9.8. INCOMMENSURATE AND COMMENSURATE MODULATED STRUCTURES

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

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

and

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

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

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

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

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† See footnote on p. 913.

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references