International Tables for Crystallography (2016). Vol. A, Section 1.3.3, pp. 28–31.

Examples

(i) The lattice **L** spanned by the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

has metric tensor

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

The inverse of the metric tensor is

$$\boldsymbol{G}^* = \boldsymbol{G}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Interpreting the columns of $\boldsymbol{G}^{-1}$ as coordinate vectors with respect to the original basis, one concludes that the reciprocal basis is given by

$$\mathbf{a}^* = \mathbf{a} - \mathbf{b}, \quad \mathbf{b}^* = \tfrac{1}{2}(-2\mathbf{a} + 3\mathbf{b}), \quad \mathbf{c}^* = \tfrac{1}{2}\mathbf{c}.$$

Inserting the columns for **a**, **b**, **c**, one obtains

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \quad \mathbf{c}^* = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

For the direct computation, the matrix $\boldsymbol{B}$ with the basis vectors **a**, **b**, **c** as columns is

$$\boldsymbol{B} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

and has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 1 & 1 & -2 \\ 1 & -1 & 0 \end{pmatrix}.$$

The rows of this matrix are indeed the vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ as computed above.

(ii) The body-centred cubic lattice **L** has the vectors

$$\mathbf{a} = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{c} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

as primitive basis.

The matrix

$$\boldsymbol{B} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

with the basis vectors **a**, **b**, **c** as columns has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The rows of $\boldsymbol{B}^{-1}$ are the vectors

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{c}^* = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

showing that the reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice.

1.3.3. The structure of space groups

1.3.3.1. Point groups of space groups

The multiplication rule for symmetry operations

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$$

shows that the mapping $\Pi : (\boldsymbol{W}, \boldsymbol{w}) \longmapsto \boldsymbol{W}$ which assigns a space-group operation to its linear part is actually a group homomorphism, because the first component of the combined operation is simply the product of the linear parts of the two operations. As a consequence, the linear parts of a space group form a group themselves, which is called the point group of $\mathcal{G}$. The kernel of the homomorphism Π consists precisely of the translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}$, and since kernels of homomorphisms are always normal subgroups (*cf.* Section 1.1.6), the translation subgroup $\mathcal{T}$ forms a normal subgroup of $\mathcal{G}$. According to the *homomorphism theorem* (see Section 1.1.6), the point group is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$.

Definition

The *point group* $\mathcal{P}$ of a space group $\mathcal{G}$ is the group of linear parts of operations occurring in $\mathcal{G}$. It is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$ of $\mathcal{G}$ by the translation subgroup $\mathcal{T}$.

When $\mathcal{G}$ is considered with respect to a coordinate system, the operations of $\mathcal{P}$ are simply 3×3 matrices.

The point group plays an important role in the analysis of the macroscopic properties of crystals: it describes the symmetry of the set of face normals and can thus be directly observed. It is usually obtained from the *diffraction record* of the crystal, where adding the information about the translation subgroup explains the sharpness of the Bragg peaks in the diffraction pattern.

Although we have already deduced that the translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ forms a normal subgroup in $\mathcal{G}$ because it is the kernel of the homomorphism mapping each operation to its linear part, it is worth investigating this fact by an explicit computation. Let $t = (\boldsymbol{I},\ \boldsymbol{t})$ be a translation in $\mathcal{T}$ and $W = (\boldsymbol{W},\ \boldsymbol{w})$ an arbitrary operation in $\mathcal{G}$, then one has

$$\begin{aligned} W t W^{-1} &= (\boldsymbol{W},\ \boldsymbol{w})(\boldsymbol{I},\ \boldsymbol{t})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{W},\ \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{I},\ -\boldsymbol{w} + \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w}) = (\boldsymbol{I},\ \boldsymbol{W}\boldsymbol{t}), \end{aligned}$$

which is again a translation in $\mathcal{G}$, namely by $\boldsymbol{W}\boldsymbol{t}$. This little computation shows an important property of the translation subgroup with respect to the point group, namely that every vector from the translation lattice is mapped again to a lattice vector by each operation of the point group of $\mathcal{G}$.

Proposition. Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and translation subgroup $\mathcal{T}$ and let $\mathbf{L} = \{\boldsymbol{t} \mid (\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}\}$ be the lattice of translations in $\mathcal{T}$. Then $\mathcal{P}$ acts on the lattice $\mathbf{L}$, *i.e.* for every $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{t} \in \mathbf{L}$ one has $\boldsymbol{W}\boldsymbol{t} \in \mathbf{L}$.

A point group that acts on a lattice is a subgroup of the full group of symmetries of the lattice, obtained as the group of orthogonal mappings that map the lattice to itself. With respect to a primitive basis, the group of symmetries of a lattice consists of all integral basis transformations that fix the metric tensor of the lattice.

Definition

Let **L** be a three-dimensional lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis **a**, **b**, **c**.

(i) An *automorphism* of **L** is an isometry mapping **L** to itself. Written with respect to the basis **a**, **b**, **c**, an automorphism of **L** is an integral basis transformation fixing the metric tensor of **L**, *i.e.* it is an integral matrix $\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z})$ with $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$.

(ii) The group

$$\mathcal{B} := Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$$

of all automorphisms of **L** is called the *automorphism group* or *Bravais group* of **L**. Note that $Aut(\mathbf{L})$ acts on the coordinate columns of **L**, which are simply columns with integral coordinates.

Since the isometries in the Bravais group of a lattice preserve distances, the possible images of the vectors in a basis are vectors of the same lengths as the basis vectors. But due to its discreteness, a lattice contains only finitely many lattice vectors up to a given length. This means that a lattice automorphism can only permute the finitely many vectors up to the maximum length of a basis vector. Thus, there can only be finitely many automorphisms of a lattice. This argument proves the following important fact:

Theorem. The Bravais group of a lattice is finite. As a consequence, point groups of space groups are finite groups.

As subgroups of the Bravais group of a lattice, point groups can be realized as integral matrix groups when written with respect to a primitive basis. For a centred lattice, it is possible that the Bravais group of a lattice contains non-integral matrices, because the centring vector is a column with non-integral entries. However, in dimensions two and three the conventional bases are chosen such that the Bravais groups of all lattices are integral when written with respect to a conventional basis.

Information on the Bravais groups of the primitive lattices in two- and three-dimensional space is displayed in Tables 1.3.3.1 and 1.3.3.2. The columns of the tables contain the names of the lattices, the metric tensor with respect to the conventional basis (with only the upper half given, the lower half following by the symmetry of the metric tensor), the Hermann–Mauguin symbol for the type of the Bravais group and generators of the Bravais group (given in the shorthand notation introduced in Section 1.2.2.1 and the corresponding Seitz symbols discussed in Section 1.4.2.2).

The finiteness and integrality of the point groups has important consequences. For example, it implies the *crystallographic restriction* that rotations in space groups of two- and three-dimensional space can only have orders 1, 2, 3, 4 or 6. On the one hand, an integral matrix clearly has an integral trace.[1] But a matrix $\boldsymbol{W}$ with the property that $\boldsymbol{W}^k = \boldsymbol{I}$ can be diagonalized over the complex numbers and the diagonal entries have to be kth roots of unity, *i.e.* powers of $\zeta_k = \exp(2\pi i/k)$. Since diagonalization does not change the trace, the sum of these kth roots of unity still has to be an integer and in particular these roots of unity have to occur in complex conjugate pairs. In dimension 2 this means that the two diagonal entries are complex conjugate and the only possible ways to obtain an integral trace are $\zeta_1 + \zeta_1^{-1} = 2$, $\zeta_2 + \zeta_2^{-1} = -2$, $\zeta_3 + \zeta_3^{-1} = -1$, $\zeta_4 + \zeta_4^{-1} = 0$ and $\zeta_6 + \zeta_6^{-1} = 1$. In dimension 3 the third diagonal entry does not have a complex conjugate partner, and therefore has to be ± 1.

[1] The trace of a matrix is the sum of its diagonal entries.

Table 1.3.3.1
Automorphism groups of two-dimensional primitive lattices

Lattice	Metric tensor	Bravais group	
		Hermann–Mauguin symbol	Generators
Oblique	$\begin{pmatrix} g_{11} & g_{12} \\ & g_{22} \end{pmatrix}$	2	2: $\bar{x}, \bar{y}$
Rectangular	$\begin{pmatrix} g_{11} & 0 \\ & g_{22} \end{pmatrix}$	$2mm$	2: $\bar{x}, \bar{y}$ m_{10}: $\bar{x}, y$
Square	$\begin{pmatrix} g_{11} & 0 \\ & g_{11} \end{pmatrix}$	$4mm$	4^+: $\bar{y}, x$ m_{10}: $\bar{x}, y$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} \\ & g_{11} \end{pmatrix}$	$6mm$	6^+: $x - y, x$ m_{21}: $\bar{x}, \bar{x} + y$

Thus the possible orders in dimension 3 are the same as in dimension 2.

A much stronger result was obtained by H. Minkowski (1887). He gave an explicit bound for the maximal power p^m of a prime p which can divide the order of an n-dimensional finite integral matrix group. In dimension 2 this theorem implies that the orders of the point groups divide 24 and in dimension 3 the orders of the point groups divide 48. The Bravais groups $4mm$ (of order 8) and $6mm$ (of order 12) of the square and hexagonal lattices in dimension 2 and the Bravais group $m\bar{3}m$ (of order 48) of the cubic lattice in dimension 3 show that Minkowski's result is the best possible in these dimensions.

1.3.3.2. Coset decomposition with respect to the translation subgroup

The translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ can be used to distribute the operations of $\mathcal{G}$ into different classes by grouping together all operations that differ only by a translation. This results in the decomposition of $\mathcal{G}$ into cosets with respect to $\mathcal{T}$ (see Section 1.1.4 for details of cosets).

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$.

(i) The *right coset* $\mathcal{T}W$ of an operation $W \in \mathcal{G}$ with respect to $\mathcal{T}$ is the set $\{tW \mid t \in \mathcal{T}\}$.
Analogously, the set $W\mathcal{T} = \{Wt \mid t \in \mathcal{T}\}$ is called the *left coset* of W with respect to $\mathcal{T}$.

(ii) A set $\{W_1, \ldots, W_m\}$ of operations in $\mathcal{G}$ is called a system of *coset representatives* relative to $\mathcal{T}$ if every operation W in $\mathcal{G}$ is contained in exactly one coset $\mathcal{T}W_i$.

(iii) Writing $\mathcal{G}$ as the disjoint union

$$\mathcal{G} = \mathcal{T}W_1 \cup \ldots \cup \mathcal{T}W_m$$

is called the *coset decomposition of* $\mathcal{G}$ *relative to* $\mathcal{T}$.

If the translation subgroup $\mathcal{T}$ is a subgroup of index $[i]$ in $\mathcal{G}$, a set of coset representatives for $\mathcal{G}$ relative to $\mathcal{T}$ consists of $[i]$ operations $W_1, W_2, \ldots, W_{[i]}$, where W_1 is assumed to be the identity element e of $\mathcal{G}$. The cosets of $\mathcal{G}$ relative to $\mathcal{T}$ can be imagined as columns of an infinite array with $[i]$ columns, labelled by the coset representatives, as displayed in Table 1.3.3.3.

Table 1.3.3.2
Automorphism groups of three-dimensional primitive lattices

Lattice	Metric tensor	Bravais group: Hermann–Mauguin symbol	Bravais group: Generators
Triclinic	$\begin{pmatrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{pmatrix}$	$\bar{1}$	$\bar{1}$: $\bar{x}, \bar{y}, \bar{z}$
Monoclinic	$\begin{pmatrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	$2/m$	2_{010}: $\bar{x}, y, \bar{z}$ m_{010}: $x, \bar{y}, z$
Orthorhombic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	mmm	m_{100}: $\bar{x}, y, z$ m_{010}: $x, \bar{y}, z$ m_{001}: $x, y, \bar{z}$
Tetragonal	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$4/mmm$	4_{001}: $\bar{y}, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}, y, z$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$6/mmm$	6_{001}: $x-y, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}+y, y, z$
Rhombohedral	$\begin{pmatrix} g_{11} & g_{12} & g_{12} \\ & g_{11} & g_{12} \\ & & g_{11} \end{pmatrix}$	$\bar{3}m$	$\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ $m_{1\bar{1}0}$: y, x, z
Cubic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{pmatrix}$	$m\bar{3}m$	m_{001}: $x, y, \bar{z}$ $\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ m_{110}: $\bar{y}, \bar{x}, z$

Table 1.3.3.3
Right-coset decomposition of $\mathcal{G}$ relative to $\mathcal{T}$

$W_1 = e$	W_2	W_3	...	$W_{[i]}$
t_1	$t_1 W_2$	$t_1 W_3$	...	$t_1 W_{[i]}$
t_2	$t_2 W_2$	$t_2 W_3$	...	$t_2 W_{[i]}$
t_3	$t_3 W_2$	$t_3 W_3$	...	$t_3 W_{[i]}$
t_4	$t_4 W_2$	$t_4 W_3$	...	$t_4 W_{[i]}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$

Remark: We can assume some enumeration $t_1, t_2, t_3, \ldots$ of the operations in $\mathcal{T}$ because the translation vectors form a lattice. For example, with respect to a primitive basis, the coordinate vectors of the translations in $\mathcal{G}$ are simply columns $\begin{pmatrix} l \\ m \\ n \end{pmatrix}$ with integral components l, m, n. A straightforward enumeration of these columns would start with

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} \bar{1} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \bar{1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix},$$
$$\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \ldots$$

Writing out the matrix–column pairs, the coset $\mathcal{T}(\boldsymbol{W}, \boldsymbol{w})$ consists of the operations of the form $(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})$ with $\boldsymbol{t}$ running over the lattice translations of $\mathcal{T}$. This means that the operations of a coset with respect to the translation subgroup all have the same linear part, which is also evident from a listing of the cosets as columns of an infinite array, as in the example above.

Proposition

Let $W = (\boldsymbol{W}, \boldsymbol{w})$ and $W' = (\boldsymbol{W}', \boldsymbol{w}')$ be two operations of a space group $\mathcal{G}$ with translation subgroup $\mathcal{T}$.

(1) If $\boldsymbol{W} \neq \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are disjoint, *i.e.* their intersection is empty.

(2) If $\boldsymbol{W} = \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are equal, because WW'^{-1} has linear part $\boldsymbol{I}$ and is thus an operation contained in $\mathcal{T}$.

The one-to-one correspondence between the point-group operations and the cosets relative to $\mathcal{T}$ explicitly displays the isomorphism between the point group $\mathcal{P}$ of $\mathcal{G}$ and the factor group $\mathcal{G}/\mathcal{T}$. This correspondence is also exploited in the listing of the general-position coordinates. What is given there are the coordinate triplets for coset representatives of $\mathcal{G}$ relative to $\mathcal{T}$, which correspond to the first row of the array in Table 1.3.3.3. As just explained, the other operations in $\mathcal{G}$ can be obtained from these coset representatives by adding a lattice translation to the translational part.

Furthermore, the correspondence between the point group and the coset decomposition relative to $\mathcal{T}$ makes it easy to find a system of coset representatives $\{W_1, \ldots, W_m\}$ of $\mathcal{G}$ relative to $\mathcal{T}$. What is required is that the linear parts of the W_i are precisely the operations in the point group of $\mathcal{G}$. If $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_m$ are the different operations in the point group $\mathcal{P}$ of $\mathcal{G}$, then a system of coset representatives is obtained by choosing for every linear part $\boldsymbol{W}_i$ a translation part $\boldsymbol{w}_i$ such that $W_i = (\boldsymbol{W}_i, \boldsymbol{w}_i)$ is an operation in $\mathcal{G}$.

It is customary to choose the translation parts $\boldsymbol{w}_i$ of the coset representatives such that their coordinates lie between 0 and 1, excluding 1. In particular, if the translation part of a coset representative is a lattice vector, it is usually chosen as the zero vector $\boldsymbol{o}$.

Note that due to the fact that $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, a system of coset representatives for the right cosets is at the same time a system of coset representatives for the left cosets.

1.3.3.3. Symmorphic and non-symmorphic space groups

If a coset with respect to the translation subgroup contains an operation of the form $(\boldsymbol{W}, \boldsymbol{w})$ with $\boldsymbol{w}$ a vector in the translation lattice, it is clear that the same coset also contains the operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part. On the other hand, if a coset does not contain an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$, this may be caused by an inappropriate choice of origin. For example, the operation $(-\boldsymbol{I}, (1/2, 1/2, 1/2))$ is turned into the inversion $(-\boldsymbol{I}, (0, 0, 0))$ by moving the origin to 1/4, 1/4, 1/4 (*cf.* Section 1.5.1.1 for a detailed treatment of origin-shift transformations).

Depending on the actual space group $\mathcal{G}$, it may or may not be possible to choose the origin such that every coset with respect to $\mathcal{T}$ contains an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$.

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$. If it is possible to choose the coordinate system such that every coset of $\mathcal{G}$ with respect to $\mathcal{T}$ contains an operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part, $\mathcal{G}$ is called a *symmorphic* space group, otherwise $\mathcal{G}$ is called a *non-symmorphic* space group.

One sees that the operations with trivial translation part form a subgroup of $\mathcal{G}$ which is isomorphic to a subgroup of the point group $\mathcal{P}$. This subgroup is the group of operations in $\mathcal{G}$ that fix the origin and is called the *site-symmetry group* of the origin (site-symmetry groups are discussed in detail in Section 1.4.4). It is the distinctive property of symmorphic space groups that they contain a subgroup which is isomorphic to the full point group. This may in fact be seen as an alternative definition for symmorphic space groups.

Proposition. A space group $\mathcal{G}$ with point group $\mathcal{P}$ is symmorphic if and only if it contains a subgroup isomorphic to $\mathcal{P}$. For a non-symmorphic space group $\mathcal{G}$, every finite subgroup of $\mathcal{G}$ is isomorphic to a proper subgroup of the point group.

Note that every finite subgroup of a space group is a subgroup of the site-symmetry group for some point, because finite groups cannot contain translations. Therefore, a symmorphic space group is characterized by the fact that it contains a site-symmetry group isomorphic to its point group, whereas in non-symmorphic space groups all site-symmetry groups have orders strictly smaller than the order of the point group.

Symmorphic space groups can easily be constructed by choosing a lattice $\mathbf{L}$ and a point group $\mathcal{P}$ which acts on $\mathbf{L}$. Then $\mathcal{G} = \{(\boldsymbol{W}, \boldsymbol{w}) \mid \boldsymbol{W} \in \mathcal{P}, \boldsymbol{w} \in \mathbf{L}\}$ is a space group in which the coset representatives can be chosen as $(\boldsymbol{W}, \boldsymbol{o})$.

Non-symmorphic space groups can also be constructed from a lattice $\mathbf{L}$ and a point group $\mathcal{P}$. What is required is a system of coset representatives with respect to $\mathcal{T}$ and these are obtained by choosing for each operation $\boldsymbol{W} \in \mathcal{P}$ a translation part $\boldsymbol{w}$. Owing to the translations, it is sufficient to consider vectors $\boldsymbol{w}$ with components between 0 and 1. However, the translation parts cannot be chosen arbitrarily, because for a point-group operation of order k, the operation $(\boldsymbol{W}, \boldsymbol{w})^k$ has to be a translation $(\boldsymbol{I}, \boldsymbol{t})$ with $\boldsymbol{t} \in \mathbf{L}$. Working this out, this imposes the restriction that

$$(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \in \mathbf{L}.$$

Once translation parts $\boldsymbol{w}$ are found that fulfil all these restrictions, one finally has to check whether the space group obtained this way is (by accident) symmorphic, but written with respect to an inappropriate origin. A change of origin by $\boldsymbol{p}$ is realized by conjugating the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ by the translation $(\boldsymbol{I}, -\boldsymbol{p})$ (*cf.* Section 1.5.1 on transformations of the coordinate system) which gives

$$(\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).$$

Thus, the space group just constructed is symmorphic if there is a vector $\boldsymbol{p}$ such that $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p} + \boldsymbol{w} \in \mathbf{L}$ for each of the coset representatives $(\boldsymbol{W}, \boldsymbol{w})$.

The above considerations also show how every space group can be assigned to a symmorphic space group in a canonical way, namely by setting the translation parts of coset representatives with respect to $\mathcal{T}$ to $\boldsymbol{o}$. This has the effect that screw rotations are turned into rotations and glide reflections into reflections. The Hermann–Mauguin symbol (see Section 1.4.1 for a detailed discussion of Hermann–Mauguin symbols) of the symmorphic space group to which an arbitrary space group is assigned is simply obtained by replacing any screw rotation symbol N_m by the corresponding rotation symbol N and every glide reflection symbol a, b, c, d, e, n by the symbol m for a reflection. A space group is found to be symmorphic if no such replacement is required, *i.e.* if the Hermann–Mauguin symbol only contains the symbols 1, 2, 3, 4, 6 for rotations, $\bar{1}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ for rotoinversions and m for reflections.

Example

The space groups with Hermann-Mauguin symbols $P4mm$, $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$ are all assigned to the symmorphic space group with Hermann–Mauguin symbol $P4mm$.

1.3.4. Classification of space groups

In this section we will consider various ways in which space groups may be grouped together. For the space groups themselves, the natural notion of equivalence is the classification into *space-group types*, but the point groups and lattices from which the space groups are built also have their own classification schemes into *geometric crystal classes* and *Bravais types of lattices*, respectively.

Some other types of classifications are relevant for certain applications, and these will also be considered. The hierarchy of the different classification levels and the numbers of classes on the different levels in dimension 3 are displayed in Fig. 1.3.4.1.

1.3.4.1. Space-group types

The main motivation behind studying space groups is that they allow the classification of crystal structures according to their symmetry properties. Since many properties of a structure can be derived from its group of symmetries alone, this allows the investigation of the properties of many structures simultaneously.

On the other hand, even for the same crystal structure the corresponding space group may look different, depending on the chosen coordinate system (see Chapter 1.5 for a detailed discussion of transformations to different coordinate systems). Because it is natural to regard two realizations of a group of symmetry operations with respect to two different coordinate systems as equivalent, the following notion of equivalence between space groups is natural.