This set of vectors is a vector module M^*. The vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ 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.

A vector 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 lattice Λ^* of main reflections 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 are main reflections 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 of Λ^*).

An element R of K then transforms the basic vectors $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$, $\mathbf{q}$ into ones of the form (9.8.1.15). If one denotes, as in (9.8.1.2), $\mathbf{q}$ by $\mathbf{a}_4^*$, this implies

$$R\mathbf{a}_i^* = \sum_{j=1}^{4} \Gamma^*(R)_{ji}\mathbf{a}_j^*, \quad i = 1, \ldots, 4, \tag{9.8.1.16}$$

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

$$\Gamma^*(R) = \begin{pmatrix} \Gamma_E^*(R) & \Gamma_M^*(R) \\ 0 & \varepsilon(R) \end{pmatrix}, \quad \text{where } \varepsilon(R) = \pm 1. \tag{9.8.1.17}$$

This matrix represents the orthogonal transformation R when referred to the basis vectors $\mathbf{a}_i^*$ $(i = 1, 2, 3, 4)$ of the vector module M^*. As in the case of lattices, two vector 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 vector modules. Equivalent vector 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 as in (9.8.1.15). Within such a larger vector module, the actual diffraction peaks then obey *centring conditions*. For a vector module associated with 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 describe the diffraction spots by means of the non-primitive lattice basis $\mathbf{a}_1^*, \frac{1}{2}\mathbf{a}_2^*, \mathbf{a}_3^*$ and by the modulation wavevector $\alpha\mathbf{a}_1^*$.

Crystallographic point groups are denoted generally by the same letter K.

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

$$H_s = \sum_{i=1}^{4} h_i a_{si}^*, \tag{9.8.1.18}$$

where [*cf.* (9.8.1.14)] m has now been replaced by h_4 and

$$a_{si}^* = (\mathbf{a}_i^*, 0), \quad i = 1, 2, 3; \quad a_{s4}^* = (\mathbf{q}, 1). \tag{9.8.1.19}$$

As will be explained in Section 9.8.4, these vectors span the four-dimensional reciprocal lattice for a periodic structure having as three-dimensional intersection (say defined by the hyperplane $t = 0$) the modulated crystal structure (a specific example has been given in Subsection 9.8.1.3). 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

$$R_s a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj} \quad (i = 1, 2, 3, 4), \tag{9.8.1.20a}$$

where $\Gamma(R)$ is the transpose of the matrix $\Gamma^*(R^{-1})$ appearing in (9.8.1.17) and therefore for incommensurate one-dimensionally modulated structures it has the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \varepsilon(R) \end{pmatrix}. \tag{9.8.1.20b}$$

9.8.1.4.3. *Four-dimensional crystallography*

Let us summarize the results obtained in the previous paragraph. 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 (sometimes also denoted by 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 $\varepsilon = \pm 1$ and they act on the four-dimensional lattice basis as

$$(R, \varepsilon)a_{si} = \sum_{j=1}^{4} \Gamma(R)_{ji} a_{sj}, \quad i = 1, \ldots, 4, \tag{9.8.1.21}$$

where ε stands for $\varepsilon(R)$ as in (9.8.1.20*b*). So the point-group symmetry operations are crystallographic and given by pairs of a three-dimensional crystallographic point-group transformation and a one-dimensional $\varepsilon = \pm 1$, respectively. The case $\varepsilon = -1$ corresponds to an *inversion of the phase of the modulation function*.

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

Two point groups K_s and K_s' belong to the same *geometric crystal class* if their three-dimensional (external) parts (forming the point group K_E and K_E', respectively) are in the same three-dimensional crystal class [*i.e.* are conjugated subgroups of $O(3)$] and their one-dimensional internal parts (forming the point groups K_I and K_I', respectively) are equal. The latter condition implies that corresponding point-group elements have the same value of ε.

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.

Also, the notion of *arithmetic equivalence* can be generalized to these four-dimensional point groups, as they admit the same faithful integral representation $\Gamma(K)$ given above. This means

references