)-dimensional superspace groups.* The number labelling the superspace group is denoted by $n.m$, where n is the number attached to the three-dimensional basic space group and m numbers the various superspace groups having the same basic space group. The symbol of the basic space group, the symbol for the four-dimensional point group K_s, the number of the four-dimensional Bravais class to which the superspace group belongs (Table 9.8.3.4) and the superspace-group symbol are also given. The superspace-group symbol is given in the short notation, *i.e.* for the basic space group one uses the short symbol from *International Tables for Crystallography*, Volume A, and then the values of v_4^0 are given for each of the generators in this symbol, unless all these values are zero. Then, instead of writing a number of zeros, one omits them all. Finally, the special reflection conditions due to non-primitive translations are given, for $hk\ell m$ if $\mathbf{q}^r{=}0$ and for $HKLm$ otherwise. Recall the $HKLm$ are the indices with respect to a conventional basis $\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{c}_c^*$, $\mathbf{q}^i$ as in Table 9.8.3.4. The reflection conditions due to centring translations are given in Table 9.8.3.10.

No.	Basic space group	Point group K_s	Bravais class No.	Group symbol	Special reflection conditions
1.1	$P1$	(1,1)	1	$P1(\alpha\beta\gamma)$	
2.1	$P\bar{1}$	$(\bar{1},\bar{1})$	1	$P\bar{1}(\alpha\beta\gamma)$	

This is the beginning of Table 9.8.3.5 in ITCC 1999

Table 9.8.3.10: *Centring reflection conditions for (3+1)-dimensional Bravais classes.* The centring reflection conditions are given for the 24 Bravais classes, belonging to six systems (with number and symbol according to Table 9.8.3.6). If $\mathbf{q}^r{=}0$ these are the usual conditions for $hk\ell m$, the indices of the reflections expressed with respect to $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, $\mathbf{q}$. Otherwise, the conditions are for $HKLm$ with respect to a conventional basis $\mathbf{a}_c^*$, $\mathbf{b}_c^*$, $\mathbf{c}_c^*$, $\mathbf{q}^i$ of the vector module M^*. The relation between the indices $HKLm$ and $hk\ell m$ is given in the fourth column. Planar monoclinic and axial monoclinic mean a monoclinic lattice of main reflections and with $\mathbf{q}^i$ in the mirror plane, or along the unique axis, respectively.

System	$\mathbf{q}^i$ vector	Reflection conditions	Relation of indices.	Bravais class No.	Bravais class Symbol
Triclinic	$(\alpha\beta\gamma)$			1	$\bar{1}P(\alpha\beta\gamma)$
Planar monoclinic	$(\alpha\beta 0)$			2	$2/mP(\alpha\beta 0)$
		$L+m=2n$	$L=2\ell+m$	3	$2/mP(\alpha\beta\frac{1}{2})$
		$h+\ell=2n$		4	$2/mB(\alpha\beta 0)$

This is the beginning of Table 9.8.3.6 in ITCC 1999

both are equal to three. Accordingly,

$$Span_R(\Lambda) = V \quad \text{and} \quad \Lambda \equiv \mathbb{Z}^3. \tag{9.8.4.2}$$

The elements of $\mathbb{Z}^3$ are triples of integers that correspond to the coordinates n_i of the lattice points. The Bragg reflection peaks of such a crystal structure are at the positions of the reciprocal lattice Λ^*, also of dimension and rank equal to three. Furthermore, the Fourier wavevectors $\mathbf{H}$ belong to Λ^* (after identification of reciprocal lattice vectors with lattice points):

$$\mathbf{H} = \sum_{i=1}^{3} h_i \mathbf{a}_i^*, \quad h_i \ \text{ integers}, \tag{9.8.4.3}$$

where $\{\mathbf{a}_i^*\}$ is the reciprocal basis

$$\mathbf{a}_i.\mathbf{a}_j^* = \delta_{ij}.$$

The two corresponding metric tensors

$$g_{ik} = \mathbf{a}_i.\mathbf{a}_k \quad \text{and} \quad g_{ik}^* = \mathbf{a}_i^*.\mathbf{a}_k^*, \tag{9.8.4.4}$$

are positive definite and dual:

$$\sum_{k=1}^{3} g_{ik} g_{kj}^* = \delta_{ij}.$$

We now consider crystal structures defined in the same three-dimensional Euclidean space V with Fourier wavevectors that are integral linear combinations of $n = 3+d$ fundamental ones $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$:

$$\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}_i^*, \quad h_i \text{ integers}. \tag{9.8.4.5}$$

The components $(h_1, \ldots, h_n)$ are the indices labelling the corresponding Bragg reflection peaks. For a modulated structure the vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ span the reciprocal lattice of the basic structure.

A crystal with diffraction peaks at positions (9.8.4.5) is *quasiperiodic*. Mathematically it is considered to be quasiperiodic even if n equals the dimension (lattice periodicity), but usually one means that n is larger than the dimension. Then the crystal is *aperiodic*. For modulated structures the term *incommensurate* crystal is used in the aperiodic case. The description above can still be convenient in the case that the basis vectors are not independent over the rational numbers, *i.e.* when there are combinations $\sum_i q_i \mathbf{a}_i^*=0$ with rational numbers q_i not all equal to zero. A typical example is that of a superstructure arising from the commensurate modulation of a basic structure with lattice periodicity.

Let us denote by M^* the set of all integral linear combinations of the vectors $\mathbf{a}_i^*$ $(i = 1, \ldots, n)$. These n vectors form a *basis* of the vector module M^*, which has *rank* equal to n. The *dimension* of M^* is the dimension of the Euclidean space spanned by M^*:

$$Span_R(M^*) = V \quad \text{and} \quad M^* \equiv \mathbb{Z}^n. \tag{9.8.4.6}$$

The elements of $\mathbb{Z}^n$ are precisely the set of indices h_i introduced above. Mathematically, M^* has the structure of a (free Abelian) $\mathbb{Z}$-module. Its elements are vectors. So we call M^* a *vector module* or *Fourier module* because it contains the wavevectors of the Fourier components of the structure.

Lattices and vector modules are free $\mathbb{Z}$-modules. For such a module, there exists a dual one that is also free and of the same rank. In the periodic crystal case, that duality can be expressed by a scalar product, but for an aperiodic crystal this does not work. It is possible to keep the metrical duality by enlarging the space and considering the Fourier module M^* as the projection of an n-dimensional (reciprocal) lattice Σ^* in an n-dimensional Euclidean space V_s.

$$\Lambda^* \to M^*, \quad Span_R(\Sigma^*) = V_s, \quad \Sigma^* \equiv \mathbb{Z}^n, \tag{9.8.4.7}$$

with the orthogonal projection π_E of V_s onto V defined by

$$M^* = \pi_E \Sigma^*. \tag{9.8.4.8}$$

Then the diffraction peaks, each belonging to an element of the Fourier module, correspond to vectors of the reciprocal lattice Σ^*. The space V is often called *external*, *physical space*, or *parallel space* and denoted by V_E, its orthocomplement is called *internal* or *perpendicular space* and is denoted by V_I. The relation between the basis vectors in V_s and V_E is

$$a^*_{si} = (\mathbf{a}^*_i, \mathbf{a}^*_{Ii}), \quad i = 1, \ldots, n, \tag{9.8.4.9}$$

where the a^*_{si} form a basis of Σ^* and the $\mathbf{a}^*_i$ one for M^*. The vectors $\mathbf{a}^*_{Ii}$ span V_I.

The crystal density ρ in V can also be embedded as ρ_s in V_s by identifying the Fourier components $\hat{\rho}$ at points of M^* and of Σ^*:

$$\hat{\rho}_s(h_1, \ldots, h_n) = \hat{\rho}(h_1, \ldots, h_n). \tag{9.8.4.10}$$

If the density function in V is defined as

$$\rho(\mathbf{r}) = \sum_{\mathbf{k} \in M^*} \hat{\rho}(\mathbf{k}) \exp(2\pi i \mathbf{k}.\mathbf{r}), \quad \mathbf{k} = \sum_{i=1}^{n} h_i \mathbf{a}^*_i, \tag{9.8.4.11}$$

then the function ρ_s is given by

$$\rho_s(r_s) = \sum_{k_s \in \Sigma^*} \hat{\rho}(\pi_E k_s) \exp(2\pi i k_s.r_s). \tag{9.8.4.12}$$

This ρ_s is invariant under translations of the n-dimensional lattice Σ with basis

$$a_{si} = (\mathbf{a}_i, \mathbf{a}_{Ii}), \tag{9.8.4.13}$$

dual to (9.8.4.9). In the commensurate case, this correspondence requires that the given superstructure be considered as the limit of an incommensurate crystal, for which the embedding is one-to one.

As discussed below, point-group symmetries R of the diffraction pattern, when expressed in terms of transformation of the set of indices, define n-dimensional integral matrices. They form finite groups, and for that reason can be considered as n-dimensional orthogonal transformations R_s in V_s leaving invariant the Euclidean metric tensors

$$g_{sik} = a_{si}.a_{sk} \quad \text{and} \quad g^*_{sik} = a^*_{si}.a^*_{sk}. \tag{9.8.4.14}$$

For *modulated crystals*, there is a set of main reflections belonging to a three-dimensional reciprocal lattice. For that case, the embedding can be specialized by making the choice

$$\begin{aligned} a^*_{si} &= (\mathbf{a}^*_i, 0) \qquad i = 1,2,3, \\ a^*_{s(3+j)} &= (\mathbf{a}^*_{3+j}, \mathbf{d}^*_j) \quad j = 1,2,\ldots,d = n-3, \end{aligned} \tag{9.8.4.15}$$

and, correspondingly,

$$\begin{aligned} a_{si} &= (\mathbf{a}_i, \mathbf{a}_{Ii}) \qquad i = 1,2,3, \\ a_{s(3+j)} &= (0, \mathbf{d}_j) \qquad j = 1,2,\ldots,d, \end{aligned} \tag{9.8.4.16}$$

with $\mathbf{d}^*_i.\mathbf{d}_k{=}\delta_{ik}$ and $\mathbf{a}^*_i.\mathbf{a}_k{=}\delta_{ik}$. Such bases for modulated structures are called *standard lattice bases*.

9.8.4.2. Point groups

9.8.4.2.1. Laue class

Definition 1. The *Laue point group* P_L of the diffraction pattern is the point group in three dimensions that transforms each Bragg peak into a peak of the same intensity (if no anomalous dispersion occurs).

Because all diffraction vectors are of the form (9.8.4.5), the action of an element of the Laue group is given by

$$R\mathbf{a}^*_i = \sum_{j=1}^{n} \Gamma^*(R)_{ji}\mathbf{a}^*_j, \quad i = 1,\ldots,n. \tag{9.8.4.17}$$

The n-dimensional matrices $\Gamma^*(R)$ form a finite group of integral matrices $\Gamma^*(K)$ for K equal to P_L or one of its subgroups. A theorem in algebra states that then there is a basis in n dimensions such that the transformations R on that basis are orthogonal and represent n-dimensional orthogonal transformations R_s. The corresponding group is an n-dimensional crystallographic group denoted by K_s. Because R is already an orthogonal transformation on V, R_s is reducible and can be presented as pair (R, R_I) of orthogonal transformations, in 3 and $(n-3)$ dimensions, respectively. The basis on which R_s acts according to $\Gamma^*(R)$ is given by (9.8.4.9). It spans a lattice Σ^* that is the reciprocal of the

lattice Σ with basis (9.8.4.13). The pairs (R, R_I), sometimes also noted (R_E, R_I), leave Σ invariant:

$$(R, R_I)(\mathbf{a}_i.\mathbf{a}_{Ii}) = (R\mathbf{a}_i, R_I\mathbf{a}_{Ii}) = \sum_{j=1}^{n} \Gamma(R)_{ji}(\mathbf{a}_j, \mathbf{a}_{Ij}), \tag{9.8.4.18}$$

where $\Gamma(R)$ is the transpose of $\Gamma^*(R^{-1})$.

For *modulated* crystals, one may distinguish a lattice of main reflections, the remaining reflections being called satellites. The main reflections are, generally, more intense. Therefore, main reflections are transformed into main reflections by elements of the Laue group. On a standard lattice basis (9.8.4.16), the matrices $\Gamma(R)$ take the special form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix}. \tag{9.8.4.19}$$

The transformation of main reflections and satellites is then given by $\Gamma^*(R)$, the relation with $\Gamma(R)$ being (as already said)

$$\Gamma^*(R) = \text{Transpose}[\Gamma(R^{-1})].$$

Accordingly, on a standard basis one has

$$\Gamma^*(R) = \begin{pmatrix} \Gamma^*_E(R) & \Gamma^*_M(R) \\ 0 & \Gamma^*_I(R) \end{pmatrix}. \tag{9.8.4.20}$$

The set of matrices $\Gamma_E(R)$ for elements R of K forms a crystallographic point group in three dimensions, denoted K_E, having elements R of $O(3)$, and the corresponding set of matrices $\Gamma_I(R)$ forms one in d dimensions denoted by K_I with elements R_I of $O(d)$.

For a modulated crystal, one can choose the $\mathbf{a}_i^*$ $(i = 1, 2, 3)$ of a standard basis. These span the reciprocal lattice of the basic structure. One can then express the additional vectors $\mathbf{a}^*_{3+j}$ (which correspond to the modulation wave vectors) in terms of the basis of the lattice of main reflections:

$$\mathbf{a}^*_{3+j} = \sum_{i=1}^{3} \sigma_{ji}\mathbf{a}^*_i, \quad j = 1, 2, \ldots, d. \tag{9.8.4.21}$$

The three components of the jth row of the $(d\times 3)$-dimensional matrix σ are just the three components of the jth modulation wavevector $\mathbf{q}_j$=$\mathbf{a}^*_{3+j}$ with respect to the basis $\mathbf{a}^*_1$, $\mathbf{a}^*_2$, $\mathbf{a}^*_3$. It is easy to show that the internal components $\mathbf{a}_{Ii}$ $(i = 1, 2, 3)$ of the corresponding dual standard basis can be expressed as

$$\mathbf{a}_{Ii} \;=\; -\sum_{j=1}^{d} \sigma_{ji}\mathbf{d}_j, \quad i = 1, 2, 3. \tag{9.8.4.22}$$

This follows directly from (9.8.4.21) and the definition of the standard reciprocal basis. From (9.8.4.18 and 9.8.4.19), a simple relation can be deduced between σ and the three constituents $\Gamma_E(R)$, $\Gamma_I(R)$, and $\Gamma_M(R)$ of the matrix $\Gamma(R)$:

$$\sigma\Gamma_E(R) - \Gamma_I(R)\sigma = \Gamma_M(R). \tag{9.8.4.23}$$

Notice that the elements of $\Gamma_M(R)$ are integers, whereas σ has, in general, irrational entries. This requires that the irrational part of σ gives zero when inserted in the left-hand side of (9.8.4.23). It is therefore possible to decompose σ into parts σ^i and σ^r as follows.

$$\sigma = \sigma^i + \sigma^r, \quad \text{with} \quad \sigma^i = \frac{1}{N}\sum_R \Gamma_I(R)\sigma\Gamma_E^{-1}, \tag{9.8.4.24}$$

where the sum is over all elements of the Laue group of order N. It follows from this definition that

$$\Gamma_I(R)\sigma^i\Gamma_E(R)^{-1} = \sigma^i. \tag{9.8.4.25}$$

This implies

$$\Gamma_M(R) = \sigma^r\Gamma_E(R) - \Gamma_I(R)\sigma^r. \tag{9.8.4.26}$$

The matrix σ^r has rational entries and is called the rational part of σ. The part σ^i is the irrational (or invariant) part.

The above equations simplify for the case $d = 1$. The elements σ_{1i} are the three components of the wavevector $\mathbf{q}$, the row matrix $\sigma\Gamma_E(R)$ has the components of $R^{-1}\mathbf{q}$ and $\Gamma(R) = \epsilon(R) = \pm 1$ since, for $d = 1$, $\mathbf{q}$ can only be transformed to $\pm\mathbf{q}$. One has the corresponding relations:

$$\mathbf{q} = \mathbf{q}^i + \mathbf{q}^r, \quad \text{with} \quad \mathbf{q}^i \equiv \frac{1}{N}\sum_R \epsilon(R)R\mathbf{q}, \tag{9.8.4.27}$$

and

$$R\mathbf{q} = \epsilon(R)\mathbf{q} \ \ \text{(modulo the reciprocal lattice } \Lambda^*); \quad R\mathbf{q}^i = \epsilon(R)\mathbf{q}^i. \tag{9.8.4.28}$$

The reciprocal lattice vector that gives the difference between $R\mathbf{q}$ and $\epsilon(R)\mathbf{q}$ has as components the elements of the row matrix $\Gamma_M(R)$.

9.8.4.2.2. Geometric and arithmetic crystal classes for modulated crystals

According to what has been said, in the case of modulated crystals a standard basis can be chosen for M^* and Σ^*. According to equation (9.8.4.17), for each three-dimensional point-group operation R that leaves the diffraction pattern invariant, there is a point-group transformation R_E in the physical space (such that $R = R_E$), and a point-group transformation R_I in the internal space, such that the pair (R_E, R_I) is a (3+d)-dimensional orthogonal transformation R_s leaving a (3+d)-dimensional lattice Σ invariant. For incommensurate crystals, this internal transformation is unique and follows from the transformation by R of the modulation wavevectors.There is exactly one R_I for each R, because in the incommensurately modulated case, the correspondence between M^* and Σ^* is uniquely fixed by the embedding rule (9.8.4.10). Because the matrices $\Gamma(R)$ and the corresponding transformations in the (3+d)-dimensional space form a group, this implies hat there is a mapping from the group K_E of elements R_E to the group K_I of elements R_I, and this mapping is a homomorphism. A point group K_s of a (3+d) dimensional lattice constructed

for a modulated crystal, therefore, consists of a three-dimensional crystallographic point group K_E, a d-dimensional crystallographic point group K_I, and a homomorphism from K_E to K_I.

Definition 2. Two (3+d)-dimensional point groups K_s and K'_s for modulated phases are *geometrically equivalent* if they are connected by a pair of orthogonal transformations (T_E, T_I) in V_E and V_I, respectively, such that for every R_s from the first group here is an element R'_s of the second group such that $R_E T_E = T_E R'_E$ and $R_I T_I = T_I R'_I$.

A point group determines a set of groups of matrices, one for each standard basis of each lattice left invariant. On a basis of an invariant lattice, the point group gives a group of integral matrices, an *arithmetic point group*.

Definition 3. Two arithmetic point groups for modulated crystals are *arithmetically equivalent* if they are obtained from each other by a transformation from one standard basis to another standard basis.

The arithmetic equivalence class of a (3+d)-dimensional point group is fully determined by a three-dimensional point group and a standard basis for the vector module M^* because of relation (9.8.4.17).

In three dimensions, there are 32 geometrical crystal class and 73 arithmetic crystal classes. In one dimension, these numbers are both equal to two. Therefore, one finds all (3+1)-dimensional point groups of incommensurately modulated structures by considering all triples of one of the 32 (73) point groups, one of the two one-dimensional point groups, and all homomorphisms from the first to the second.

Analogously, in (3+d) dimensions, one takes one of the 32 (or 73) groups, one of the d-dimensional groups, and all homomorphisms [homomorphism: mapping ϕ from a group A to a group B such that for elements a_1 and a_2 from A one has $\phi(a_1).\phi(a_2) = \phi(a_1.a_2)$] from the first to the second. If one takes all triples of a three-dimensional group, a d-dimensional group, and a homomorphism from the first to the second, one finds groups that are possibly equivalent. The equivalent ones still have to be eliminated in order to arrive at a list of non-equivalent groups.

9.8.4.3. Systems and Bravais classes

9.8.4.3.1. Holohedry

The Laue group of the diffraction pattern is a three-dimensional point group that leaves the positions and the intensities of the diffraction spots as a set invariant, thus the vector module M^* as well. As discussed in Subsection 9.8.4.2, each of the elements of the Laue group can be combined with an orthogonal transformation in the internal space. The resulting point group in 3+d dimensions leaves the lattice Σ^* invariant for which the module M^* is the projection. Conversely, if one has a point group that leaves the (3+d)-dimensional lattice invariant, its three-dimensional (external) part with elements $R_E = R$

leaves the vector module invariant.

Definition 4. The holohedry of a lattice Σ^* is the subgroup of the direct product $O(3) \times O(d)$, *i.e.* the group of all pairs of orthogonal transformations $R_s = (R, R_I)$ that leave the lattice invariant.

This choice is possible because the point groups are reducible, *i.e.* leave the subspaces V and V_I of the direct sum space V_s invariant. In the case of an incommensurate crystal, the projection of Σ^* on M^* is one-to-one as one can see as follows. The vector

$$H_s = \sum_{i=1}^{3} h_i(\mathbf{a}_i^*, 0) + \sum_{j=1}^{d} m_j(\mathbf{q}_j, \mathbf{d}_j^*) \qquad (9.8.4.29)$$

of Σ^* is projected on $\mathbf{H}=\sum_i h_i\mathbf{a}_i^* + \sum_j m_j\mathbf{q}_j$. The vectors projected on the null vector satisfy, therefore, the relation $\sum_i h_i\mathbf{a}_i^* + \sum_j m_j\mathbf{q}_j=0$. For an incommensurate phase, the basis vectors are rationally independent, which means that $h_i=0$ and $m_j=0$ for any i and j. Consequently, one and only one vector of Σ^* is projected on each given vector of M^*.

Suppose now $R=1$. This transformation leaves the components of every vector belonging to M^* in V invariant. If R_I is the corresponding orthogonal transformation in V_I of an element R_s of the point group, a vector with component $\mathbf{H}_I$ is transformed into a vector with component H_I'. Since a given $\mathbf{H}$ is the component of only one vector of Σ^*, this implies $\mathbf{H}_I=\mathbf{H}_I$'. Consequently, R_I is also the identity transformation. Therefore, for incommensurate modulated phases, there are no point-group elements with $R_E = 1$ and $R_I \neq 1$. For commensurate crystal structures embedded in the superspace, this is different: point-group elements with internal component different from the identity associated with an external component equal to unity can occur.

For modulated crystal structures, the holohedral point group can be expressed with respect to a lattice basis of standard form (9.8.4.16). It is then faithfully represented by integral matrices that are of the form indicated in (9.8.4.19) and (9.8.4.20).

9.8.4.3.2. Crystallographic systems

Definition 5. A *crystallographic system* is a set of lattices having geometrically equivalent holohedral point groups.

In this way, a given holohedral point group (and even each crystallographic point group) belongs to exactly one system. Two lattices belong to the same system if there are orthonormal bases in V and in V_I, respectively, such that the holohedral point groups of the two lattices are represented by the same set of matrices.

9.8.4.3.3. Bravais classes

Definition 6. Two lattices belong to the same *Bravais class* if their holohedral point groups are arithmetically equivalent.

This means that each of them admits a lattice basis of standard form such that their holohedral point group is represented by the same set of integral matrices.

9.8.4.4. Superspace groups

9.8.4.4.1. Symmetry elements

The elements of a (3+d)-dimensional superspace group are pairs of Euclidean transformations in three and d dimensions:

$$g_s = (\{R|\mathbf{v}\}, \{R_I|\mathbf{v}_I\}) \in E(3) \times E(d), \tag{9.8.4.30}$$

i.e. are elements of the direct product of the corresponding Euclidean groups. The elements $\{R|\mathbf{v}\}$ form a three-dimensional space group, but the same does not hold for for the elements $\{R_I|\mathbf{v}_I\}$ of $E(d)$. This is because the internal translations $\mathbf{v}_I$ also contain the 'compensating' transformations associated with the corresponding translation $\mathbf{v}$ in V. In other words, a basis of the lattice Σ does not simply split into one basis for V and one for V_I.

As for elements of a three-dimensional space group, the translational component $v_s = (\mathbf{v}, \mathbf{v}_I)$ of the element g_s can be decomposed into an intrinsic part v_s^0 and an origin-dependent part v_s^a:

$$(\mathbf{v}, \mathbf{v}_I) = (\mathbf{v}^0, \mathbf{v}_I^0) + (\mathbf{v}^a, \mathbf{v}_I^a),$$

with

$$v_s^0 = (\mathbf{v}^0, \mathbf{v}_I^0) = \frac{1}{n} \sum_{m=1}^{n} (R^m\mathbf{v}, R_I^m\mathbf{v}_I), \tag{9.8.4.31}$$

where n denotes the order of the element R. In particular, for d=1 the intrinsic part $\mathbf{v}_I^0$ of $\mathbf{v}_I$ is equal to $\mathbf{v}_I$ if $\epsilon(R) = R_I = +1$ and vanishes when $\epsilon = -1$. The latter means that for d=1 there is always an origin in internal space such that the internal shift $\mathbf{v}_I$ can be chosen to be zero for an element with ϵ=-1.

The internal part of the intrinsic translation can itself be decomposed into two parts. One part stems from the presence of a translation in the external space. The lattice of the (3+d)-dimensional space group has basis vectors

$$(\mathbf{a}, \mathbf{a}_{Ii}), \quad (0, \mathbf{d}_j), \quad i = 1, 2, 3; \quad j = 1, \ldots, d. \tag{9.8.4.32}$$

The internal part of the first three basis vectors is

$$\mathbf{a}_{Ii} \;=\; -\,\Delta\mathbf{a}_i \;=\; -\sum_{j=1}^{d} \sigma_{ji}\mathbf{d}_j \tag{9.8.4.33}$$

according to equation (9.8.4.22). The three-dimensional translation $\mathbf{v}$=$\sum_i v_i\mathbf{a}_i$ then entails a d-dimensional translation $-\Delta\mathbf{v}$ in V_I given by

$$\Delta\mathbf{v} = \Delta\left(\sum_{i=1}^{3} v_i\mathbf{a}_i\right) = \sum_{i=1}^{3} v_i\Delta\mathbf{a}_i. \tag{9.8.4.34}$$

These are the so-called *compensating translations*. Hence, the internal translation $\mathbf{v}_I$ can be decomposed as

$$\mathbf{v}_I \;=\; -\Delta\mathbf{v} + \delta, \tag{9.8.4.35}$$

where $\delta = \sum_{j=1}^{d} v_{3+j}\mathbf{d}_j$.

This decomposition, however, does still depend on the origin. Consider the case d=1. Then an origin shift $\mathbf{s}$ in the three-dimensional space changes the translation $\mathbf{v}$ to $\mathbf{v}+(1-R)\mathbf{s}$ and its internal part $-\Delta\mathbf{v} = -\mathbf{q}.\mathbf{v}$ to $-\mathbf{q}.\mathbf{v} - \mathbf{q}.(1-R)\mathbf{s}$. This implies that for the case that $\epsilon = 1$ the part δ changes to $\delta + \mathbf{q}.(1-R)\mathbf{s} = \delta + \mathbf{q}^r.(1-R)\mathbf{s}$, because $\mathbf{q}^i$ is invariant under R. Therefore, δ changes, in general. The internal translation

$$\delta - \mathbf{q}^r.\mathbf{v}, \tag{9.8.4.36}$$

however, is invariant under an origin shift in V_E.

Definition 7. *Equivalent superspace groups.* Two superspace groups for modulated phases are equivalent if they are isomorphic and have point groups that are arithmetically equivalent.

Another definition leading to the same superspace-group types considers equivalency with respect to affine transformations among bases of standard form.

This means that two equivalent superspace groups admit standard bases such that the two space groups are represented by the same set of (4+d)-dimensional affine transformation matrices. We recall that an n-dimensional Euclidean transformation $g_s = \{R_s|v_s\}$ if referred to a basis of space can be represented by an (n+1)-dimensional matrix, of the form

$$A(g_s) \;=\; \begin{pmatrix} R_s & v_s \\ 0 & 1 \end{pmatrix} \tag{9.8.4.37}$$

with R_s an $n \times n$ matrix and v_s an n-dimensional column matrix, all with real entries.

9.8.4.4.2. Equivalent positions and modulation relations

A (3+d)-dimensional space group that leaves a function invariant maps points in (3+d)-space to points where the function has the same value. The atomic positions of a modulated crystal represent such a pattern, and the superspace group leaving the crystal invariant leads to a partition into equivalent atomic positions. These relations can be formulated either in (3+d)-dimensional space, or, equally well, in three-dimensional space. As a simple case, we first consider a crystal with a one-dimensional occupation modulation: this implies d=1. Again, as in 9.8.1.3.2, we omit the basis vectors $\mathbf{d}_1$ and $\mathbf{d}_1^*$ and give only the corresponding components.

An element of the (3+1)-dimensional superspace group is a pair

$$g_s = (\{R|\mathbf{v}\}, \{\epsilon|v_I\}) \tag{9.8.4.38}$$

of Euclidean transformations in V_E and V_I, respectively. This element maps a point $r_s = (\mathbf{r}, r_I)$ to one at $(R\mathbf{r} + \mathbf{v}, \epsilon r_I + v_I)$. Suppose the probability for the position $\mathbf{n}+\mathbf{r}_j$ to

be occupied by an atom of species A is given by

$$P_A(\mathbf{n}, j, r_I) \;=\; p_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j)+r_I], \tag{9.8.4.39}$$

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

$$P_A(\mathbf{n}', j', r_I) = P_A[\mathbf{n}, j, \epsilon(r_I - v_I). \tag{9.8.4.40}$$

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

$$P_A(\mathbf{n}', j', 0) = P_A(\mathbf{n}, j, -\epsilon v_I). \tag{9.8.4.41}$$

In terms of the modulation function this means

$$p_j[(\mathbf{q}.\mathbf{n}' + \mathbf{r}_{j'})] = p_j[\mathbf{q}.(\mathbf{n}+\mathbf{r}_j) - \epsilon v_I]. \tag{9.8.4.42}$$

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

$$p_{j'}(x) = p_j\left(\epsilon(x-\delta) + \mathbf{K}.(\mathbf{r}_{j'} - \mathbf{v})\right), \quad \text{where} \quad R\mathbf{q} = \epsilon\mathbf{q} + \mathbf{K}. \tag{9.8.4.43}$$

Analogously, for a displacive modulation, the position $\mathbf{n}+\mathbf{r}_j$ with displacement $\mathbf{u}_j(t_o)$, where $t_0 = \mathbf{q}.(\mathbf{n}+\mathbf{r}_j)$, is transformed to $\mathbf{n}'+\mathbf{r}_{j'}$ with displacement

$$\mathbf{u}_{j'}(t_0') = R\mathbf{u}_j(t_0 - \epsilon v_I). \tag{9.8.4.44}$$

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

$$\mathbf{u}_{j'}(x) = R\mathbf{u}_j\left(\epsilon x - \epsilon\delta + \mathbf{K}.(\mathbf{r}_{j'} - \mathbf{v})\right), \quad \text{where } R\mathbf{q} = \epsilon\mathbf{q} + \mathbf{K}. \tag{9.8.4.45}$$

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:

$$S_{\mathbf{H}} = \sum_n f_n(\mathbf{H}) \exp(2\pi i \mathbf{H}.\mathbf{r}_n), \tag{9.8.4.46}$$

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 $\exp(2\pi i H_s.r_{sn})$ over all particles in the unit cell Ω 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 very special 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)

$$\begin{aligned} S_{\mathbf{H}} &= \sum_A \sum_j \int_\Omega \mathrm{d}\mathbf{t} f_A(\mathbf{H}) P_{Aj}(\mathbf{t}) \\ &\times \exp\left(2\pi i(\mathbf{H}, \mathbf{H}_I).(\mathbf{r}_j + \mathbf{u}_j(\mathbf{t}), \mathbf{t})\right), \end{aligned} \tag{9.8.4.47}$$

where the first sum is over 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 the 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

$$p_j(t) = 1; \quad \mathbf{u}_j(t) = \mathbf{U}_j \sin[2\pi(\mathbf{q}.\mathbf{r}_j + t + \phi_j)]. \tag{9.8.4.48}$$

According to this equation, the structure factor is

$$\begin{aligned} S_{\mathbf{H}} &= \sum_j \int_0^1 \mathrm{d}t f_j(\mathbf{H}) \exp(2\pi i \mathbf{H}.\mathbf{r}_j) \exp(2\pi i m t) \\ &\times \exp[2\pi i \mathbf{H}.\mathbf{U}_j \sin 2\pi(\mathbf{q}.\mathbf{r}_j + t + \phi_j)]. \end{aligned} \tag{9.8.4.49}$$

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

$$S_{\mathbf{H}} = \sum_j f_j(\mathbf{H}) \exp(2\pi i \mathbf{K}.\mathbf{r}_j) J_{-m}(2\pi \mathbf{H}.\mathbf{U}_j) \exp(-2\pi i m \phi_j). \tag{9.8.4.50}$$

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

$$\begin{aligned} S_{\mathbf{H}} &= \sum_j \int_0^1 \mathrm{d}t f_j(\mathbf{H}) p_j(\mathbf{q}.\mathbf{r}_j + t + \psi_j) \exp[2\pi i(\mathbf{H}.\mathbf{r}_j + mt)] \\ &\times \exp(-2\pi i \mathbf{H}.\mathbf{u}_j(\mathbf{q}.\mathbf{r}_j + t + \phi_j)]. \end{aligned} \tag{9.8.4.51}$$

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

$$\begin{aligned} p_j(\mathbf{q}.\mathbf{r}_j + \quad t \quad + \psi_j) \exp[2\pi i \mathbf{H}.\mathbf{u}_j(\mathbf{q}.\mathbf{r}_j + t + \phi_j)] \\ = \sum_k C_{j,k}(\mathbf{H}) \exp[2\pi i k(\mathbf{q}.\mathbf{r}_j + t)]. \end{aligned} \tag{9.8.4.52}$$

and consequently the structure factor becomes

$$S_{\mathbf{H}} = \sum_j f_j(\mathbf{H}) \exp(2\pi i \mathbf{K}.\mathbf{r}_j) C_{j,-m}(\mathbf{H}), \text{ where } \mathbf{H} = \mathbf{K} + m\mathbf{q}. \tag{9.8.4.53}$$

The diffraction from incommensurate modulated crystal structures has been treated in de Wolff (1974), Yamamoto (1982*a*, *b*), Pačiorek & Kucharczyk (1985), Petriček, Coppens & Becker (1985), Petriček & Coppens (1988), Perez-Mato *et al.* (1986,1987), and Steurer (1987). Based on the techniques described above, two computer programs have been developed: REMOS (Yamamoto 1982*a*, *b*) and JANA2000 (Petriček 2000). For a review see van Smaalen (2007).

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 (to which intergrowth compounds belong). Disregarding modulations, one can describe these crystals as composed of two or more 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 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 for the corresponding subsystem 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 $\mathbf{a}_i^*$ ($i = 1, \ldots, n$) form a basis set such that every $\mathbf{a}_{\nu i}^*$ can be expressed as an integral linear combination of them:

$$\mathbf{a}_{\nu i}^* = \sum_{k=1}^{n} Z_{ik}^\nu \mathbf{a}_k^*, \quad Z_{ik}^\nu \text{ integers}, \tag{9.8.5.2}$$

with $n = 3{+}d_0$ and $d_0 > 0$. Then the vectors of the diffraction pattern of the unmodulated system are again of the form (9.8.4.5) and generate a Fourier module M_0^* of dimension three and rank ($3{+}d_0$), which can be considered as projection of a ($3{+}d_0$)-dimensional lattice Σ_0^*.

We now assume that one can choose $\mathbf{a}_{Ii}^*{=}0$ for i=1,2,3 and we denote $\mathbf{a}_{I3+j}^*$ by $\mathbf{d}_j^*$. This corresponds to assuming the existence of a subset of Bragg reflections at the positions of a three-dimensional reciprocal lattice Λ^*. Then there is a standard basis for the lattice Σ_0, which is the reciprocal of Σ_0^*, given by

$$(\mathbf{a}_i, \mathbf{a}_{Ii}), \quad (0, \mathbf{d}_j), \quad i = 1, 2, 3, \quad j = 1, \ldots, d_0. \tag{9.8.5.3}$$

In order to find the ($3{+}d_0$)-dimensional periodic structure for which the composite crystal is the three-dimensional intersection, one associates with a translation $\mathbf{t}$ in internal space V_I three-dimensional independent shifts, one for each subsystem. These shifts of the subsystems replace the phase shifts adopted for the modulated structures: V_I is now the space of the variable relative positions of the subsystems. Again, a translation in superspace can give rise to a non-Euclidean transformation in the three-dimensional space of the crystal, because of the variation in the relative positions among subsystems. Each subsystem,

however, is rigidly translated. For the basis vectors $\mathbf{d}_j$, the shift of the subsystem ν is defined in terms of projection operators π_ν:

$$\pi_\nu \mathbf{d}_j = \sum_{i=1}^{3} Z^\nu_{i3+j} \mathbf{a}_{\nu i}, \quad j = 1, 2, \ldots, d_0. \tag{9.8.5.4}$$

Then an arbitrary translation $\mathbf{t}=\sum_j t_j \mathbf{d}_j$ in V_I displaces the subsystem ν over a vector $\sum_j t_j(\pi_\nu \mathbf{d}_j)$. A translation $(\mathbf{a},\mathbf{a}_I+\mathbf{d})$ belonging to the $(3+d_0)$-dimensional lattice Σ_0 induces for the subsystem ν a relative translation in physical space over $\mathbf{a}+\pi_\nu(\mathbf{a}_I+\mathbf{d})$. The statement is that this translation is a vector of the lattice Λ_ν and leaves therefore the subsystem ν invariant. So the lattice translations belonging to Σ_0 form a group of symmetry operations for the composite crystal as a whole.

The proof is as follows. If $\mathbf{k}$ belongs to Λ^*_ν, the vector $(\mathbf{k},\mathbf{k}_I)$ belongs to Σ_0. In particular, for $\mathbf{k}=\mathbf{a}^*_{\nu i}$, one has, because of (9.8.5.2) and (9.8.5.4),

$$\mathbf{a}^*_{\nu i}.\pi_\nu \mathbf{d}_j = Z^\nu_{i3+j}, \quad j = 1, \ldots, d_0, \tag{9.8.5.5}$$

and

$$\mathbf{k}_I = \sum_{j=1}^{d_0} Z^\nu_{i3+j} \mathbf{d}^*_j \quad \text{and therefore} \quad \mathbf{k}_I.\mathbf{d}_j = Z^\nu_{i3+j}.$$

Note that one has $\mathbf{k}_I.\mathbf{t}=\mathbf{k}.\pi_\nu \mathbf{t}$, for any $\mathbf{t}$ from V_I as π_ν is a linear operator. Because of the linearity, this holds for every $\mathbf{k}$ from Λ^*_ν as well. Since $(\mathbf{k},\mathbf{k}_I)$ belongs to Σ^*_0 and $(\mathbf{a},\mathbf{a}_I+\mathbf{d})$ to Σ_0, one has for their inner product:

$$\mathbf{k}.\mathbf{a} + \mathbf{k}_I.\mathbf{a}_I + \mathbf{k}_I.\mathbf{d} = \mathbf{k}.(\mathbf{a} + \pi_\nu \mathbf{a}_I + \pi_\nu \mathbf{d}) \equiv 0 \ \text{ modulo } 1,$$

which implies that $\mathbf{a}+\pi_\nu \mathbf{a}_I+\pi_\nu \mathbf{d}$ is an element of Λ_ν.

In conclusion, one may state that the composite structure is the intersection with the physical space ($\mathbf{t}=0$) of a pattern having atomic positions given by

$$(\mathbf{n}_\nu + \mathbf{r}_{\nu j} - \pi_\nu \mathbf{t}, \mathbf{t}) \quad \text{for any} \quad \mathbf{t} \quad \text{of} \quad V_I. \tag{9.8.5.6}$$

Such a pattern is invariant under the $(3+d_0)$-dimensional lattice Σ_0. Again, orthogonal transformations R of $O(3)$ leaving the Fourier module M^*_0 invariant can be extended to orthogonal transformations R_s of $O(3) \times O(d_0)$ allowing to give a Euclidean structure to the superspace. One can then consider the superspace-group symmetry of the basic structure defined by atomic positions (9.8.5.6). A superspace-group element induces (in three-dimensional space) for the subsystem ν the transformation

$$g_s : \mathbf{n}_\nu + \mathbf{r}_{\nu j} \rightarrow R\mathbf{n}_\nu + R\mathbf{r}_{\nu j} + \mathbf{v} + R\pi_\nu R_I^{-1} \mathbf{v}_I, \tag{9.8.5.7}$$

changing the position $\mathbf{n}_\nu+\mathbf{r}_{\nu j}$ into an equivalent one of the composite structure, not necessarily, however, within the same subsystem ν.

Finally, in general, the composite structure will be modulated, because of the interaction between the subsystems. The modulation of subsystem ν will, generally, contain

the wavevectors of the reciprocal lattices of the other subsystems. If there are two subsystems, the reflections $\mathbf{a}^*_{\nu i}$ $(i = 1, 2, 3)$ are the main reflections of subsystems 1 and 2, some are common, others belong to either of the two. As an example, take a composite crystal with two subsystems, one with a basic structure with reciprocal lattice spanned by $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$, the other with $\mathbf{a}^*$, $\mathbf{b}^*$, and $\gamma\mathbf{c}^*$. Then a general reflection is

$$h_1\mathbf{a}^* + h_2\mathbf{b}^* + h_3\mathbf{c}^* + h_4\gamma\mathbf{c}^*.$$

The reflections with $h_3 = h_4 = 0$ are common to both subsystems, those with h_4=0 belong to the first, those with $h_3 = 0$ to the second system, and those with both $h_3 \neq 0$ and $h_4 \neq 0$ are sum reflections. They stem from the modulation of one subsystem by the interaction with the other.

For the case of a one-dimensional modulation of each subsystem (as in the example above), the positions are

$$\mathbf{n}_\nu + \mathbf{r}_{\nu j} + \mathbf{u}_{\nu j}[\mathbf{q}_\nu.(\mathbf{n}_\nu + \mathbf{r}_{\nu j})]. \tag{9.8.5.8}$$

In principle, it is possible to have modulation wavevectors not coming from the interaction with the other subsystems, for example due to interaction with the electrons. Then one should add still more wavevectors, and the rank becomes 3+d with $d \geq d_0$.One can write

$$\mathbf{q}_\nu = \sum_{j=1}^{3+d} Q^\nu_j \mathbf{a}^*_j, \quad Q^\nu_j \text{ integers.} \tag{9.8.5.9}$$

The peaks of the diffraction pattern are at the positions of the Fourier module M^*, which can be considered as the projection of a (3+d)-dimensional reciprocal lattice Σ^*, which is the reciprocal of the lattice Σ that leaves invariant the pattern of modulated atomic positions in superspace given by

$$(\mathbf{n}_\nu + \mathbf{r}_{\nu j} - \pi_\nu\mathbf{t} + \mathbf{u}_{\nu j}[\mathbf{q}_\nu.(\mathbf{n}_\nu + \mathbf{r}_{\nu j} - \pi_\nu\mathbf{t}) + \mathbf{q}_{I\nu}.\mathbf{t}],\ \mathbf{t}) \quad (\text{any } \mathbf{t} \text{ of } V_I) \tag{9.8.5.10}$$

with $\pi_\nu\mathbf{d}_j$=0 if $j > d_0$, and where $\mathbf{q}_{I\nu}$ is the internal part of the (3+d)-dimensional vector that projects on $\mathbf{q}_\nu$. The symmetry of this pattern is a (3+d)-dimensional superspace group G_s. The transformation induced in the modulated composite crystal by an element g_s of G_s is now readily written down. For the case $d = d_0 = 1$ and $g_s = (\{R|\mathbf{v}\}, \{\epsilon|\Delta\})$, the position $\mathbf{n}_\nu$+$\mathbf{r}_{\nu j}$ is transformed into

$$R(\mathbf{n}_\nu + \mathbf{r}_{\nu j}) + \mathbf{v} + \epsilon R\pi_\nu\Delta\mathbf{d}_1, \tag{9.8.5.11}$$

and the modulation $\mathbf{u}_{\nu j}(\mathbf{q}_\nu.(\mathbf{n}_\nu + \mathbf{r}_{\nu j}))$ into

$$R\mathbf{u}_{\nu j}\left(\mathbf{q}_\nu.(\mathbf{n}_\nu + \mathbf{r}_{\nu j} + \epsilon\pi_\nu\Delta\mathbf{d}_1) - \epsilon\mathbf{q}_{I\nu}.\Delta\mathbf{d}_1\right).$$

This shows how the superspace-group approach can be applied to a (modulated) composite structure.

9.8.5.2. Modulated structures of rank higher than four

The general description of modulated structures, and its foundation are not limited to structures of rank four, as has been shown in Section 9.8.4. Also the notation for crystal classes, Bravais classes and superspace groups may directly be generalised to situations where the rank of the Fourier module is higher than four. However, the number of classes and types increases rapidly with higher rank. Therefore, its is not feasible to present tables of superspace groups for the higher-dimensional cases. We present here tables of Bravais classes for ranks four, five and six (Janner, Janssen & de Wolff, 1983). The notation of superspace groups corresponding to these Bravais classes then may be derived from this.

In the Tables 9.8.5.1 - 9.8.5.10 Bravais classes in (3+1)-, (3+2)-, and (3+3)-dimensional spaces are denoted by a one-line symbol. The symbol consists of that for the physical component $\Gamma_E(K)$ and the basis modulation vector(s). The latter are given with respect to the standard conventional bases in ITCA. The action of K on the modulation wave vectors give the components in internal space. This group $\Gamma_I(K)$ is given as well. Next, a conventional basis for the Fourier module is indicated. The centering reflection conditions are given in the last column.

The basis of the Fourier module consists of 3 wave vectors that satisfy the conditions for the corresponding centering, given in the one-line symbol. Furthermore, the remaining basis vectors may be constructed using the action of the point group on the modulation wave vectors. A conventional basis then is obtained by vectors belonging to the main reflections and satisfying the reflection conditions, and the irrational parts $\mathbf{q}_j^i$ of the modulation wave vectors in the primitive basis. From the matrix for transforming the conventional to the primitive basis, follow the reflection conditions.

Consider, as example, the (3+2)-dimensional case $mmmC(10\gamma, 00\nu)$. The orthorhombic conventional basis of the main reflections is $\mathbf{a}_1^*$=(100), $\mathbf{a}_2^*$=(010), and $\mathbf{a}_3^*$=(001). A primitive basis of the main reflections is given by (110),($\bar{1}$10) and (001), and for the satellites (10γ) and (00ν). The irrational parts of the latter two vectors are (00γ) and (00ν). Therefore the conventional basis for the Fourier module is given by (100), (010), (001), (00γ) and (00ν). The transformation matrix from the conventional to the primitive basis and its inverse transpose are

$$S = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}; \quad (S^{-1})^{\mathrm{T}} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then the reflection condition is $H + K + M_1 = 2n$ (=even) for $\mathbf{H}$=$H\mathbf{a}_1^* + K\mathbf{a}_2^* + L\mathbf{a}_3^* + M_1\mathbf{a}_4^* + M_2\mathbf{a}_5^*$, because the centering is $\frac{1}{2}\frac{1}{2}0\frac{1}{2}0$. The arithmetic crystal class is determined by the matrices for the action of the generators on the basis: m_x transforms the primitive basis vectors to ($\bar{1}$10), (110), (001), ($\bar{1}0\gamma$) and (00ν). Therefore the matrix $\Gamma(m_x)$ is given

by

$$\Gamma(m_x) \;=\; = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Analogously, we get the matrices for the other two generators:

$$\Gamma(m_y) \;=\; = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix};\; \Gamma(m_z) \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

The corresponding (3+2)-dimensional point group has the generators $(R_E, R_I) = (m_x, 1_2)$, $(m_y, 1_2)$ and $(m_z, 2)$, where 1_2 is the identity in two dimensions, and 2 is the two-fold rotation in 2 dimensions.

With the matrices of the generators, one may determine the possible superspace groups. One of them has a vector $(0, \frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2})$ associated with the first generator, and zero for the other two. Then the symbol for this superspace group is $Cnmm(10\gamma, 00\nu)n00$: its point group is $mmm(112)$, the external part of the non-primitive translation $(0\frac{1}{2}\frac{1}{2})$ for m_x is indicated, in the usual way by n, the internal part $(0\frac{1}{2})$ by the second n.

As said before, it does not make sense to produce printed tables of superspace groups in dimensions five and higher, but this illustrates the idea. However, lists of superspace groups can be found on the internet: see the websites http://quasi.nims.go.jp/yamamoto/spgr.html and http://superspace.epfl.ch. Information comparable to that in Vol. A of the *International Tables for Crystallography* could be obtained from specialized software only. This can be realized in arbitrary dimensions (Thiers, Ephraïm, Janssen & Janner, 1993), and has partially been implemented in software on the EPFL website.

9.8.5.3. General quasiperiodic crystals

Incommensurately modulated crystals form only a special case of general quasiperiodic crystals. A quasiperiodic crystal is a matter distribution for which the idealised density function may be written as

$$\rho(\mathbf{r}) \;=\; \sum_{\mathbf{k}\in M^*} \hat{\rho}(\mathbf{k}) \exp(i\mathbf{k}.\mathbf{r}) \quad \text{with} \quad M^* = Span_Z(\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*). \tag{9.8.5.12}$$

If $n > 3$, the structure is aperiodic. Again, a quasiperiodic function may be seen as the intersection of a periodic function in n-dimensional space with a three-dimensional hyperplane, the physical space. The periodic function is

$$\rho(\mathbf{r}_s) \;=\; \sum_{\mathbf{k}_s\in\Sigma^*} \hat{\rho}(\pi_E\mathbf{k}_s) \exp(i\mathbf{k}_s.\mathbf{r}_s), \tag{9.8.5.13}$$

Table 9.8.5.1: *(3+1)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=1.* First column: one-line symbol. Second column: the transformations in internal space corresponding to the generators in the one-line symbol. Third column: a choice of a conventional basis, in components with respect to the standard basis in the ITCA for three-dimensional space groups. Because, generally, this conventional basis is not a primitive basis, there are reflection conditions, which are given in column four. With respect to the conventional basis given here, the diffraction peaks are at $\mathbf{H}=H\mathbf{a}_1^*+K\mathbf{a}_2^*+L\mathbf{a}_3^*+M\mathbf{a}_4^*$. The information given in this table is essentially the same as that in Table (9.8.3.4).

Triclinic				$mmmC(00\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$H+K=2n$
$\bar{1}P(\alpha\beta\gamma)$	$\bar{1}$	$100, 010, 001, \alpha\beta\gamma$	None	$mmmC(10\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$H+K+M=2n$
Monoclinic				$mmmA(00\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$K+L=2n$
$2/mP(\alpha\beta 0)$	$\bar{1}1$	$100, 010, 001, \alpha\beta 0$	None	$mmmA(\frac{1}{2}0\gamma)$	$11\bar{1}$	$\frac{1}{2}00, 010, 001, 00\gamma$	$H+M, K+L=2n$
$2/mP(\alpha\beta\frac{1}{2})$	$\bar{1}1$	$100, 010, 00\frac{1}{2}, \alpha\beta 0$	$L+M=2n$	$mmmF(00\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$H+K, K+L=2n$
$2/mB(\alpha\beta\bar{0})$	$\bar{1}1$	$100, 010, 00\bar{1}, \alpha\beta 0$	$H+L=2n$	$mmmF(10\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$K+L, H+K+M=2n$
$2/mP(00\gamma)$	$1\bar{1}$	$100, 010, 001, 00\gamma$	None	Tetragonal			
$2/mP(\frac{1}{2}0\gamma)$	$1\bar{1}$	$\frac{1}{2}00, 010, 001, 00\gamma$	$H+M=2n$	$4/mmmP(00\gamma)$	$1\bar{1}11$	$100, 010, 001, 00\gamma$	None
$2/mB(00\gamma)$	$1\bar{1}$	$100, 010, 001, 00\gamma$	$H+L=2n$	$4/mmmP(\frac{1}{2}\frac{1}{2}\gamma)$	$1\bar{1}11$	$\frac{1}{2}\frac{1}{2}0, \frac{\bar{1}}{2}\frac{1}{2}0, 001, 00\gamma$	$H+K+M=2n$
$2/mB(0\frac{1}{2}\gamma)$	$1\bar{1}$	$100, 0\frac{1}{2}0, 001, 00\gamma$	$H+L, K+M=2n$	$4/mmmI(00\gamma)$	$1\bar{1}11$	$100, 010, 001, 00\gamma$	$H+K+L=2n$
Orthorhombic				Trigonal			
$mmmP(00\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	None	$\bar{3}mR(00\gamma)$	$\bar{1}1$	$100, 010, 001, 00\gamma$	$H-K-L=3n$
$mmmP(0\frac{1}{2}\gamma)$	$11\bar{1}$	$100, 0\frac{1}{2}0, 001, 00\gamma$	$K+M=2n$	$\bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma)$	$\bar{1}11$	$\frac{1}{3}\frac{1}{3}0, \frac{2}{3}\frac{\bar{1}}{3}0, 001, 00\gamma$	$H-K-M=3n$
$mmmP(\frac{1}{2}\frac{1}{2}\gamma)$	$11\bar{1}$	$\frac{1}{2}\frac{1}{2}0, \frac{\bar{1}}{2}\frac{1}{2}0, 001, 00\gamma$	$H+K+M=2n$	Hexagonal			
$mmmI(00\gamma)$	$11\bar{1}$	$100, 010, 001, 00\gamma$	$H+K+L=2n$	$6/mmmP(00\gamma)$	$1\bar{1}11$	$100, 010, 001, 00\gamma$	None

where M^* is the projection of an n-dimensional reciprocal lattice Σ^*: $M^*=\pi_E\Sigma^*$. The direct lattice in n dimensions then is Σ. In the general case, however, this lattice does not have a split basis. Contrary to the case of modulated crystals, one can not find a basis with $d=n-3$ basis vectors belonging to the internal space V_I, because, generally, the integer representation of the point group is not Z-reducible into a three-dimensional and a d-dimensional integer representation. But, just as in the case of modulated crystals, the symmetry group of the n-dimensional density function is an n-dimensional superspace group. It is a superspace group, because the physical space V_E is left invariant by the point group of the symmetry group. Therefore, the point group elements still can be written as $R=(R_E,R_I)$. There is an orthogonal basis in superspace on which the elements are

$$R \;=\; \begin{pmatrix} R_E & 0 \\ 0 & R_I \end{pmatrix}, \tag{9.8.5.14}$$

but there is, generally, no basis on which the elements are

$$\Gamma(R) \;=\; \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix} \tag{9.8.5.15}$$

with integer entries.

So, in n-dimensional space one may distinguish three types of space groups: the general n-dimensional space groups, in general without invariant 3-dimensional space for the point group, the superspace groups, for which there is such an invariant space, but generally without split basis, and superspace groups for modulated structures, with an invariant physical space and having a lattice with a split basis.

Table 9.8.5.2: *(3+2)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=2: Triclinic and Monoclinic basic structure.* First column: one-line symbol. Second column: internal point group. Third column: a choice of conventional basis, with components with respect to the standard conventional bases for three-dimensional space groups, as given in ITCA. Fourth column: reflection conditions for the reflections $H\mathbf{a}_1^* + K\mathbf{a}_2^* + L\mathbf{a}_3^* + M_1\mathbf{a}_4^* + M_2\mathbf{a}_5^*$.

Triclinic							
$\bar{1}P(\alpha\beta\gamma, \lambda\mu\nu)$	$2p$	$100, 010, 001, \alpha\beta\gamma, \lambda\mu\nu$	None				
Monoclinic							
$2/mP(\alpha\beta 0, \lambda\mu 0)$	$21p$	$100, 010, 001, \alpha\beta 0, \lambda\mu 0$	None	$2/mP(\alpha\beta\frac{1}{2}, \lambda\mu 0)$	$21p$	$100, 010, 00\frac{1}{2}, \alpha\beta 0, \lambda\mu 0$	$L + M_1 = 2n$
$2/mB(\alpha\beta 0, \lambda\mu 0)$	$21p$	$100, 010, 001, \alpha\beta 0, \lambda\mu 0$	$H + L = 2n$	$2/mP(00\gamma, 00\nu)$	$12p$	$100, 010, 001, 00\gamma, 00\nu$	None
$2/mP(\frac{1}{2}0\gamma, 00\nu)$	$12p$	$\frac{1}{2}00, 010, 001, 00\gamma, 00\nu$	$H + M_1 = 2n$	$2/mP(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu)$	$12p$	$\frac{1}{2}00, 0\frac{1}{2}0, 001, 00\gamma, 00\nu$	$H + M_1, K + M_2 = 2n$
$2/mB(00\gamma, 00\nu)$	$12p$	$100, 010, 001, 00\gamma, 00\nu$	$H + L = 2n$	$2/mB(0\frac{1}{2}\gamma, 00\nu)$	$12p$	$100, 0\frac{1}{2}0, 001, 00\gamma, 00\nu$	$H + L, K + M_1 = 2n$
$2/mP(\alpha\beta 0, 00\nu)$	mmp	$100, 010, 001, \alpha\beta 0, 00\nu$	None	$2/mP(\alpha\beta\frac{1}{2}, 00\nu)$	mmp	$100, 010, 00\frac{1}{2}, \alpha\beta 0, 00\nu$	$L + M_1 = 2n$
$2/mP(\alpha\beta 0, \frac{1}{2}0\nu)$	mmp	$\frac{1}{2}00, 010, 001, \alpha\beta 0, 00\nu$	$H + M_2 = 2n$	$2/mP(\alpha\beta\frac{1}{2}, \frac{1}{2}0\nu)$	mmp	$\frac{1}{2}00, 010, 00\frac{1}{2}, \alpha\beta 0, 00\nu$	$H + M_2, L + M_1 = 2n$
$2/mB(\alpha\beta 0, 00\nu)$	mmp	$100, 010, 001, \alpha\beta 0, 00\nu$	$H + L = 2n$	$2/mB(\alpha\beta 0, 0\frac{1}{2}\nu)$	mmp	$100, 0\frac{1}{2}0, 001, \alpha\beta 0, 00\nu$	$H + L, K + M_2$
$2/mP(\alpha\beta\gamma)$	mmc	$100, 010, 001, \alpha\beta 0, 00\gamma$	$M_1 + M_2 = 2n$	$2/mB(\alpha\beta\gamma)$	mmc	$100, 010, 001, \alpha\beta 0, 00\gamma$	$H + L, M_1 + M_2 = 2n$

Table 9.8.5.3: *(3+2)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=2: Orthorhombic basic structure.*

Orthorhombic							
$mmmP(00\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	None	$mmmP(0\frac{1}{2}\gamma, 00\nu)$	$112p$	$100, 0\frac{1}{2}0, 001, 00\gamma, 00\nu$	$K+M_1=2n$
$mmmP(\frac{1}{2}\frac{1}{2}\gamma, 00\nu)$	$112p$	$\frac{1}{2}\frac{1}{2}0, \bar{\frac{1}{2}}\frac{1}{2}0, 001, 00\gamma, 00\nu$	$H+K+M_1=2n$	$mmmP(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu)$	$112p$	$\frac{1}{2}00, 0\frac{1}{2}0, 001, 00\gamma, 00\nu$	$H+M_1, K+M_1=2n$
$mmmI(00\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$K+K+L=2n$	$mmmC(00\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$H+K=2n$
$mmmC(10\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$H+K+M_1=2n$	$mmmA(00\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$K+L=2n$
$mmmA(\frac{1}{2}0\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$K+L,H+M_1=2n$	$mmmF(00\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$H+K,K+L=2n$
$mmmF(10\gamma, 00\nu)$	$112p$	$100, 010, 001, 00\gamma, 00\nu$	$H+K+M_1,K+L=2n$	$mmmP(0\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	None
$mmmP(\frac{1}{2}\beta 0, 00\nu)$	$1mmp$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\nu$	$H+M_1=2n$	$mmmP(0\beta\frac{1}{2}, 00\nu)$	$1mmp$	$100, 010, 00\frac{1}{2}, 0\beta 0, 00\nu$	$L+M_1=2n$
$mmmP(\frac{1}{2}\beta\frac{1}{2}, 00\nu)$	$1mmp$	$\frac{1}{2}0\frac{1}{2}, 010, \bar{\frac{1}{2}}0\frac{1}{2}, 0\beta 0, 00\nu$	$H+L+M_1=2n$	$mmmP(\frac{1}{2}\beta 0, \frac{1}{2}0\nu)$	$1mmp$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\nu$	$H+M_1+M_2=2n$
$mmmP(\frac{1}{2}\beta 0, 0\frac{1}{2}\nu)$	$1mmp$	$\frac{1}{2}00, 0\frac{1}{2}0, 001, 0\beta 0, 00\nu$	$H+M_1,K+M_2=2n$	$mmmP(0\beta\frac{1}{2}, 0\frac{1}{2}\nu)$	$1mmp$	$100, 0\frac{1}{2}0, 00\frac{1}{2}, 0\beta 0, 00\nu$	$K+M_2,L+M_1=2n$
$mmmP(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}0\nu)$	$1mmp$	$\frac{1}{2}00, 010, 00\frac{1}{2}, 0\beta 0, 00\nu$	$H+M_1+M_2,L+M_1=2n$	$mmmP(\frac{1}{2}\beta\frac{1}{2}, 0\frac{1}{2}\nu)$	$1mmp$	$\frac{1}{2}0\frac{1}{2}, 0\frac{1}{2}0, \bar{\frac{1}{2}}0\frac{1}{2}, 0\beta 0, 00\nu$	$H+L+M_1,K+M_2=2n$
$mmmP(\bar{\frac{1}{2}}\beta\bar{\frac{1}{2}}, \bar{\frac{1}{2}}\frac{1}{2}\nu)$	$1mmp$	$0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \bar{\frac{1}{2}}\frac{1}{2}0, 0\beta 0, 00\nu$	$H+K+M_1,H+L+M_2=2n$	$mmmI(0\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$H+K+L=2n$
$mmmC(0\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$H+K=2n$	$mmmC(0\beta\frac{1}{2}, 00\nu)$	$1mmp$	$100, 010, 00\frac{1}{2}, 0\beta 0, 00\nu$	$H+K,L+M_1=2n$
$mmmC(0\beta 0, 10\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$H+K+M_2=2n$	$mmmC(0\beta\frac{1}{2}, 10\nu)$	$1mmp$	$100, 010, 00\frac{1}{2}, 0\beta 0, 00\nu$	$H+K+M_2,L+M_1=2n$
$mmmA(0\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$K+L=2n$	$mmmA(\frac{1}{2}\beta 0, 00\nu)$	$1mmp$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\nu$	$K+L,H+M_1=2n$
$mmmA(\frac{1}{2}\beta 0, \frac{1}{2}0\nu)$	$1mmp$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\nu$	$K+L,H+M_1+M_2=2n$	$mmmF(0\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$H+K,K+L=2n$
$mmmF(1\beta 0, 00\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$K+L,H+L+M_1=2n$	$mmmF(1\beta 0, 10\nu)$	$1mmp$	$100, 010, 001, 0\beta 0, 00\nu$	$K+L,H+L+M_1+M_2=2n$
$mmmP(0\beta\gamma)$	$1mmc$	$100, 010, 001, 0\beta 0, 00\gamma$	$M_1+M_2=2n$	$mmmP(\frac{1}{2}\beta\gamma)$	$1mmc$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\gamma$	$H+M_1,M_1+M_2=2n$
$mmmC(0\beta\gamma)$	$1mmc$	$100, 010, 001, 0\beta 0, 00\gamma$	$H+K,M_1+M_2=2n$	$mmmA(0\beta\gamma)$	$1mmc$	$100, 010, 001, 0\beta 0, 00\gamma$	$K+L,M_1+M_2=2n$
$mmmA(\frac{1}{2}\beta\gamma)$	$1mmc$	$\frac{1}{2}00, 010, 001, 0\beta 0, 00\gamma$	$K+L,H+M_1,H+M_2=2n$	$mmmF(0\beta\gamma)$	$1mmc$	$100, 010, 001, 0\beta 0, 00\gamma$	$H+K,K+L,M_1+M_2=2n$
$mmmI(0\beta\gamma)$	$1mmc$	$100,010,001,0\beta 0,00\gamma$	$H+K+L,M_1+M_2=2n$				

This variety of space groups has also consequences for the notation. The notation for superspace groups for modulated crystals, as described here, is based on the properties of the point groups and the lattices with respect to the physical space. The point group was indicated by its physical component K_E, a 3-dimensional point group, and the basic modulation wavevectors, from which the component K_I follows. The non-primitive translations could be split into components along the 3 basis vectors corresponding to the basic structure, and components along the other basis vectors lying in V_I. This leads to symbols like $P2(00\gamma)s$. For general quasiperiodic structures, the point group elements are still couples of orthogonal transformations, but each point group may have an associated non-primitive translation with (intrinsic) components along any lattice vector, and this lattice vector is generally not in one of the two spaces V_E or V_I. Then the symbol of the same space group should be $P2_u(1)$.

Table 9.8.5.4: *(3+2)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=2: Tetragonal basic structure.*

Tetragonal							
$4/mP(\alpha\beta 0)$	$41p$	$100, 010, 001, \alpha\beta 0, -\beta\alpha 0$	None	$4/mP(\alpha\beta\frac{1}{2})$	$41p$	$100, 010, 00\frac{1}{2}, \alpha\beta 0, -\beta\alpha 0$	$L+M_1+M_2=2n$
$4/mI(\alpha\beta 0)$	$41p$	$100, 010, 001, \alpha\beta 0, -\beta\alpha 0$	$H+K, K+L=2n$	$4/mmmP(00\gamma, 00\nu)$	$1211p$	$100, 010, 001, 00\gamma, 00\nu$	None
$4/mmmP(\frac{1}{2}\frac{1}{2}\gamma, 00\nu)$	$1211p$	$\frac{1}{2}\frac{1}{2}0, \bar{\frac{1}{2}}\frac{1}{2}0, 001, 00\gamma, 00\nu$	$H+K+M_1=2n$	$4/mmmI(00\gamma, 00\nu)$	$1211p$	$100, 010, 001, 00\gamma, 00\nu$	$H+K, K+L=2n$
$4/mmmP(\alpha 00)$	$41mmp$	$100, 010, 001, \alpha 00, 0\alpha 0$	None	$4/mmmP(\alpha\frac{1}{2}0)$	$41mmp$	$\frac{1}{2}00, 0\frac{1}{2}0, 001, \alpha 00, 0\alpha 0$	$H+M_2, K+M_1=2n$
$4/mmmP(\alpha 0\frac{1}{2})$	$41mmp$	$100, 010, 00\frac{1}{2}, \alpha 00, 0\alpha 0$	$L+M_1+M_2=2n$	$4/mmmP(\alpha\frac{1}{2}\frac{1}{2})$	$41mmp$	$0\frac{1}{2}\frac{1}{2}0, \bar{\frac{1}{2}}0\frac{1}{2}, 001, \alpha 00, 0\alpha 0$	$H+M_1, K+M_2=2n$
$4/mmmI(\alpha 00)$	$41\dot{m}mp$	$100, 010, 001, \alpha 00, 0\alpha 0$	$H+K+L=2n$	$4/m\dot{m}mP(\alpha\alpha 0)$	$41m\dot{m}p$	$100, 010, 001, \alpha\alpha 0, \bar{\alpha}\alpha 0$	None
$4/m\dot{m}mP(\alpha\alpha\frac{1}{2})$	$41m\dot{m}p$	$100, 010, 00\frac{1}{2}, \alpha\alpha 0, \bar{\alpha}\alpha 0$	$L+M_1+M_2=2n$	$4/m\dot{m}mI(\alpha\alpha 0)$	$41m\dot{m}p$	$100, 010, 001, \alpha\alpha 0, \bar{\alpha}\alpha 0$	$H+K+L$
$4/m\dot{m}mI(\alpha\alpha 1)$	$41m\dot{m}p$	$100, 010, 001, \alpha\alpha 0, \bar{\alpha}\alpha 0$	$H+K+L+M_1+M_2=2n$				

Table 9.8.5.5: *(3+2)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=2: Trigonal and Hexagonal basic structure.*

Trigonal							
$\bar{3}P(\alpha\beta\frac{1}{3})$	$6p$	$100, 010, 00\frac{1}{3}, \alpha\beta 0, (\alpha+\beta)\bar{\alpha}0$	L-M_1-M_2=3n	$\bar{3}R(\alpha\beta 0)$	$6p$	$100, 010, 001, \alpha\beta 0, (\alpha+\beta)\bar{\alpha}0$	$2H+K+L=3n$
$\bar{3}1mP(\bar{\frac{1}{3}}\frac{1}{3}\gamma, 00\nu)$	$211p$	$100, 010, 001, 00\gamma, 00\nu$	H-K-M_1=3n	$3mR(00\gamma, 00\nu)$	$21p$	$100, 010, 001, 00\gamma, 00\nu$	$2H+K+L=3n$
$\bar{3}1mP(\alpha\alpha\frac{1}{3})$	$61mp$	$100, 010, 001, \alpha\alpha 0, 2\bar{\alpha}\alpha 0$	H-K-M_1=3n	$\bar{3}mR(\alpha\alpha 0)$	$6\dot{m}p$	$100, 010, 001, \alpha\alpha, 2\bar{\alpha}\alpha 0$	$2H+K+L=3n$
$\bar{3}m1P(\alpha 0\frac{1}{3})$	$6m1p$	$100, 010, 00\frac{1}{3}, \alpha 00, \bar{\alpha}\alpha 0$	L-M_1=3n	$\bar{3}mR(\alpha 00)$	$6mp$	$100, 010, 001, \alpha 00, \bar{\alpha}\alpha 0$	$2H+K+L=3n$
Hexagonal							
$6/mP(\alpha\beta 0)$	$61p$	$100, 010, 001, \alpha\beta 0, (\alpha+\beta)\bar{\alpha}0$	None	$6/mmmP(00\gamma, 00\nu)n2dimnsio$	$1211p$	$100, 010, 001, 00\gamma, 00\nu$	None
$6/mmmP(\alpha 00)$	$6\dot{m}mp$	$100, 010, 001, \alpha 00, \bar{\alpha}\alpha 0$	None	$6/mmmP(\alpha\alpha 0)$	$61m\dot{m}p$	$100, 010, 001, \alpha\alpha, 2\bar{\alpha}\alpha 0$	None

Let us summarize the notation for general quasiperiodic symmetry groups. The point group is reducible in a three- and a d-dimensional part. Both are point groups. Therefore, the point group is of the form (K_E, K_I). The first component is given by its standard symbol for three dimensions. This holds as well for the second component, but the number of symbols here should be equal to that for the first component and the nth symbol for the first should correspond to the nth symbol for the second component. This can be done by introducing symbols '1' and by choosing a non-standard setting for K_I. An example is 4/mmm(41mm).

Sometimes ii is convenient to use a short symbol. Consider the point group $5m(5^2m)$. The first part is a non-crystallographic point group in three dimensions. This implies that for having a crystallographic operation, the second part contains necessarily 5^2. Therefore, in such a context one may omit the second part and use a *short symbol*: $5m$ instead of the *long symbol*.

In the symbol for an arithmetic crystal class, the point group symbol gets a prefix indicating the centering. Finally, the symbol for a superspace group requires an indication of the (intrinsic) non-primitive translations. These are given with respect to a conventional basis. Because, generally, there is not a lattice in either V_E or V_I, one cannot split the translation into an internal or external part and a remainder. Therefore, the symbol for the non-primitive translation is attached to the symbols for the elements of K_E. An example is P$5a(5^2m)$, a five-dimensional superspace group with point group $5m(5^2m)$, P-centering, and a non-primitive translation $\frac{1}{2}\mathbf{a}_1$ along the unique axis $\mathbf{a}_1$ associated with the point group element $m(m)$.

Finally, for a general type space group, the point group does not consist of pairs (R_E, R_I). Symbols for such space groups were recommended by an IUCr commission

Table 9.8.5.6: *(3+3)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=3: Triclinic and Monoclinic basic structure.*

Triclinic								
1	$\bar{1}P(\alpha\beta\gamma,\lambda\mu\nu,\zeta\eta\theta)$	$\bar{1}P$						
Monoclinic								
2	$2/mP(\alpha\beta 0,\lambda\mu 0,\zeta\eta 0)$	$\bar{1}1P$	3	$2/mP(\alpha\beta\frac{1}{2},\lambda\mu 0,\zeta\eta 0)$	$\bar{1}1P$	4	$2/mB(\alpha\beta 0,\lambda\mu 0,\zeta\eta 0)$	$\bar{1}1P$
5	$2/mP(00\gamma,00\nu,00\theta)$	$1\bar{1}P$	6	$2/mP(\frac{1}{2}0\gamma,00\nu,00\theta)$	$1\bar{1}P$	7	$2/mP(\frac{1}{2}0\gamma,0\frac{1}{2}\nu,00\theta)$	$1\bar{1}P$
8	$2/mP(\frac{1}{2}0\gamma,0\frac{1}{2}\nu,\frac{1}{2}0\theta)$	$1\bar{1}P$	9	$2/mB(00\gamma,00\nu,00\theta)$	$1\bar{1}P$	10	$2/mB(0\frac{1}{2}\gamma,00\nu,00\theta)$	$1\bar{1}P$
11	$2/mP(\alpha\beta 0,\lambda\mu 0,00\theta)$	$2/mP$	12	$2/mP(\alpha\beta\frac{1}{2},\lambda\mu 0,00\theta)$	$2/mP$	13	$2/mP(\alpha\beta 0,\lambda\mu 0,\frac{1}{2}0\theta)$	$2/mP$
14	$2/mP(\alpha\beta\frac{1}{2},\lambda\mu 0,\frac{1}{2}0\theta)$	$2/mP$	15	$2/mB(\alpha\beta 0,\lambda\mu 0,00\theta)$	$2/mP$	16	$2/mB(\alpha\beta 0,\lambda\mu 0,0\frac{1}{2}\theta)$	$2/mP$
17	$2/mP(\alpha\beta 0,\lambda\mu\nu)$	$2/mA$	18	$2/mP(\alpha\beta\frac{1}{2},\lambda\mu\nu)$	$2/mA$	19	$2/mB(\alpha\beta 0,\lambda\mu\nu)$	$2/mA$
20	$2/mP(\alpha\beta 0,00\nu,00\theta)$	$m/2P$	21	$2/mP(\alpha\beta\frac{1}{2},00\nu,00\theta)$	$m/2P$	22	$2/mP(\alpha\beta 0,\frac{1}{2}0\nu,00\theta)$	$m/2P$
23	$2/mP(\alpha\beta\frac{1}{2},\frac{1}{2}0\nu,00\theta)$	$m/2P$	24	$2/mB(\alpha\beta 0,00\nu,00\theta)$	$m/2P$	25	$2/mB(\alpha\beta 0,0\frac{1}{2}\nu,00\theta)$	$m/2P$
26	$2/mP(\alpha\beta\gamma,00\nu)$	$m/2C$	27	$2/mP(\alpha\beta\gamma,\frac{1}{2}0\nu)$	$m/2C$	28	$2/mB(\alpha\beta\gamma,00\nu)$	$m/2C$
29	$2/mB(\alpha\beta\gamma,0\frac{1}{2}\nu)$	$m/2C$						

(Janssen *et al.*, 1999, 2002). For the same group one gets the symbol $P2_u$, which is equivalent with $P2_z$. The latter, however, is the superspace group $P2_1(00\gamma)$, which is not equivalent with $P2(00\gamma)s$ as superspace group, because the non-primitive translation is in physical space for one, and in internal space for the other. This illustrates the fact that the definitions of equivalence should be different for the different cases.

A more extensive treatment of the crystallography of aperiodic crystals can be found in Janssen (1988), Yamamoto (1996), Janssen, Chapuis & de Boissieu (2007), and van Smaalen (2007).

9.8.5.4. Tilings and quasicrystals

Examples of quasiperiodic structures that cannot be considered as modulated structures are quasicrystals. Whereas the point groups of modulated structures have components in physical space which are 3-dimensional crystallographic groups (because they leave the basic structure invariant), this is no longer the case for the crystals that are not modulated structures. This is illustrated by the fact that quasicrystals may have such components which are not crystallographic in three dimensions. For example, they may contain five-fold rotation elements.

The point groups for incommensurately modulated crystals belong to one of the isomorphism classes C_n (cyclic), D_n (dihedral), T (tetrahedral) and O (octahedral), and their direct products with C_2, where $n = 1, 2, 3, 4$, or 6. The reason is that rotation elements of 2- and 3-dimensional crystallographic point groups have traces for their matrices equal to $2\cos(2\pi m/n)$ (in 2 dimensions) or $1+2\cos(2\pi m/n)$ (in 3 dimensions). Because these traces are integer for crystallographic groups, the restriction of n to the mentioned values follows. In spaces of higher dimensions and having a 2- or 3-dimensional invariant subspace (the physical space), these restrictions become different. Each rotation is a com-

Table 9.8.5.7: *(3+3)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=3: Orthorhombic basic structure.*

Orthorhombic								
30	$mmmP(00\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	31	$mmmP(0\frac{1}{2}\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	32	$mmmP(\frac{1}{2}\frac{1}{2}\gamma, 00\nu, 00\theta)$	$11\bar{1}P$
33	$mmmP(\frac{1}{2}0\gamma, 0\frac{1}{2}\nu, 00\theta)$	$11\bar{1}P$	34	$mmmI(00\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	35	$mmmC(00\gamma, 00\nu, 00\theta)$	$11\bar{1}P$
36	$mmmC(10\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	37	$mmmA(00\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	38	$mmmA(\frac{1}{2}0\gamma, 00\nu, 00\theta)$	$11\bar{1}P$
39	$mmmF(00\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	40	$mmmF(10\gamma, 00\nu, 00\theta)$	$11\bar{1}P$	41	$mmmP(0\beta 0, 00\nu, 00\theta)$	$1m/2P$
42	$mmmP(\frac{1}{2}\beta 0, 00\nu, 00\theta)$	$1m/2P$	43	$mmmP(0\beta\frac{1}{2}, 00\nu, 00\theta)$	$1m/2P$	44	$mmmP(0\beta 0, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$
45	$mmmP(0\beta 0, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$	46	$mmmP(\frac{1}{2}\beta\frac{1}{2}, 00\nu, 00\theta)$	$1m/2P$	47	$mmmP(\frac{1}{2}\beta 0, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$
48	$mmmP(\frac{1}{2}\beta 0, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$	49	$mmmP(0\beta\frac{1}{2}, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$	50	$mmmP(0\beta\frac{1}{2}, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$
51	$mmmP(0\beta 0, \frac{1}{2}\frac{1}{2}\nu, 00\theta)$	$1m/2P$	52	$mmmP(0\beta 0, 0\frac{1}{2}\nu, \frac{1}{2}0\theta)$	$1m/2P$	53	$mmmP(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$
54	$mmmP(\frac{1}{2}\beta\frac{1}{2}, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$	55	$mmmP(\frac{1}{2}\beta 0, \frac{1}{2}\frac{1}{2}\nu, 00\theta)$	$1m/2P$	56	$mmmP(\frac{1}{2}\beta 0, 0\frac{1}{2}\nu, \frac{1}{2}0\theta)$	$1m/2P$
57	$mmmP(0\beta\frac{1}{2}, \frac{1}{2}\frac{1}{2}\nu, 00\theta)$	$1m/2P$	58	$mmmP(0\beta\frac{1}{2}, 0\frac{1}{2}\nu, \frac{1}{2}0\theta)$	$1m/2P$	59	$mmmP(\frac{1}{2}\beta\frac{1}{2}, \frac{1}{2}\frac{1}{2}\nu, 00\theta)$	$1m/2P$
60	$mmmP(\frac{1}{2}\beta\frac{1}{2}, 0\frac{1}{2}\nu, \frac{1}{2}0\theta)$	$1m/2P$	61	$mmmI(0\beta 0, 00\nu, 00\theta)$	$1m/2P$	62	$mmmC(0\beta 0, 00\nu, 00\theta)$	$1m/2P$
63	$mmmC(0\beta\frac{1}{2}, 00\nu, 00\theta)$	$1m/2P$	64	$mmmC(0\beta 0, 10\nu, 00\theta)$	$1m/2P$	65	$mmmC(0\beta\frac{1}{2}, 10\nu, 00\theta)$	$1m/2P$
66	$mmmB(0\beta 0, 00\nu, 00\theta)$	$1m/2P$	67	$mmmB(1\beta 0, 00\nu, 00\theta)$	$1m/2P$	68	$mmmB(0\beta 0, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$
69	$mmmB(1\beta 0, 0\frac{1}{2}\nu, 00\theta)$	$1m/2P$	70	$mmmA(0\beta 0, 00\nu, 00\theta)$	$1m/2P$	71	$mmmA(\frac{1}{2}\beta 0, 00\nu, 00\theta)$	$1m/2P$
72	$mmmA(0\beta 0, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$	73	$mmmA(\frac{1}{2}\beta 0, \frac{1}{2}0\nu, 00\theta)$	$1m/2P$	74	$mmmF(0\beta 0, 00\nu, 00\theta)$	$1m/2P$
75	$mmmF(1\beta 0, 00\nu, 00\theta)$	$1m/2P$	76	$mmmF(0\beta 0, 10\nu, 00\theta)$	$1m/2P$	77	$mmmF(1\beta 0, 10\nu, 00\theta)$	$1m/2P$
78	$mmmP(00\gamma, 0\mu\nu)$	$1m/2A$	79	$mmmP(\frac{1}{2}0\gamma, 0\mu\nu)$	$1m/2A$	80	$mmmP(0\frac{1}{2}\gamma, 0\mu\nu)$	$1m/2A$
81	$mmmP(00\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$	82	$mmmP(\frac{1}{2}\frac{1}{2}\gamma, 0\mu\nu)$	$1m/2A$	83	$mmmP(\frac{1}{2}0\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$
84	$mmmP(0\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$	85	$mmmP(\frac{1}{2}\frac{1}{2}\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$	86	$mmmI(00\gamma, 0\mu\nu)$	$1m/2A$
87	$mmmC(00\gamma, 0\mu\nu)$	$1m/2A$	88	$mmmC(10\gamma, 0\mu\nu)$	$1m/2A$	89	$mmmB(00\gamma, 0\mu\nu)$	$1m/2A$
90	$mmmB(0\frac{1}{2}\gamma, 0\mu\nu)$	$1m/2A$	91	$mmmA(00\gamma, 0\mu\nu)$	$1m/2A$	92	$mmmA(\frac{1}{2}0\gamma, 0\mu\nu)$	$1m/2A$
93	$mmmA(00\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$	94	$mmmA(\frac{1}{2}0\gamma, \frac{1}{2}\mu\nu)$	$1m/2A$	95	$mmmF(00\gamma, 0\mu\nu)$	$1m/2A$
96	$mmmF(10\gamma, 0\mu\nu)$	$1m/2A$	97	$mmmP(\alpha 00, 0\mu 0, 00\theta)$	$mmmP$	98	$mmmP(\alpha\frac{1}{2}0, 0\mu 0, 00\theta)$	$mmmP$
99	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, 0\mu 0, 00\theta)$	$mmmP$	100	$mmmP(\alpha\frac{1}{2}0, \frac{1}{2}\mu 0, 00\theta)$	$mmmP$	101	$mmmP(\alpha\frac{1}{2}0, 0\mu\frac{1}{2}, 00\theta)$	$mmmP$
102	$mmmP(\alpha\frac{1}{2}0, 0\mu 0, 0\frac{1}{2}\theta)$	$mmmP$	103	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu 0, 00\theta)$	$mmmP$	104	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, 0\mu\frac{1}{2}, 00\theta)$	$mmmP$
105	$mmmP(\alpha\frac{1}{2}0, \frac{1}{2}\mu 0, \frac{1}{2}0\theta)$	$mmmP$	106	$mmmP(\alpha\frac{1}{2}0, 0\mu\frac{1}{2}, \frac{1}{2}0\theta)$	$mmmP$	107	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu\frac{1}{2}, 00\theta)$	$mmmP$
108	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu 0, \frac{1}{2}0\theta)$	$mmmP$	109	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu 0, 0\frac{1}{2}\theta)$	$mmmP$	110	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, 0\mu\frac{1}{2}, 0\frac{1}{2}\theta)$	$mmmP$
111	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu\frac{1}{2}, \frac{1}{2}0\theta)$	$mmmP$	112	$mmmP(\alpha\frac{1}{2}\frac{1}{2}, \frac{1}{2}\mu\frac{1}{2}, \frac{1}{2}\frac{1}{2}\theta)$	$mmmP$	113	$mmmI(\alpha 00, 0\mu 0, 00\theta)$	$mmmP$
114	$mmmC(\alpha 00, 0\mu 0, 00\theta)$	$mmmP$	115	$mmmC(\alpha 0\frac{1}{2}, 0\mu 0, 00\theta)$	$mmmP$	116	$mmmC(\alpha 00, 0\mu 0, 01\theta)$	$mmmP$
117	$mmmC(\alpha 0\frac{1}{2}, 0\mu\frac{1}{2}, 00\theta)$	$mmmP$	118	$mmmC(\alpha 0\frac{1}{2}, 0\mu 0, 01\theta)$	$mmmP$	119	$mmmC(\alpha 0\frac{1}{2}, 0\mu\frac{1}{2}, 01\theta)$	$mmmP$
120	$mmmF(\alpha 00, 0\mu 0, 00\theta)$	$mmmP$	121	$mmmF(\alpha 01, 0\mu 0, 00\theta)$	$mmmP$	122	$mmmF(\alpha 01, 0\mu 1, 00\theta)$	$mmmP$
123	$mmmF(\alpha 01, 0\mu 1, 01\theta)$	$mmmP$	124	$mmmP(\alpha\beta 0, 00\gamma)$	$mmmC$	125	$mmmP(\alpha\beta\frac{1}{2}, 00\gamma)$	$mmmC$
126	$mmmP(\alpha\beta 0, 0\frac{1}{2}\gamma)$	$mmmC$	127	$mmmP(\alpha\beta\frac{1}{2}, 0\frac{1}{2}\gamma)$	$mmmC$	128	$mmmP(\alpha\beta 0, \frac{1}{2}\frac{1}{2}\gamma)$	$mmmC$
129	$mmmP(\alpha\beta\frac{1}{2}, \frac{1}{2}\frac{1}{2}\gamma)$	$mmmC$	130	$mmmI(\alpha\beta 0, 00\gamma)$	$mmmC$	131	$mmmC(\alpha\beta 0, 00\gamma)$	$mmmC$
132	$mmmC(\alpha\beta\frac{1}{2}, 00\gamma)$	$mmmC$	133	$mmmC(\alpha\beta 0, 10\gamma)$	$mmmC$	134	$mmmC(\alpha\beta\frac{1}{2}, 10\gamma)$	$mmmC$
135	$mmmC(0\beta\gamma, \alpha 00)$	$mmmC$	136	$mmmC(0\beta\gamma, \alpha 0\frac{1}{2})$	$mmmC$	137	$mmmF(\alpha\beta 0, 00\gamma)$	$mmmC$
138	$mmmF(\alpha\beta 0, 10\gamma)$	$mmmC$	139	$mmmP(0\beta\gamma, \lambda 0\gamma)$	$mmmI$	140	$mmmP(\frac{1}{2}\beta\gamma, \lambda 0\gamma)$	$mmmI$
141	$mmmP(\frac{1}{2}\beta\gamma, \lambda\frac{1}{2}\gamma)$	$mmmI$	142	$mmmP(\frac{1}{2}\beta\gamma, \lambda\frac{1}{2}\gamma+\frac{1}{2})$	$mmmI$	143	$mmmI(0\beta\gamma, \lambda 0\gamma)$	$mmmI$
144	$mmmC(0\beta\gamma, \lambda 0\gamma)$	$mmmI$	145	$mmmC(0\beta\gamma, \lambda 0\gamma+\frac{1}{2})$	$mmmI$	146	$mmmF(0\beta\gamma, \lambda 0\gamma)$	$mmmI$
147	$mmmF(0\beta\gamma, \lambda 0\gamma+1)$	$mmmI$	148	$mmmP(\alpha\beta\gamma)$	$mmmF$	149	$mmmI(\alpha\beta\gamma)$	$mmmF$
150	$mmmC(\alpha\beta\gamma)$	$mmmF$	151	$mmmF(\alpha\beta\gamma)$	$mmmF$			

bination of rotations in mutually perpendicular 2-dimensional spaces. Now the restriction is that the sum over all values of $2\cos(2\pi m_i/n_i)$ is an integer. For example, the direct sum of a rotation over $2\pi/5$ and one over $4\pi/5$ has trace $2(\cos(2\pi/5)+\cos(4\pi/5)) = -1$, which is an integer. Therefore, a five-fold rotation may become crystallographic in 4 dimensions:

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & -1 & -1 & -1 \end{pmatrix}.$$

The same holds for 8-, 10- and 12-fold rotations. In general, the minimal dimension for which an n-fold rotation may be crystallographic is given by the Euler function $\Phi(n)$, which has as value for an integer n the number of integers smaller than n which have no common divisor with n. In this way, all finite orthogonal groups in 2 and 3 dimensions have a crystallographic realisation, and 2- or 3-dimensional invariant subspace, in a space of sufficiently high dimension. Besides the cyclic and dihedral groups for arbitrary n,

Table 9.8.5.8: *(3+3)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=3: Tetragonal basic structure.*

Tetragonal					
152	$4/mP(\alpha\beta 0, 00\theta)$	$4/mP$	153	$4/mP(\alpha\beta\frac{1}{2}, 00\theta)$	$4/mP$
154	$4/mP(\alpha\beta 0, \frac{1}{2}\frac{1}{2}\theta)$	$4/mP$	155	$4/mP(\alpha\beta\frac{\bar{1}}{2}, \frac{1}{2}\frac{1}{2}\theta)$	$4/mP$
156	$4/mI(\alpha\beta 0, 00\theta)$	$4/mP$	157	$4/mP(\alpha\beta\gamma)$	$4/mI$
158	$4/mI(\alpha\beta\gamma)$	$4/mI$	159	$4/mmmP(00\gamma, 00\nu, 00\theta)$	$1\bar{1}11P$
160	$4/mmmP(\frac{1}{2}\frac{1}{2}\gamma, 00\nu, 00\theta)$	$1\bar{1}11P$	161	$4/mmmI(00\gamma, 00\nu, 00\theta)$	$1\bar{1}11P$
162	$4/mmmP(\alpha 00, 00\theta)$	$4/mmmP$	163	$4/mmmP(\alpha\frac{1}{2}0, 00\theta)$	$4/mmmP$
164	$4/mmmP(\alpha 0\frac{1}{2}, 00\theta)$	$4/mmmP$	165	$4/mmmP(\alpha\frac{1}{2}\frac{1}{2}, 00\theta)$	$4/mmmP$
166	$4/mmmP(\alpha 00, \frac{1}{2}\frac{1}{2}\theta)$	$4/mmmP$	167	$4/mmmP(\alpha\frac{\bar{1}}{2}0, \frac{1}{2}\frac{1}{2}\theta)$	$4/mmmP$
168	$4/mmmP(\alpha 0\frac{1}{2}, \frac{\bar{1}}{2}\frac{1}{2}\theta)$	$4/mmmP$	169	$4/mmmP(\alpha\frac{\bar{1}}{2}\frac{1}{2}, \frac{\bar{1}}{2}\frac{1}{2}\theta)$	$4/mmmP$
170	$4/mmmI(\alpha 00, 00\theta)$	$4/mmmP$	171	$4/mmmP(\alpha\alpha 0, 00\theta)$	$4/m\ddot{m}\dot{m}P$
172	$4/mmmP(\alpha\alpha\frac{1}{2}, 00\theta)$	$4/m\ddot{m}\dot{m}P$	173	$4/mmmP(\alpha\alpha 0, \frac{1}{2}\frac{1}{2}\theta)$	$4/m\ddot{m}\dot{m}P$
174	$4/mmmP(\alpha\alpha\frac{\bar{1}}{2}, \frac{1}{2}\frac{1}{2}\theta)$	$4/m\ddot{m}\dot{m}P$	175	$4/mmmI(\alpha\alpha 0, 00\theta)$	$4/m\ddot{m}\dot{m}P$
176	$4/mmmI(\alpha\alpha 1, 00\theta)$	$4/m\ddot{m}\dot{m}P$	177	$4/mmmP(0\beta\gamma)$	$4/mmmI$
178	$4/mmmP(\frac{1}{2}\beta\gamma)$	$4/mmmI$	179	$4/mmmI(0\beta\gamma)$	$4/mmmI$
180	$4/mmmP(\alpha\alpha\gamma)$	$4/m\ddot{m}\dot{m}I$	181	$4/mmmI(\alpha\alpha\gamma)$	$4/m\ddot{m}\dot{m}I$

there is the icosahedral group for which the minimal dimension is 6.

Extension of a crystallographic point group in n dimensions with a lattice group $\mathbb{Z}^n$ leads to the n-dimensional space groups. When the point group has an invariant 2- or 3-dimensional subspace, the space groups are superspace groups. The point groups are (K_E, K_I) with elements (R_E, R_I) and the lattice is $\mathbb{Z}^n$.

As an example, we consider the 3-dimensional group 8mm. This group is the external part of a superspace point group 8mm(8^3mm) with generators:

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \end{pmatrix}; \quad B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

With respect to an orthogonal basis with 2 basis vectors in V_E and 2 in V_I, the matrices for A and B and the 4 basis vectors of the invariant lattice are:

$$A_\perp = \begin{pmatrix} \cos(\frac{\pi}{4}) & \sin(\frac{\pi}{4}) & 0 & 0 \\ -\sin(\frac{\pi}{4}) & \cos(\frac{\pi}{4}) & 0 & 0 \\ 0 & 0 & \cos(\frac{3\pi}{4}) & -\sin(\frac{3\pi}{4}) \\ 0 & 0 & \sin(\frac{3\pi}{4}) & \cos(\frac{3\pi}{4}) \end{pmatrix}; \quad B_\perp = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix};$$

$$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}.$$

Table 9.8.5.9: *(3+3)-dimensional Bravais classes for incommensurate crystal phases with internal dimension d=3: Trigonal and Hexagonal basic structure.*

Trigonal								
182	$\bar{3}P(\alpha\beta\frac{1}{3},00\theta)$	$\bar{3}P$	183	$\bar{3}P(\alpha\beta0,\frac{1}{3}\frac{1}{3}\theta)$	$\bar{3}P$	184	$\bar{3}P(\alpha\beta\frac{1}{3},\frac{1}{3}\frac{1}{3}\theta)$	$\bar{3}P$
185	$\bar{3}R(\alpha\beta0,00\theta)$	$\bar{3}P$	186	$\bar{3}P(\alpha\beta\gamma)$	$\bar{3}R$	187	$\bar{3}R(\alpha\beta\gamma)$	$\bar{3}R$
188	$\bar{3}1mP(\frac{1}{3}\frac{1}{3}\gamma,00\nu,00\theta)$	$\bar{1}11P$	189	$\bar{3}mR(00\gamma,00\nu,00\theta)$	$\bar{1}1P$	190	$\bar{3}1mP(\alpha00,\frac{1}{3}\frac{1}{3}\nu)$	$\bar{3}1mP$
191	$\bar{3}m1P(\alpha0\frac{1}{3},00\nu)$	$\bar{3}m1P$	192	$\bar{3}mR(\alpha00,00\nu)$	$\bar{3}\dot{m}P$	193	$\bar{3}1mP(\alpha\alpha\frac{1}{3},00\nu)$	$\bar{3}1\dot{m}P$
194	$\bar{3}1mP(\alpha\alpha0,\frac{1}{3}\frac{1}{3}\nu)$	$\bar{3}1\dot{m}P$	195	$\bar{3}1mP(\alpha\alpha\frac{1}{3},\frac{1}{3}\frac{1}{3}\nu)$	$\bar{3}1\dot{m}P$	196	$\bar{3}mR(\alpha\alpha0,00\nu)$	$\bar{3}\ddot{m}P$
197	$\bar{3}1mP(\alpha\alpha\gamma)$	$\bar{3}1mR$	198	$\bar{3}m1P(\alpha0\gamma)$	$\bar{3}m1R$	199	$\bar{3}mR(\alpha0\gamma)$	$\bar{3}mR$
Hexagonal								
200	$6/mP(\alpha\beta\gamma)$	$6/mP$	201	$6/mmmP(00\gamma,00\nu,00\theta)$	$1\bar{1}11P$	202	$6/mmmP(\alpha0\gamma)$	$6/mmmP$
203	$6/mmmP(\alpha\alpha\gamma)$	$6/m\ddot{m}\dot{m}P$						

Table 9.8.5.10: *(3+3)-dimensionale Bravais classes for incommensurate crystal phases with internal dimension d=3: Cubic basic structure.*

Cubic								
204	$m\bar{3}P(\alpha\frac{1}{2}0)$	$m\bar{3}P$	205	$m\bar{3}F(\alpha10)$	$m\bar{3}P$	206	$m\bar{3}P(\frac{1}{2}\beta\beta+\frac{1}{2})$	$m\bar{3}I$
207	$m\bar{3}F(0\beta\beta+1)$	$m\bar{3}I$	208	$m\bar{3}mP(\alpha00)$	$m\bar{3}mP$	209	$m\bar{3}mP(\alpha\frac{1}{2}\frac{1}{2})$	$m\bar{3}mP$
210	$m\bar{3}mI(\alpha00)$	$m\bar{3}mP$	211	$m\bar{3}mF(\alpha00)$	$m\bar{3}mP$	212	$m\bar{3}mP(0\beta\beta)$	$m\bar{3}mI$
213	$m\bar{3}mI(0\beta\beta)$	$m\bar{3}mI$	214	$m\bar{3}mF(0\beta\beta)$	$m\bar{3}mI$	215	$m\bar{3}mP(\alpha\alpha\alpha)$	$m\bar{3}mF$
216	$m\bar{3}mI(\alpha\alpha\alpha)$	$m\bar{3}mF$	217	$m\bar{3}mF(\alpha\alpha\alpha)$	$m\bar{3}mF$			

For the arithmetic point group generated by A and B there are 2 superspace groups, one symmorphic and one non-symmorphic. The generators of the latter are (in lattice coordinates):

$$\left\{\left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \end{array}\right)\middle|\left(\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \end{array}\right)\right\},\quad \left\{\left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \end{array}\right)\middle|\left(\begin{array}{c} \frac{1}{2} \\ 0 \\ 0 \\ 0 \end{array}\right)\right\}$$

The symbols for these two superspace groups are P8mm(8^3mm) and P8am(8^3mm).

The Bravais classes of the 5- and 6-dimensional Bravais classes relevant for quasicrystals are given in Table 9.8.5.11. The superspace groups for the icosahedral, pentagonal, and decagonal families are in given in Tables 9.8.5.12 and 9.8.5.13. For the octagonal and dodecagonal groups see (Janssen, 1988).

9.8.5.5. The incommensurate versus the commensurate case

As said earlier, it sometimes makes sense to use the description as developed for incommensurate crystal phases for a (commensurate) superstructure. In fact, very often the modulation wavevector also shows in addition to continuously varying (incommensurate)

Table 9.8.5.11: *A selection of 5- and 6-dimensional Bravais classes for quasicrystals.* In each second line a basis of the reciprocal lattice Σ^* is given.

System	Centering	K_E	K_I	Condition	Symbol
Pentagonal	P	$\bar{5}$m	$\bar{5}$m	None	$\bar{5}$m($\bar{5}^3$)R
					$(a\cos[2\pi j/5], a\sin[2\pi j/5], b)$, $j = 0, \ldots, 4$
Decagonal	P	10/mmm	10/mmm	None	10/mmm(10^3/mmm)P
					$(a\cos[2\pi j/5], a\sin[2\pi j/5], 0), (0, 0, b)$ $j = 1, \ldots, 4$
Octagonal	P	8/mmm	8/mmm	None	8/mmm(8^3/mmm)P
					$(a\cos[2\pi j/8], a\sin[2\pi j/8], 0), (0, 0, b)$ $j = 0, \ldots, 3$
Octagonal	I	8/mmm	8/mmm	$\sum_i h_i$=2n	8/mmm(8^3/mmm)I
					$(a\cos[2\pi j/8], a\sin[2\pi j/8], b)$ $j = 0, \ldots, 4$
Dodecagonal	P	12/mmm	12/mmm	None	12/mmm(12^5/mmm)P
					$(a\cos[2\pi j/12], a\sin[2\pi j/12], 0), (0, 0, b)$ $j = 0, \ldots, 4$
Icosahedral	P	$\bar{5}\bar{3}$m	$\bar{5}\bar{3}$m	None	$\bar{5}\bar{3}$m($\bar{5}\bar{3}$m)P
					$a(\tau 10)$, $a(-\tau 10)$, $a(0\tau 1)$, $a(0\tau\text{-}1)$, $a(10\tau)$, $a(-10\tau)$
Icosahedral	I	$\bar{5}\bar{3}$m	$\bar{5}\bar{3}$m	$\sum_i h_i = 2n$	$\bar{5}\bar{3}$m($\bar{5}\bar{3}$m)I
					$a(\tau 10)$, $a(-\tau 10)$, $a(0\tau 1)$, $a(0\tau\text{-}1)$, $a(10\tau)$, $a(-10\tau)$
Icosahedral	F	$\bar{5}\bar{3}$m	$\bar{5}\bar{3}$m	$h_i + h_j$=2n	$\bar{5}\bar{3}$m($\bar{5}\bar{3}$m)F
					$a(\tau 10)$, $a(-\tau 10)$, $a(0\tau 1)$, $a(0\tau\text{-}1)$, $a(10\tau)$, $a(-10\tau)$

values, several rational values at various phase transitions of a given crystal or in different compounds of a given structural family. In these cases, there is a three-dimensional space-group symmetry. Generally, the space groups of the various phases are different. The description as used for incommensurate phases then gives the possibility of a more unified characterization for the symmetry of related modulated crystal phases. In fact, the theory of higher-dimensional space groups for modulated structures is largely independent of the assumption of irrationality. Only some of the statements need to be adapted. The most important change is that there is no longer a one-to-one correspondence between the points of the reciprocal lattice Σ^* and its projection on V defining the positions of the Bragg peaks. Furthermore, the projection of the lattice Σ on the space V_I forms a discrete set. The latter means the following. For an incommensurate modulation, the incommensurate structure, which is the intersection of a periodic structure with the hyperplane $\mathbf{r}_I$=0, is also the intersection of the same periodic structure with a hyperplane $\mathbf{r}_I$=constant, where this constant is of the form

$$\sum_{i=1}^{3} h_i \mathbf{a}_{Ii} + \sum_{j=1}^{d} m_j \mathbf{a}_{I3+j}. \tag{9.8.5.16}$$

Because for an incommensurate structure these vectors form a dense set in V_I, the phase of the modulation function with respect to the basic structure is not determined. For a commensurate modulation, however, the points (9.8.5.16) form a discrete set, even belong to a lattice, and the phase (or the phases) of the modulation are determined within vectors of this lattice. Notice that the grid of this lattice becomes finer as the denominators in the rational components become larger.

When G_s is a (3+d)-dimensional superspace group, its elements, in general, do not leave the physical space V invariant. The subgroup of all elements that do leave V invariant, when restricted to V, is a group of distance-preserving transformations in three dimensions and thus a subgroup of $E(3)$, the three-dimensional Euclidean group. In general, this subgroup is not a three-dimensional space group. It is so when the modulation wavevectors all have rational components only, *i.e.* when σ is a matrix with rational entries. Because the phase of the modulation function is now determined (within a given rational number smaller than 1), the space group depends in general on this phase. As an example, consider a one-dimensional modulation of a basic structure with orthorhombic space group $Pcmn$. Suppose that the modulation wavevector is $\gamma\mathbf{c}^*$. then the mirror $R = m_z$ perpendicular to the c axis is combined with $R_I = \epsilon = -1$. Suppose, furthermore, that the glide reflection perpendicular to the a axis and the b mirror are both combined with a phase shift $\frac{1}{2}$. In terms of the coordinates x, y, z with respect to the a, b, and c axes, and internal coordinate t, the generators of the (3+1)-dimensional superspace group $Pcmn(00\gamma)ss0$ act as

$$\begin{aligned}
&(a)\ (x,y,z,t) &&\rightarrow\ (x+k, y+\ell, z+m, t-\gamma m+n), \\
&(b)\ (x,y,z,t) &&\rightarrow\ (-x+k+\frac{1}{2}, y+\ell, z+\frac{1}{2}+m, t-\gamma/2-\gamma m+\frac{1}{2}+n), \\
&(c)\ (x,y,z,t) &&\rightarrow\ (x+k, -y+\ell+\frac{1}{2}, z+m, t-\gamma m+\frac{1}{2}+n),
\end{aligned} \tag{9.8.5.17}$$

$$(d)\ (x,y,z,t) \ \rightarrow \ (x+\frac{1}{2}+k, y+\frac{1}{2}+\ell, -z+\frac{1}{2}+m, -t-\gamma/2-\gamma m+n),$$
$$k,\ell,m,n \text{ integers.}$$

Note that these positions are referred to a split basis (*i.e.* of basis vectors lying either in V or in V_I) and not to a basis of the lattice Σ. When the superstructure is the intersection of a periodic structure with the plane $t = t_0$, its three-dimensional space group follows from equation (9.8.5.17) by the requirement $t' = t_0$. When γ has the rational value r/s with r and s relatively prime, the conditions for each of the generators to give an element of the three-dimensional space group are, respectively:

$$\begin{aligned} -rm+sn &= 0 \qquad (a)\\ -2rm+2sn &= r-s \qquad (b)\\ -2rm+2sn &= -s \qquad (c)\\ -2rm+2sn &= 4st, \qquad (d) \end{aligned} \qquad (9.8.5.18)$$

for m, n, r, s integers and t real. These conditions are never satisfied simultaneously. It depends on the parity of both r and s which element occurs, and for the elements with $\epsilon = -1$ it also depends on the value of the 'phase' t, or more precisely on the product $\phi = 4st$. The translation group is determined by the first condition as in 9.8.5.18(a). Its generators are **a**, **b** and s**c**, where the last vector is the external part of the lattice vector s(**c**,$-r/s$)+r(0,1). The other space-group elements can be derived in the same way. The possible space groups are:

$\gamma = r/s$	ϕ even integer	ϕ odd integer	otherwise
r even, s odd	$11\frac{2_1}{n}$	$2_12_12_1$	112_1
r odd, s even	$1\frac{2_1}{c}1$	2_1cn	$1c1$
r odd, s odd	$\frac{2_1}{c}11$	$c2_1n$	$c11$

In general, the three-dimensional space groups compatible with a given (3+d)-dimensional superspace group can be determined using analogous equations.

As one can see from the table above, the orthorhombic (3+d)-dimensional superspace group leads in several cases to monoclinic three-dimensional space groups. The lattice of main reflections, however, still has orthorhombic point-group symmetry. Description in the conventional way by means of three-dimensional groups then neglects some of the structural features present. Even if the orthorhombic symmetry is slightly broken, the orthorhombic basic structure is a better characterization than a monoclinic one. In that case the superspace-group symmetry is also only an approximation.

When the denominators of the wavevector components become small, additional symmetry operations become possible. Because the one-to-one correspondence between Σ^* and M^* is no longer present, there may occur symmetry elements with trivial action in V but with nontrivial transformation in V_I. For $d = 1$, these possibilities are given in Table 9.8.3.5.

A. Glossary of symbols

M^*	Vector module in m-dimensional reciprocal space (m=1,2,3; normally m=3), isomorphic to $\mathbb{Z}^n$ with $n \geq m$. The dimension of M^* is m, its rank n.
$\mathbf{a}_i^*$	$(i = 1, \ldots, n)$ Basis of a vector module (or Fourier module) M^* of rank n; if $n = 4$ and $\mathbf{q}$ is a modulation wavevector, the basis of M^* is chosen as $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, $\mathbf{q}$, with the first three a basis of the lattice of main reflections.
Λ^*	Lattice of main reflections, m-dimensional reciprocal lattice.
$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$	(Conventional) basis of Λ^* for $m = 3$.
Λ	Direct m-dimensional lattice, dual to Λ^*.
V_s	Superspace; Euclidean space of dimension $n = m+d$; $V_s = V_E \oplus V_I$.
V	Physical or external space of dimension m (=1,2,3), also denoted as V_E.
V_I	Internal or perpendicular space of dimension d.
Σ^*	Reciprocal lattice in n-dimensional space, whose orthogonal projection on V_E is M^*.
Σ	Lattice in n-dimensional space for which Σ^* is the reciprocal.
a_{si}^*	Lattice basis of Σ^* in V_s $(i = 1, \ldots, n)$; if $n = 4$ and the crystal is modulated, this basis can be chosen as ($\mathbf{a}^*$,0), ($\mathbf{b}^*$,0), ($\mathbf{c}^*$,0), ($\mathbf{q}$,1) and is called standard. An equivalent notation is ($\mathbf{q}$,1)=($\mathbf{q}$,$\mathbf{d}^*$); for $n = 3 + d$, the general form of a standard basis is ($\mathbf{a}^*$,0), ($\mathbf{b}^*$,0),($\mathbf{c}^*$,0), ($\mathbf{q}_1$,$\mathbf{d}_1^*$),. . .,($\mathbf{q}_d$,$\mathbf{d}_d^*$).
a_{si}	$(i = 1, \ldots, n)$ Lattice basis of Σ in V_s dual to $\{a_{si}^*\}$; if $n = 4$, the standard basis is ($\mathbf{a}$, -$\mathbf{q}$.$\mathbf{a}$), ($\mathbf{b}$, -$\mathbf{q}$.$\mathbf{b}$), ($\mathbf{c}$, -$\mathbf{q}$.$\mathbf{c}$), (0,1)=(0,$\mathbf{d}$); for $n = 3 + d$, a standard basis is dual to the standard basis given above.
$\mathbf{q}_j$	Modulation wavevectors $\mathbf{q}_j = \sum_{i=1}^{3} \sigma_{ji} \mathbf{a}_i^*$; if $n = 4$, $\mathbf{q}$=$\alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$; $\sigma = (\alpha, \beta, \gamma)$; if $n = 4$, $\mathbf{q}$=$\mathbf{q}^i$+$\mathbf{q}^r$, with $\mathbf{q}^i$=$(1/N) \sum_R \epsilon(R) R\mathbf{q}$, where $\epsilon(R) = \pm 1$, and N is the order of K.
$\mathbf{H}$	Bragg reflections: $\mathbf{H}$=$\sum_i h_i \mathbf{a}_i^* = (h_1, \ldots, h_n)$; when $n = 4$, $\mathbf{H}$=$h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^* + m\mathbf{q}$.
H_s	Embedding of $\mathbf{H}$ in V_s: for $\mathbf{H}$=$\sum_i h_i \mathbf{a}_i^*$ one has $H_s = \sum_i h_i a_{si}^*$.
P_L	Laue point group.
$O(m)$	Orthogonal group in m dimensions.
R	Orthogonal point-group transformation.
K	Point group, crystallographic subgroup of $O(m)$.
R_s	Point-group element in superspace: $R_s = (R, R_I)$. For $n = 4$, $R_I = \pm 1$.
K_s	Point group, crystallographic subgroup of $O(m) \times O(d)$.
K_E	External part of K_s.

K_I	Internal part of K_s.
$\mathbf{r}_0(\mathbf{n},j)$	Atomic position in the basic structure: $\mathbf{n}+\mathbf{r}_j$.
$\mathbf{r}(\mathbf{n},j)$	Atomic position in displacively modulated structure.
$\mathbf{u}_j(x)$	Modulation function, with $\mathbf{u}_j(x)=\mathbf{u}_j(x+1)$.
$p_j(x)$	Modulation function for occupation modulation.
g	Euclidean transformation in m dimensional physical space: $g = \{R\|\mathbf{v}\}$.
g_s	Superspace-group transformation: $(\{R\|\mathbf{v}\},\{R_I\|\mathbf{v}_I\})$.
$\mathbf{v}^0$	Intrinsic (origin independent) translation part.
$\mathbf{v}_I$	Internal shift, for $d=1$: $v_I = \Delta = \delta$-$\mathbf{q}.\mathbf{v}$.
v_4^0	Intrinsic internal shift for $d=1$: $v_4^0 = \delta - \mathbf{q}^r.\mathbf{v}$.
$\Gamma^*(R)$	Point group transformation with respect to the basis of M^*.
$\Gamma(R)$	Rotational part of a superspace-group transformation, with respect to a basis of Σ.
$\Gamma_E(R)$	External part of $\Gamma(R)$ (for modulated crystals).
$\Gamma_I(R)$	Internal part of $\Gamma(R)$ (for modulated crystals).
$\Gamma_M(R)$	Mixed part of $\Gamma(R)$ (for modulated crystals).
$S_{\mathbf{H}}$	Structure factor.
$f_j(\mathbf{H})$	Atomic scattering factor for atom j.

B. Basic definitions

[i] *Vector module*, $\mathbb{Z}$*-module* or *Fourier module*. A vector module is the set of all integral linear combinations of a finite number of vectors in a vector space. The *dimension* of the module is the dimension (m) of the subspace generated by it over the real numbers. Its *rank* (n) is the minimal number of rationally independent vectors that generate the module. If this rank is equal to the dimension, the module is also a lattice. The term *Fourier module* is used for the vector module in reciprocal space generated by the wave vectors of the Fourier transform of a crystallographic structure. A reciprocal lattice is a special case of a Fourier module, for which $n = m$. Both vector and Fourier modules are special cases of a free Abelian $\mathbb{Z}$-module, an abelian group without elements of finite order (except the identity) on which the ring $\mathbb{Z}$ of integers acts associatively and distributively. For modulated structures the Fourier module is spanned by the m basis vectors of the basic structure, and $d = n - m$ modulation wave vectors. d is called the *dimension of the modulation*.

[ii] *Superspace.* A superspace V_s is an n-dimensional Euclidean space that is the direct sum $V_E \oplus V_I$ of an m-dimensional *external* or *physical space* V_E and a d-dimensional *internal space* V_I. V_E is also denoted by V.

[iii] *Split basis.* For the space $V_s = V_E \oplus V_I$, this is a basis with m basis vectors in V_E and $d = n - m$ basis vectors in V_I.

[iv] *Standard basis.* A standard basis for (the direct space) V_s is one having the last d basis vectors lying in V_I, where d is the dimension of V_I. A standard basis in reciprocal space is one with the first m basis vectors lying in V_E. For a modulated phase the lattice basis may be chosen as a standard basis.

[v] *Conventional basis.* For a lattice Λ, it is a basis such that (i) the lattice generated by it is contained in Λ as a sublattice and (ii) there is the standard relationship between the basis vectors (*e.g.* for a cubic lattice a conventional basis consists of three mutually perpendicular vectors of the same length).
The lattice Λ is obtained from the lattice spanned by the conventional basis by adding *centring vectors*. [For example, the bcc lattice is obtained from the conventional cubic lattice by centring the unit cell with $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$.]
The reciprocal basis for the conventional basis is a conventional basis for a reciprocal lattice Λ^*.
For $(m + d)$-dimensional modulated structures, a conventional basis for the lattice Σ satisfies the same conditions (i) and (ii) as formulated above. In addition, however, one requires that the basis is standard and such that the non-vanishing external components satisfy the relations of an (m=3) conventional basis and that the corresponding internal components only involve the irrational components of the modulation wavevector(s). Again a conventional basis for Σ^* is dual to the same for Σ.

[vi] *Holohedry.* The holohedry of a vector module in m dimensions is the subgroup of $O(m)$ (the orthogonal transformations of the same dimension) that leaves the vector module invariant.
The holohedry of an (m+d)-dimensional lattice is the subgroup of $O(m)\times O(d)$ that leaves the lattice invariant.

[vii] *Point group.* An $(m+d)$-dimensional crystallographic point group $K_s = (K_E, K_I)$ is a subgroup of $O(m)\times O(d)$. With respect to a standard lattice basis (in the case of a modulated crystal) its elements $R_s = (R, R_I)$ are of the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix},$$

where all the entries are integers and R is an element of an m-dimensional point group K, which is actually the same as K_E. For an incommensurate modulated crystal, K_s and K are isomorphic groups. If d=1, then $\Gamma_I(R) = \epsilon(R) = \pm 1$.

[viii] *Geometric crystal class.* Two point groups $K_s = (K_E, K_I)$ and $K'_s = (K'_E, K'_I)$ of pairs (R_E, R_I) of orthogonal transformations are geometrically equivalent if and only if there are orthogonal transformations T_E and T_I of $O(m)$ and $O(d)$, respectively, such that $R'_E{=}T_E.R_E.T_E^{-1}$ and $R'_I{=}T_I.R_I.T_I^{-1}$ for some group homomorphism $(R_E, R_I) \rightarrow (R'_E, R'_I)$. For d=1, that condition takes a simpler form because $R_I = \epsilon = \pm 1$. Then $R_I = R'_I$ for corresponding group elements.

[ix] *Arithmetic crystal class.* A group of integral matrices $\Gamma(R)^*$ [for $R \in K$ of $O(m)$] is determined on a basis $\{\mathbf{a}_i^*; i = 1, \ldots, n\} = \mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, $\mathbf{q}_1, \ldots \mathbf{q}_d$ of a vector module in reciprocal space by an m-dimensional point group K (here $m = 3$).
For modulated crystals, the transformations in direct space are given by matrices $\Gamma(R)$ = transpose of $\Gamma^*(R^{-1})$ which are of the form 9.8.4.19. Two groups are arithmetically equivalent if and only if there is a non-singular $(m + d)$-dimensional matrix S of the form

$$S = \begin{pmatrix} S_E & 0 \\ S_M & S_I \end{pmatrix}$$

with integral entries such that $\Gamma'(K') = S\Gamma(K)S^{-1}$. Here, S_E is $m \times m$ and S_I is $d \times d$-dimensional.
An alternative formulation is: The matrix groups $\Gamma(K)$ and $\Gamma'(K')$ are arithmetically equivalent if
(a) the groups K and K' are geometrically equivalent m-dimensional point groups [the corresponding $(m + d)$-dimensional groups K_s and K'_s are then also geometrically equivalent];
(b) there are vector module bases $\mathbf{a}^*, \ldots, \mathbf{q}_d$ and $\mathbf{a}^* \ldots, \mathbf{q}'_d$ such that K on the first basis gives the same group of matrices as K' on the second basis.
Two general $(m + d)$-dimensional arithmetic point groups (i.e. not in standard form) are equivalent if they are conjugated in $\mathrm{GL}(n, \mathbb{Z})$ by an element R of the form $S_1 T S_2^{-1}$ where S_1 and S_2 bring the point group on standard form, and $T = T_E \oplus T_I$ leaves V_E and V_I invariant.

[x] *Bravais class.* Two vector modules are in the same Bravais class if the groups of matrices determined by their holohedries are arithmetically equivalent. Two $(m + d)$-dimensional lattices are in the same Bravais class if their (arithmetic) holohedries are arithmetically equivalent. In both cases, one can find bases for the two structures such that the holohedries take the same matrix form. In the $(m + d)$-dimensional case of modulated crystals, the lattice bases both have to be standard.

[xi] *Superspace group.* An $(m + d)$-dimensional superspace group is an n-dimensional space group ($n = m + d$) such that its point group leaves an m-dimensional subspace invariant.
It is determined on a lattice basis by the matrices $\Gamma(R)$ of the point-group transformations and by the components $v_i(R)$ $(i = 1, \ldots, n)$ of the translational parts of its elements. The matrices $\Gamma(R)$ represent at the same time the elements R of the m-dimensional point group K and the corresponding elements R_s of the n-dimensional point groups K_s.
Two $(m + d)$-dimensional superspace groups are equivalent if there is an origin and a lattice basis for each group such that the collection $\{\Gamma(R), v_s(R)\}$ is the same for both groups, under the condition that the corresponding basis transformation leaves V_E invariant.

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Table 9.8.5.12: *6-dimensional superspace groups for icosahedral crystals.*

Short Symbol	Long Symbol	Generators	Conditions
P532	P532($5^2$32)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$	None
P$5_1$32	P$5_1$32($5^2$32)	$(x + \frac{1}{5}, z, u + \frac{1}{5}, v, w, y - \frac{1}{5})$ $(w, x, v, \bar{z}, \bar{u}, y)$	$h_1h_2h_2h_2h_2h_2 : h_1 = 5n$
P$\bar{5}\bar{3}$m	P$\bar{5}\bar{3}$m($\bar{5}^2\bar{3}$m)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$ $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}, \bar{w})$	None
P$\bar{5}\bar{3}$d	P$\bar{5}\bar{3}$d($\bar{5}^2\bar{3}$m)	$(x, z + \frac{1}{2}, u + \frac{1}{2}, v + \frac{1}{2}, w + \frac{1}{2}, y)$ $(w, x, v, \bar{z}, \bar{u}, y)$ $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}, \bar{w})$	$h_1h_2h_3\bar{h}_3h_2h_1 : h_2$=even
I532	I532($5^2$32)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$	$\sum h_i =$ even
I$5_1$32	I$5_1$32($5^2$32)	$(x + \frac{1}{5}, z + \frac{1}{5}, u - \frac{1}{5}, v + \frac{2}{5}, w - \frac{1}{5}, y - \frac{1}{5})$ $(w, x, v, \bar{z}, \bar{u}, y)$	$\sum h_i =$ even $h_1h_2h_2h_2h_2h_2 : h_1$=5n
I$\bar{5}\bar{3}$m	I$\bar{5}\bar{3}$m($\bar{5}^2\bar{3}$m)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$ $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}, \bar{w})$	$\sum h_i =$ even
F532	F532($5^2$32)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$	$h_i + h_j =$ even
F$5_1$32	F$5_1$32($5^2$32)	$(x, z + \frac{1}{2}, u + \frac{1}{2}, v + \frac{1}{2}, w + \frac{1}{2}, y)$ $(w, x, v, \bar{z}, \bar{u}, y)$	$h_i + h_j =$ even $h_1h_2h_2h_2h_2h_2 : h_1$=5n
F$\bar{5}\bar{3}$m	F$\bar{5}\bar{3}$m($\bar{5}^2\bar{3}$m)	(x, z, u, v, w, y) $(w, x, v, \bar{z}, \bar{u}, y)$ $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}, \bar{w})$	$h_i + h_j =$ even
F$\bar{5}\bar{3}$d	F$\bar{5}\bar{3}$d($\bar{5}^2\bar{3}$m)	$(x, z + \frac{1}{4}, u, v, w + \frac{1}{4}, y + \frac{1}{2})$ $(w, x, v, \bar{z}, \bar{u}, y)$ $(\bar{x}, \bar{y}, \bar{z}, \bar{u}, \bar{v}, \bar{w})$	$h_i + h_j =$ even $h_1h_2h_3\bar{h}_3h_2h_1 : h_2$=even

Table 9.8.5.13: *5-dimensional superspace groups for pentagonal and decagonal quasicrystals.*

Short Symbol	Long Symbol	Conditions	Short Symbol	Long Symbol	Conditions
R5	R5(5^2)	None	R5m	R5m(5^2m)	None
R5a	R5a(5^2m)	$h_1h_2h_3h_3h_2$: h_1=even	R52	R52(5^2m)	None
R$\bar{5}$	R$\bar{5}$(10))	None	R$\bar{5}$m	R$\bar{5}$m(10m)	None
R$\bar{5}$a	R$\bar{5}$a(10m)	$h_1h_2h_3h_3h_2$: h_1=even			
P5	P5(5^2)	None	P5_1	P5_1(5^2)	$h_1 0000$: h_1=$5n$
P5_2	P5_2(5^2)	$h_1 0000$: h_1=$5n$	P5m	P5m(5^2m)	None
P5a	P5a(5^2m)	$h_1h_2h_3h_3h_2$: h_1=$2n$	P51m	P51m($5^2$1m)	None
P51a	P51a($5^2$1m)	$h_1h_2h_3h_3h_2$: h_1=$2n$	P521	P521(5^2m1)	None
P$5_1$21	P$5_1$21(5^2m1)	$h_1 0000$: h_1=$5n$	P$5_2$21	P$5_2$21(5^2m1)	$h_1 0000$: h_1=$5n$
P$\bar{5}$	P$\bar{5}$(10)	None	P$\bar{5}$m1	P$\bar{5}$m1(10m1)	None
P$\bar{5}$a1	P$\bar{5}$a1(10m1)	$h_1h_2h_3h_3h_2$: h_1=even	P$\bar{5}$1m	P$\bar{5}$1m(10 1m)	$h_1h_2h_3h_3h_2$: h_1=even
P$\bar{5}$1a	P$\bar{5}$1a(10 1m)	$h_1h_2h_3h_3h_2$: h_1=even	P10	P10(10^3)	None
P10_1	P10_1(10^3)	$h_1 0000$:h_1=$10n$	P10_2	P10_2(10^3)	$h_1 0000$:h_1=$5n$
P10_3	P10_3(10^3)	$h_1 0000$:h_1=$10n$	P10_4	P10_4(10^3)	$h_1 0000$:h_1=$5n$
P10_5	P10_5(10^3)	$h_1 0000$:h_1=$2n$	P$\overline{10}$	P$\overline{10}$(5)	None
P10/m	P10/m($10^3$1)	None	P10_5/m	P10_5($10^3$1)	$h_1 0000$:h_1 = $2n$
P10mm	P10mm(10^3mm)	None	P10_5ma	P10_5ma(10^3mm)	$h_1 0000$: $h_1$even
P10aa	P10aa(10^3mm)	$h_1h_2h_3h_3h_2$: h_1=even	P10_5am	P10_5ma(10^3mm)	$h_1 0000$: h_1=even
P10 22	P10 22(10^3mm)	None	P$10_1$22	P10_1 22(10^3mm)	$h_1 0000$: h_1=$10n$
P$10_2$22	P10_2 22(10^3mm)	$h_1 0000$: h_1=$5n$	P$10_3$22	P10_3 22(10^3mm)	$h_1 0000$: h_1=$10n$
P$10_4$22	P10_4 22(10^3mm)	$h_1 0000$: h_1=$5n$	P$10_5$22	P10_5 22(10^3mm)	$h_1 0000$: h_1=$2n$
P$\overline{10}$2m	P$\overline{10}$2m(5mm)	None	P$\overline{10}$2a	P$\overline{10}$2a(5mm)	$h_1h_2h_3h_3h_2$: h_1=even
P$\overline{10}$m2	P$\overline{10}$m2(5mm)	None	P$\overline{10}$a2	P$\overline{10}$a2(5mm)	$h_1h_2h_3h_3h_2$: h_1=even
P10/mmm	P10/mmm($10^3$1mm)	None	P10_5/ama	P10_5/ama($10^3$1mm)	$h_1 0000$: h_1=even $0h_2h_3h_4h_5$:sum=even
P10/maa	P10/maa($10^3$1mm)	$h_1h_2h_3h_4h_5$: h_1=even	P10_5/aam	P10_5/aam(10^3mm)	$h_1h_2h_3h_3h_2$: h_1=even