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.

(9.8.4.13). It is then faithfully represented by integral matrices that are of the form indicated in (9.8.4.17) and (9.8.4.18).

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 3 and d dimensions, respectively:

$$g_s = (\{R|\mathbf{v}\}, \{R_I|\mathbf{v}_I\}) \in E(3) \times E(d), \tag{9.8.4.28}$$

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 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 [see (9.8.4.32)]. 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 $\upsilon_s = (\mathbf{v}, \mathbf{v}_I)$ of the element g_s can be decomposed into an intrinsic part υ_s^o and an origin-dependent part υ_s^a:

$$(\upsilon, \upsilon_I) = (\mathbf{v}^o, \mathbf{v}_I^o) + (\mathbf{v}^a, \mathbf{v}_I^a),$$

with

$$(\mathbf{v}^o, \mathbf{v}_I^o) = \frac{1}{n}\sum_{m=1}^{n} (R^m\mathbf{v}, R_I^m\mathbf{v}_I), \tag{9.8.4.29}$$

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

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

$$(\mathbf{a}_i, \mathbf{a}_{Ii}), (0, \mathbf{d}_j), \quad i = 1, 2, 3, \quad j = 1, \ldots, d. \tag{9.8.4.30}$$

The internal part of the first three basis vectors is

$$\mathbf{a}_{Ii} = -\Delta\mathbf{a}_i = -\sum_{j=1}^{d} \sigma_{ji}\mathbf{d}_j \tag{9.8.4.31}$$

according to equation (9.8.4.20). The three-dimensional translation $\mathbf{v} = \sum_i \upsilon_i\mathbf{a}_i$ then entails a d-dimensional translation $-\Delta\mathbf{v}$ in V_I given by

$$\Delta\mathbf{v} = \Delta\left(\sum_{i=1}^{3} \upsilon_i\mathbf{a}_i\right) = \sum_{i=1}^{3} \upsilon_i\Delta\mathbf{a}_i. \tag{9.8.4.32}$$

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

$$\mathbf{v}_I = -\Delta\mathbf{v} + \boldsymbol{\delta}, \tag{9.8.4.33}$$

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

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 $-\Delta\mathbf{v} = -\mathbf{q}\cdot\mathbf{v}$ to $-\mathbf{q}\cdot\mathbf{v} - \mathbf{q}\cdot(1-R)\mathbf{s}$. This implies that for the case that $\varepsilon = 1$ the part δ changes to $\delta + \mathbf{q}\cdot(1-R)\mathbf{s} = \delta + \mathbf{q}^r\cdot(1-R)\mathbf{s}$, because $\mathbf{q}^i$ is invariant under R. Therefore, δ changes, in general. The internal translation

$$\tau = \delta - \mathbf{q}^r\cdot\mathbf{v}, \tag{9.8.4.34}$$

however, is invariant under an origin shift in V.

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

Another definition leading to the same partition of equivalent superspace groups 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 the space can be represented isomorphically by an $(n+1)$-dimensional matrix, of the form

$$A(g_s) = \begin{pmatrix} R_s & v_s \\ 0 & 1 \end{pmatrix} \tag{9.8.4.35}$$

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 to indicate 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

$$g_s = (\{R|\mathbf{v}\}, \{\varepsilon|\upsilon_I\}) \tag{9.8.4.36}$$

of Euclidean transformations in V and V_I, respectively. This element maps a point located at $r_s = (\mathbf{r}, t)$ to one at $(R\mathbf{r} + \mathbf{v}, \varepsilon t + \upsilon_I)$. Suppose the probability for the position $\mathbf{n} + \mathbf{r}_j$ to be occupied by an atom of species A is given by

$$P_A(\mathbf{n}, j, t) = p_j[\mathbf{q}\cdot(\mathbf{n} + \mathbf{r}_j) + t], \tag{9.8.4.37}$$