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

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.

since, for $d = 1$, $\mathbf{q}$ can only be transformed into $\pm\mathbf{q}$. One has the corresponding relations

$$\mathbf{q} = \mathbf{q}^i + \mathbf{q}^r, \quad \text{with} \quad \mathbf{q}^i \equiv \frac{1}{N}\sum_R \varepsilon R\mathbf{q}, \tag{9.8.4.25}$$

and

$$R\mathbf{q} \equiv \varepsilon\mathbf{q} \text{ (modulo reciprocal lattice } \Lambda^*); \quad R\mathbf{q}^i = \varepsilon\mathbf{q}^i. \tag{9.8.4.26}$$

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

9.8.4.2.2. *Geometric and arithmetic crystal classes*

According to the previous section, in the case of modulated structures a standard basis can be chosen (for M^* and correspondingly for Σ^*). According to equation (9.8.4.15), for each three-dimensional point-group operation R that leaves the diffraction pattern invariant, there is a point-group transformation R_E in the external space (the physical one, so that $R_E = R$) and a point-group transformation R_I in the internal space, such that the pair (R, 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 [see equations (9.8.4.15) and (9.8.4.18) for the $\mathbf{a}^*_{3+j}$ basis vectors]: there is exactly one R_I for each R. This is so because in the incommensurate case the correspondence between M^* and Σ^* is uniquely fixed by the embedding rule (9.8.4.10) (see Subsection 9.8.4.1). Because the matrices $\Gamma(R)$ and the corresponding transformations in the $(3+d)$-dimensional space form a group, this implies that there is a mapping from the group K_E of elements R_E to the group K_I of elements R_I that transforms products into products, *i.e.* is a group homomorphism. A point group K_s of the $(3+d)$-dimensional lattice constructed for an incommensurate 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 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 there 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.

Definition 3. Two groups of matrices 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 (9.8.4.15).

In three dimensions, there are 32 geometrically non-equivalent point groups and 73 arithmetically non-equivalent point groups. 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 (or 73) point groups, for each 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 (73) groups, one of the d-dimensional groups, and all homomorphisms 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, in general, groups that are 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^* also. 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 vector 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 the 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

$$H_s = \sum_{i=1}^{3} h_i(\mathbf{a}_i^*, 0) + \sum_{j=1}^{d} m_j(\mathbf{q}_j, \mathbf{d}_j^*) \tag{9.8.4.27}$$

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, precisely one vector of Σ^* is projected on each given vector of M^*.

Suppose now $R = 1$. This transformation leaves the component of every vector belonging to Σ^* 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 $R = R_E = 1$ 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

† See footnote on p. 913.

references