

9.8. INCOMMENSURATE AND COMMENSURATE MODULATED STRUCTURES

reciprocal space ( $V^*$  identified with  $V$ ) is one with the first  $m$  basis vectors lying in  $V$  ( $m = \text{dimension of } V$ ).

[v] *Conventional basis.* For a lattice  $\Lambda$  in three dimensions, it is a basis such that (i) the lattice generated by it is contained in  $\Lambda$  as a sublattice and (ii) there is the standard relationship between the basis vectors (e.g. for a cubic lattice a conventional basis consists of three mutually perpendicular vectors of equal length).

The lattice  $\Lambda$  is obtained from the lattice spanned by the conventional basis by adding (a small number of) *centring vectors*. [For example, the b.c.c. lattice is obtained from the conventional cubic lattice by centring the unit cell with  $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ .] The reciprocal basis for the conventional basis is a conventional basis for the reciprocal lattice  $\Lambda^*$ .

In the  $(m + d)$ -dimensional superspace, a conventional basis for the lattice  $\Sigma$  satisfies the same conditions (i) and (ii) as formulated above for the three-dimensional case. In addition, however, one requires that the basis is standard and such that the non-vanishing external components satisfy the relations of an  $(m = 3)$  conventional basis and that the corresponding internal components only involve the irrational components of the modulation vector(s) (for  $d = 1$  the basis is such that  $\mathbf{q}^r = 0$ , thus  $\mathbf{q}^i = \mathbf{q}$ ). Again a conventional basis for  $\Sigma^*$  is dual to the same for  $\Sigma$ .

[vi] *Holohedry.* The holohedry of a vector module is the group of orthogonal transformations of the same dimension that leaves the vector module invariant. The holohedry of an  $(m + d)$ -dimensional lattice is the subgroup of  $O(m) \times O(d)$  that leaves the lattice invariant.

[vii] *Point group.* An  $(m + d)$ -dimensional crystallographic point group  $K_s = (K_E, K_I)$  is a subgroup of  $O(m) \times O(d)$ . With respect to a standard lattice basis its elements  $R_s = (R, R_I)$  are of the form

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

where all the entries are integers and  $R$  is an element of an  $m$ -dimensional point group  $K$ , which is actually the same as  $K_E$ . For an incommensurate modulated crystal,  $K_s$  and  $K$  are isomorphic groups. If  $d = 1$ ,  $\Gamma_I(R) = \varepsilon = \pm 1$ .

[viii] *Geometric crystal class.* Two point groups  $K_s = (K_E, K_I)$  and  $K'_s = (K'_E, K'_I)$  of pairs  $(R_E, R_I)$  of orthogonal transformations [ $R_E$  belongs to  $O(m)$  and  $R_I$  to  $O(d)$ ] are geometrically equivalent if and only if there are orthogonal transformations  $T_E$  and  $T_I$  of  $O(m)$  and  $O(d)$ , respectively, such that  $R'_E = T_E \cdot R_E \cdot T_E^{-1}$  and  $R'_I = T_I \cdot R_I \cdot T_I^{-1}$  for some group isomorphism  $(R_E, R_I) \rightarrow (R'_E, R'_I)$ . For  $d = 1$ , that condition takes a simpler form because  $R_I = \varepsilon = \pm 1$ .

[ix] *Arithmetic crystal class.* A group of integral matrices  $\Gamma^*(R)$  [for  $R \in K$  of  $O(m)$ ] is determined on a basis  $\{\mathbf{a}_i^*; i = 1, \dots, n\} = \mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}_1, \dots, \mathbf{q}_d$  of a vector module in reciprocal space by an  $m$ -dimensional point group  $K$  (here  $m = 3$ ). For modulated crystals, the transformations in direct space are given by matrices  $\Gamma(R) = \text{transpose of } \Gamma^*(R^{-1})$  which are of the form (9.8.4.17). Two groups  $\Gamma'(K')$  and  $\Gamma(K)$  are arithmetically equivalent if and only if there is an  $(m + d)$ -dimensional matrix  $S$  of the form

$$S = \begin{pmatrix} S_E & 0 \\ S_M & S_I \end{pmatrix}$$

with integral entries and determinant  $\pm 1$  such that  $\Gamma'(K') = S\Gamma(K) \cdot S^{-1}$ . Here  $S_E$  is  $m \times m$  and  $S_I$  is  $d \times d$  dimensional. An alternative formulation is: the matrix groups  $\Gamma(K)$  and  $\Gamma'(K')$  determined as in equation (9.8.1.16) or in equation (9.8.1.21) are arithmetically equivalent if

(a) the groups  $K$  and  $K'$  are geometrically equivalent  $m$ -dimensional point groups [the corresponding  $(m + d)$ -dimensional point groups  $K_s$  and  $K'_s$  are then also geometrically equivalent];

(b) there are vector module bases  $\mathbf{a}^*, \dots, \mathbf{q}_d$  and  $\mathbf{a}'^*, \dots, \mathbf{q}'_d$  such that  $K$  on the first basis gives the same group of matrices as  $K'$  on the second basis.

[x] *Bravais class.* Two vector modules are in the same Bravais class if the groups of matrices determined by their holohedries are arithmetically equivalent. Two  $(m + d)$ -dimensional lattices are in the same Bravais class if their holohedries are arithmetically equivalent. In both cases, one can find bases for the two structures such that the holohedries take the same matrix form. In the  $(m + d)$ -dimensional case, the lattice bases both have to be standard.

[xi] *Superspace group.* An  $(m + d)$ -dimensional superspace group is an  $n$ -dimensional space group ( $n = m + d$ ) such that it has a  $d$ -dimensional lattice of internal translations. (This latter property reflects the periodicity of the modulation.) It is determined on a standard lattice basis by the matrices  $\Gamma(R)$  of the point-group transformations and by the components  $v_i(R)$  ( $i = 1, \dots, m + d$ ) of the translation parts of its elements. The matrices  $\Gamma(R)$  represent at the same time the elements  $R$  of the  $m$ -dimensional point group  $K$  and the corresponding elements  $R_s$  of the  $(n + d)$ -dimensional point groups  $K_s$ . Two  $(m + d)$ -dimensional superspace groups are equivalent if there is an origin and a standard lattice basis for each group such that the collection  $\{\Gamma(K), v_s(K)\}$  is the same for both groups. [In previous formulae,  $v_s(R)$  is often simply indicated as  $v_s$ .]

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## 9. BASIC STRUCTURAL FEATURES

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