This results in a change for τ. For example, the $(3+1)$-dimensional space group $Pmmm(\frac{1}{2}0\gamma)000 = A^{Pmmm}_{1\,1\,\bar{1}}$ has a mirror perpendicular to the a axis with associated value $\tau = 0$. The parallel mirror at a distance $a/2$ has $\mathbf{v} = \mathbf{a}$ and consequently $\tau = \frac{1}{2}$. 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.

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 $I2cb(00\gamma)0s0 = P^{I2cb}_{\bar{1}s\bar{1}}$ are $h+k+l =$ even because of the centring and $l+m =$ even and $h+m =$ even for $h0lm$ because of the two glide planes perpendicular to the b axis. When one takes for the modulation vector $\mathbf{q} = \gamma'\mathbf{c}^* = (1-\gamma)\mathbf{c}^*$, the new indices are h, k, l', and m' with $l' = l+m$ and $m' = -m$. Then the reflection conditions become $l' =$ even and $h+m =$ even for $h0l'm'$. The first of these conditions implies the symbol $I2cb(00\gamma)000 = P^{I2cb}_{\bar{1}\,1\,\bar{1}}$ for the group considered. This, however, is the symbol for the nonequivalent group with condition $h =$ even for $h0lm$. This difficulty may be avoided by sometimes using 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 periodic crystal structure is defined in a three-dimensional Euclidean space V and is invariant with respect to 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 translations are linearly independent and span a lattice Λ. The *dimension* of Λ is the dimension of the space spanned by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and the *rank* is the (smallest) number of free generators of those integral linear combinations. In the present case, both are equal to three. Accordingly,

$$\{\Lambda\} = V \quad \text{and} \quad \Lambda \approx Z^3. \tag{9.8.4.2}$$

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

$$\mathbf{a}_i \cdot \mathbf{a}_k^* = \delta_{ik}.$$

The two corresponding metric tensors g and g^*,

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

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.

A crystal is *incommensurate* when $d > 0$ and the vectors $\mathbf{a}_i^*$ linearly independent over the rational numbers. In that case, the crystal does not have lattice periodicity and is said to be *aperiodic*. The above description can still be convenient, even in the case that the vectors $\mathbf{a}_i^*$ are not independent over the rationals: one or more of them is then expressed as rational linear combinations of the others. 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 $\mathbf{a}_1^*, \ldots, \mathbf{a}_n^*$. These are said to form a *basis*. It is a set of free Abelian generators, therefore the *rank* of M^* is n. The *dimension* of M^* is the dimension of the Euclidean space spanned by M^*

$$\{M^*\} = V \quad \text{and} \quad M^* \approx Z^n. \tag{9.8.4.6}$$

The elements of Z^n are precisely the set of indices introduced above. Mathematically speaking, M^* has the structure of a (free Abelian) module. Its elements are vectors. So we call M^* a *vector module*. This nomenclature is intended as a *generic* characterization. When a series of structures is considered with different values of the components of the last d vectors with respect to the first three, the generic values of these components are irrational, but accidentally they may become rational as well. This situation typically arises when considering crystal structures under continuous variation of parameters like temperature, pressure or chemical composition. In the case of an ordinary crystal, rank and dimension are equal, the crystal structure is *periodic*, and the vector module becomes a (reciprocal) lattice.

Lattices and vector modules are, mathematically speaking, free 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 is no longer possible. It is possible to keep the metrical duality by enlarging the space and considering the vector module M^* as the projection of an n-dimensional (reciprocal) lattice Σ^* in an n-dimensional Euclidean space V_s.

$$M^* \rightarrow \Sigma^*, \quad \{\Sigma^*\} = V_s \quad \text{and} \quad \Sigma^* \approx Z^n, \tag{9.8.4.7}$$

with the orthogonal projection π_E of V_s onto V defined by

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

This corresponds to attaching to the diffraction peak with indices $(h_1, \ldots, h_n)$ the point of an n-dimensional reciprocal lattice having the same set of coordinates. The orthocomplement of V in V_s is called internal space and denoted by V_I. The embedding is uniquely defined by the relations

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

where $\{a_{si}^*\}$ is a basis of Σ^* and $\{\mathbf{a}_i^*\}$ a basis of 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 coefficients $\hat{\rho}$ at points of M^* and of Σ^* having correspondingly the same components.

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

Then ρ_s is invariant with respect to translations of the lattice Σ with basis

$$a_{si} = (\mathbf{a}_i, \mathbf{a}_{Ii}) \tag{9.8.4.11}$$

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 (9.8.4.10) is a one-to-one relation].

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 that can be considered as being n-dimensional orthogonal transformations R_s in V_s, leaving invariant the Euclidean metric tensors:

$$g_{sik} = a_{si} \cdot a_{sk} \quad \text{and} \quad g^*_{sik} = a^*_{si} \cdot a^*_{sk}. \tag{9.8.4.12}$$

The crystal classes considered in the tables suppose the existence of main reflections defining a three-dimensional reciprocal lattice. For that case, the embedding can be specialized by making the choice

$$\begin{aligned} a^*_{si} &= (\mathbf{a}^*_i, 0) \qquad i = 1, 2, 3, \\ a^*_{s(3+j)} &= (\mathbf{a}^*_{3+j}, \mathbf{d}^*_j) \qquad j = 1, 2, \ldots, d = n-3, \end{aligned} \tag{9.8.4.13}$$

and, correspondingly,

$$\begin{aligned} a_{si} &= (\mathbf{a}_i, \mathbf{a}_{Ii}) \qquad i = 1, 2, 3, \\ a_{s(3+j)} &= (0, \mathbf{d}_j) \qquad j = 1, 2, \ldots, d, \end{aligned} \tag{9.8.4.14}$$

with $\mathbf{d}^*_i \cdot \mathbf{d}_k = \delta_{ik}$ and $\mathbf{a}^*_i \cdot \mathbf{a}_k = \delta_{ik}$. These 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 every diffraction peak into a peak of the same intensity.†

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

$$R\mathbf{a}^*_i = \sum_{j=1}^{3+d} \Gamma^*(R)_{ji}\mathbf{a}^*_j, \quad i = 1, \ldots, 3+d. \tag{9.8.4.15}$$

The $(3+d)\times(3+d)$ matrices $\Gamma^*(R)$ form a finite group of integral matrices $\Gamma^*(K)$ for K equal to P_L or to one of its subgroups. A well known theorem in algebra states that then there is a basis in $3+d$ dimensions such that the matrices $\Gamma^*(R)$ on that basis are orthogonal and represent $(3+d)$-dimensional orthogonal transformations R_s. The corresponding group is a $(3+d)$-dimensional crystallographic group denoted by K_s. Because R is already an orthogonal transformation on V, R_s is reducible and can be expressed as a pair (R, R_I) of orthogonal transformations, in 3 and d dimensions, respectively. The basis on which (R, R_I) acts according to $\Gamma^*(R)$ is denoted by $\{(\mathbf{a}^*_i, \mathbf{a}^*_{Ii})\}$. It spans a lattice Σ^* that is the reciprocal of the lattice Σ with basis elements $(\mathbf{a}_i, \mathbf{a}_{Ii})$. The pairs (R, R_I), sometimes also noted (R_E, R_I), leave Σ invariant:

$$(R, R_I)(\mathbf{a}_i, \mathbf{a}_{Ii}) \equiv (R\mathbf{a}_i, R_I\mathbf{a}_{Ii}) = \sum_{j=1}^{3+d} \Gamma(R)_{ji}(\mathbf{a}_j, \mathbf{a}_{Ij}), \tag{9.8.4.16}$$

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

In many cases, one can 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 (9.8.4.13), the matrices $\Gamma(R)$ take the special form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix}. \tag{9.8.4.17}$$

The transformation of main reflections and satellites is then given by $\Gamma^*(R)$ as in (9.8.4.15), the relation with $\Gamma(R)$ being (as already said)

$$\Gamma^*(R) = \tilde{\Gamma}(R^{-1}),$$

where the tilde indicates transposition. Accordingly, on a standard basis one has

$$\Gamma^*(R) = \begin{pmatrix} \Gamma^*_E(R) & \Gamma^*_M(R) \\ 0 & \Gamma^*_I(R) \end{pmatrix}. \tag{9.8.4.18}$$

The set of matrices $\Gamma_E(R)$ for R elements 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 are modulation wavevectors) in terms of the basis of the lattice of main reflections:

$$\mathbf{a}^*_{3+j} = \sum_{i=1}^{3} \sigma_{ji}\mathbf{a}^*_i, \quad j = 1, 2, \ldots, d. \tag{9.8.4.19}$$

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

$$\mathbf{a}_{Ii} = -\sum_{j=1}^{d} \sigma_{ji}\mathbf{d}_j, \quad i = 1, 2, 3. \tag{9.8.4.20}$$

This follows directly from (9.8.4.19) and the definition of the reciprocal standard basis (9.8.4.13). From (9.8.4.16) and (9.8.4.17), 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 $\Gamma(R)$:

$$-\Gamma_I(R)\sigma + \sigma\Gamma_E(R) = \Gamma_M(R). \tag{9.8.4.21}$$

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 equation (9.8.4.21). It is therefore possible to decompose formally σ into parts σ^i and σ^r as follows.

$$\sigma = \sigma^i + \sigma^r, \quad \text{with} \quad \sigma^i \equiv \frac{1}{N}\sum_R \Gamma_I(R)\sigma\Gamma_E(R)^{-1}, \tag{9.8.4.22}$$

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

$$\Gamma_I(R)\sigma^i\Gamma_E(R)^{-1} = \sigma^i. \tag{9.8.4.23}$$

This implies

$$\Gamma_M(R) = -\Gamma_I(R)\sigma^r + \sigma^r\Gamma_E(R). \tag{9.8.4.24}$$

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

The above equations simplify for the case $d = 1$. The elements $\sigma_{1i} = \sigma_i$ 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 $\Gamma_I(R) = \varepsilon = \pm 1$

† See footnote on p. 913.