Λ^* Lattice of main reflections, m-dimensional reciprocal lattice.

$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ (Conventional) basis of Λ^* for $m = 3$.

Λ Direct m-dimensional lattice, dual to Λ^*.

V_s Superspace; Euclidean space of dimension $n = m + d$; $V_s = V \oplus V_I$.

V Physical (or external) space of dimension m ($m = 1, 2$ or 3), also indicated by V_E.

V_I Internal (or additional) space of dimension d.

Σ^* Reciprocal lattice in n-dimensional space, whose orthogonal projection on V is M^*.

Σ Lattice in n-dimensional superspace for which Σ^* is the reciprocal one.

a^*_{si} Lattice basis of Σ^* in V_s ($i = 1, \ldots, n$);
if $n = 4$, this basis can be chosen as $\{(\mathbf{a}^*, 0), (\mathbf{b}^*, 0), (\mathbf{c}^*, 0), (\mathbf{q}, 1)\}$ and is called standard. An equivalent notation is $(\mathbf{q}, 1) = (\mathbf{q}, \mathbf{d}^*)$;
for $n = 3 + d$, the general form of a standard basis is $(\mathbf{a}^*, 0)$, $(\mathbf{b}^*, 0)$, $(\mathbf{c}^*, 0)$, $(\mathbf{q}_1, \mathbf{d}^*_1), \ldots, (\mathbf{q}_j, \mathbf{d}^*_j), \ldots, (\mathbf{q}_d, \mathbf{d}^*_d)$.

a_{si} ($i = 1, \ldots, n$.) Lattice basis of Σ in V_s dual to $\{a^*_{si}\}$;
if $n = 4$, the standard basis is $(\mathbf{a}, -\mathbf{q}\cdot\mathbf{a}), (\mathbf{b}, -\mathbf{q}\cdot\mathbf{b}), (\mathbf{c}, -\mathbf{q}\cdot\mathbf{c}), (0, 1) = (0, \mathbf{d})$;
for $n = 3 + d$, a standard basis is dual to the standard one given above.

$\mathbf{q}_j$ Modulation wavevector(s) $\mathbf{q}_j = \sum_{i=1}^{3} \sigma_{ji}\mathbf{a}^*_i$;
if $n = 4$, $\mathbf{q} = \sum_{i=1}^{3} \sigma_i \mathbf{a}^*_i = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$;
$\sigma = (\alpha, \beta, \gamma)$;
if $n = 4$, $\mathbf{q} = \mathbf{q}^i + \mathbf{q}^r$, with $\mathbf{q}^i = (1/N)\sum_{R\,\text{in}\,K} \varepsilon(R)R\mathbf{q}$, where $\varepsilon(R) = R_I$, and N is the order of K.

$\mathbf{H}$ Bragg reflections: $\mathbf{H} = \sum_{i=1}^{n} h_i \mathbf{a}^*_i = (h_1, h_2, \ldots, h_n)$;
if $n = 4$, $\mathbf{H} = \sum_{i=1}^{4} h_i \mathbf{a}^*_i = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{q} = (h, k, l, m)$.

H_s Embedding of $\mathbf{H}$ in V_s: for $\mathbf{H} = (h_1, \ldots, h_n) = \sum_{i=1}^{n} h_i \mathbf{a}^*_i$, one has correspondingly $H_s = (\mathbf{H}, \mathbf{H}_I) = \sum_{i=1}^{n} h_i a^*_{si}$.

P_L Laue point group.

$O(m)$ Orthogonal group in m dimensions.

R Orthogonal point-group transformation, element of $O(m)$.

K Point group, crystallographic subgroup of $O(m)$.

R_s Superspace point-group element: $R_s = (R_E, R_I) = (R, R_I)$ element of $O(m) \times O(d)$ with $R_E = R$ external, and R_I internal part of R_s, respectively;
if $n = 4$, superspace point-group element: $[R, \varepsilon(R)]$ with $\varepsilon(R) = \pm 1$, also written (R, ε).

K_s Point group, crystallographic subgroup of $O(m) \times O(d)$.

K_E External part of K_s, crystallographic point group, subgroup of $O(m)$ with as elements the external part transformations of K_s.

K_I Internal part of K_s, crystallographic point group, subgroup of $O(d)$ with as elements the internal part transformations of K_s.

$\mathbf{r}_o(\mathbf{n}, j)$ Atomic positions in the basic structure: $\mathbf{r}_o(\mathbf{n}, j) = \mathbf{n} + \mathbf{r}_j$ with $\mathbf{n} \in \Lambda$.

$\mathbf{r}(\mathbf{n}, j)$ Atomic positions in the displacively modulated structure;
($d = 1$): $\mathbf{r}(\mathbf{n}, j) = \mathbf{r}_o(\mathbf{n}, j) + \mathbf{u}_j[\mathbf{q}\cdot\mathbf{r}(\mathbf{n}, j) + \varphi_j]$. In general, however, different phases $\varphi_{j\alpha}$ may occur for different components $u_{j\alpha}$ along the crystallographic axes.

$\mathbf{u}_j(x)$ Modulation function for displacive modulation with $\mathbf{u}_j(x + 1) = \mathbf{u}_j(x)$.

$p_j(x)$ Modulation function for occupation modulation with $p_j(x + 1) = p_j(x)$.

g Euclidean transformation in m dimensions; $g = \{R|\mathbf{v}\}$ element of the space group G with rotational part R and translational part $\mathbf{v}$.

$\mathbf{v}^o$ Intrinsic translation part (origin independent).

g_s Superspace group transformation ($d = 1$):
$g_s = \{(R, \varepsilon)|(\mathbf{v}, \Delta)\} = (\{R|\mathbf{v}\}, \{\varepsilon|\Delta\}) = \{R_s|\upsilon_s\}$ element of the superspace group G_s.
In the $(3 + d)$-dimensional case:
$g_s = \{(R, R_I)|(\mathbf{v}, \mathbf{v}_I)\} = (\{R|\mathbf{v}\}, \{R_I|\mathbf{v}_I\})$.

υ_I Internal shift ($d = 1$): $\upsilon_I = \Delta = \delta - \mathbf{q}\cdot\mathbf{v}$.

τ Intrinsic internal shift ($d = 1$): $\tau = \delta - \mathbf{q}^r\cdot\mathbf{v}$.

$\Gamma^*(R)$ Point-group transformation R with respect to a basis of M^* and at the same time superspace point-group transformation R_s with respect to a corresponding basis of Σ^*.

$\Gamma(R)$ Superspace point-group transformation with respect to a lattice basis of Σ dual to that of Σ^* leading to $\Gamma^*(R)$. The mutual relation is then $\Gamma^*(R) = \tilde{\Gamma}(R^{-1})$ with the tilde denoting transposition.

$\Gamma_E(R)$, $\Gamma_I(R)$, $\Gamma_M(R)$: external, internal, and mixed blocks of $\Gamma(R)$, respectively.

$\Gamma^*_E(R)$, $\Gamma^*_I(R)$, $\Gamma^*_M(R)$: external, internal, and mixed blocks of $\Gamma^*(R)$, respectively.

$S_{\mathbf{H}}$ Structure factor:

$$S_{\mathbf{H}} = \sum_{\mathbf{n}} \sum_{j} f_j(\mathbf{H}) \exp[2\pi i \mathbf{H}\cdot\mathbf{r}(\mathbf{n}, j)].$$

$f_j(\mathbf{H})$ Atomic scattering factor for atom j.

APPENDIX *B*
Basic definitions

In the following, we give a short definition of the most important notions appearing in the theory and of the equivalence relations used in the tables. The latter are especially adapted to the case of modulated crystal phases.

[i] *Vector module*. A set of all integral linear combinations of a finite number of vectors. The *dimension* of the vector module is the dimension (m) of the space V (also indicated as V_E and called external) generated by it over the real numbers. Its *rank* (n) is the minimal number of rationally independent vectors that generate the vector module. If this rank is equal to the dimension, the vector module is also a lattice. In general, a vector module of rank n and dimension m is the orthogonal projection on the m-dimensional space V of an n-dimensional lattice. We shall restrict ourselves mainly to the case $m = 3$ and $n = 4$, but the following definitions are valid for modulated phases of arbitrary dimension and rank. The *dimension of the modulation* (d) is $n - m$. The modulation phases span a d-dimensional space V_I (called internal or additional).

[ii] *Superspace*. V_s is an n-dimensional Euclidean space that is the direct sum of an m-dimensional *external* space V (of the crystal) and a d-dimensional *internal* space V_I (for the additional degrees of freedom). V is sometimes denoted by V_E.

[iii] *Split basis*. For the space $V_s = V \oplus V_I$, this is a basis with m basis vectors in V and $d = n - m$ basis vectors in V_I.

[iv] *Standard basis*. For the $(m + d)$-dimensional space $V_s = V \oplus V_I$, a standard basis in direct space is one having the last d basis vectors lying in V_I (d = dimension of V_I = dimension of the modulation). A standard basis in

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

[v] *Conventional basis*. For a lattice Λ in three dimensions, it is a basis such that (i) the lattice generated by it is contained in Λ 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 Λ 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 Λ^*.

In the $(m+d)$-dimensional superspace, a conventional basis for the lattice Σ 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 Σ^* is dual to the same for Σ.

[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 crystallograhic 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 $\{\mathbf{a}_i^*;\ i=1,\ldots,n\} = \mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}_1, \ldots, \mathbf{q}_d$ 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 $\Gamma(R) =$ 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 ± 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 $\mathbf{a}^*, \ldots, \mathbf{q}_d$ and $\mathbf{a}^{*\prime}, \ldots, \mathbf{q}_d'$ 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 $\upsilon_i(R)$ ($i=1,\ldots,m+d$) 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 $\{\Gamma(K), \upsilon_s(K)\}$ is the same for both groups. [In previous formulae, $\upsilon_s(R)$ is often simply indicated as υ_s.]

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9.1

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