1.3. GENERAL INTRODUCTION TO SPACE GROUPS

Definition
Let \( \mathbf{L} \) be a three-dimensional lattice with metric tensor \( \mathbf{G} \) with respect to a primitive basis \( \mathbf{a}, \mathbf{b}, \mathbf{c} \).

(i) An automorphism of \( \mathbf{L} \) is an isometry mapping \( \mathbf{L} \) to itself.

(ii) The group

\[
\mathcal{B} := \text{Aut}(\mathbf{L}) = \{ W \in \text{GL}_n(\mathbb{Z}) \mid W^T \cdot \mathbf{G} \cdot W = \mathbf{G} \}
\]

of all automorphisms of \( \mathbf{L} \) is called the automorphism group or Bravais group of \( \mathbf{L} \). Note that Aut(\( \mathbf{L} \)) acts on the coordinate columns of \( \mathbf{L} \), 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 discrete nature, 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 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. But a matrix \( W \) with the property that \( W^3 = I \) can be diagonalized over the complex numbers and the diagonal entries have to be \( 3k \)th roots of unity, i.e., powers of \( \zeta_3 = \exp(2\pi i/3) \). Since diagonalization does not change the trace, the sum of these \( 3k \) 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 \( \pm 1 \).

Table 1.3.3.1

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Metric tensor</th>
<th>Hermann–Mauguin symbol</th>
<th>Generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oblique</td>
<td>( \begin{pmatrix} s_{11} &amp; s_{12} \ s_{21} &amp; s_{22} \end{pmatrix} )</td>
<td>2</td>
<td>2: ( \bar{x}, \bar{y} )</td>
</tr>
<tr>
<td>Rectangular</td>
<td>( \begin{pmatrix} s_{11} &amp; 0 \ 0 &amp; s_{22} \end{pmatrix} )</td>
<td>2(mn)</td>
<td>2: ( \bar{x}, \bar{y} ) ( m_{12}: \bar{x}, \bar{y} )</td>
</tr>
<tr>
<td>Square</td>
<td>( \begin{pmatrix} s_{11} &amp; 0 \ 0 &amp; s_{11} \end{pmatrix} )</td>
<td>4(mm)</td>
<td>4(^c): ( \bar{y}, \bar{x} ) ( m_{12}: \bar{x}, \bar{y} )</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>( \begin{pmatrix} s_{11} &amp; -\bar{s}<em>{11} \ \bar{s}</em>{11} &amp; s_{11} \end{pmatrix} )</td>
<td>6(mm)</td>
<td>6(^c): ( x - y, x ) ( m_{21}: \bar{x}, \bar{x} + y )</td>
</tr>
</tbody>
</table>

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 \( p^n \) 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 4\(mm\) (of order 8) and 6\(mm\) (of order 12) of the square and hexagonal lattices in dimension 2 and the Bravais group 3\(3m\) (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 \( T \) 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 \( T \) (see Section 1.1.4 for details of cosets).

Definition
Let \( \mathcal{G} \) be a space group with translation subgroup \( T \).

(i) The right coset \( TW \) of an operation \( W \in \mathcal{G} \) with respect to \( T \) is the set \( \{ TW \mid t \in T \} \).

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

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

\[
\mathcal{G} = TW_1 \cup \ldots \cup TW_m
\]

is called the coset decomposition of \( \mathcal{G} \) relative to \( T \).

If the translation subgroup \( T \) is a subgroup of index \( [\mathcal{G}] \) in \( \mathcal{G} \), a set of coset representatives for \( \mathcal{G} \) relative to \( T \) consists of \([\mathcal{G}] \) operations \( W_1, W_2, \ldots, W_m \), where \( W_i \) is assumed to be the identity element \( e \) of \( \mathcal{G} \). The cosets of \( \mathcal{G} \) relative to \( T \) can be imagined as columns of an infinite array with \([\mathcal{G}] \) columns, labelled by the coset representatives, as displayed in Table 1.3.3.3.
1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.3.3.2
Automorphism groups of three-dimensional primitive lattices

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Metric tensor</th>
<th>Bravais group</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$S_{11}$</td>
<td>$S_{12}$</td>
</tr>
<tr>
<td>Triclinic</td>
<td>$g_{11}$</td>
<td>$g_{12}$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
<tr>
<td>Cubic</td>
<td>$g_{11}$</td>
<td>$g_{13}$</td>
</tr>
</tbody>
</table>

Table 1.3.3.3
Right-coset decomposition of $G$ relative to $T$

<table>
<thead>
<tr>
<th>$W_i$</th>
<th>$W_2$</th>
<th>$W_3$</th>
<th>...</th>
<th>$W_{45}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_1$</td>
<td>$t_1$</td>
<td>$t_3$</td>
<td>...</td>
<td>$t_1$</td>
</tr>
<tr>
<td>$t_2$</td>
<td>$t_2$</td>
<td>$t_3$</td>
<td>...</td>
<td>$t_2$</td>
</tr>
<tr>
<td>$t_3$</td>
<td>$t_3$</td>
<td>$t_3$</td>
<td>...</td>
<td>$t_3$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Remark: We can assume some enumeration $t_1, t_2, t_3, \ldots$ of the operations in $T$ because the translation vectors form a lattice. For example, with respect to a primitive basis, the coordinate vectors of the translations in $G$ 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

\[ \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \]

Writing out the matrix–column pairs, the coset $T(W, \mathbf{w})$ consists of the operations of the form $(I, t)(W, \mathbf{w}) = (W, \mathbf{w} + t)$ with $t$ running over the lattice translations of $T$. 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 $W = (W, \mathbf{w})$ and $W' = (W', \mathbf{w}')$ be two operations of a space group $G$ with translation subgroup $T$.

1. If $W \neq W'$, then the cosets $TW$ and $T'W'$ are disjoint, i.e., their intersection is empty.
2. If $W = W'$, then the cosets $TW$ and $T'W'$ are equal, because $WW'^{-1}$ has linear part $I$ and is thus an operation contained in $T$.

The one-to-one correspondence between the point-group operations and the cosets relative to $T$ explicitly displays the isomorphism between the point group $P$ of $G$ and the factor group $G/T$. 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 $G$ relative to $T$, which correspond to the first row of the array in Table 1.3.3.3. As just explained, the other operations in $G$ 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 $T$ makes it easy to find a system of coset representatives $\{W_1, \ldots, W_m\}$ of $G$ relative to $T$. What is required is that the linear parts of the $W_i$ are precisely the operations in the point group of $G$. If $W_1, \ldots, W_m$ are the different operations in the point group $P$ of $G$, then a system of coset representatives is obtained by choosing for every linear part $W_i$ a translation part $\mathbf{w}_i$ such that $W_i = (W_i, \mathbf{w}_i)$ is an operation in $G$.

It is customary to choose the translation parts $\mathbf{w}_i$ 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 \( o \).

Note that due to the fact that \( T \) 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. Symmorphic and non-symmorphic space groups

If a coset with respect to the translation subgroup contains an operation of the form \( (W, w) \) with \( w \) a vector in the translation lattice, it is clear that the same coset also contains the operation \( (W, o) \) with trivial translation part. On the other hand, if a coset does not contain an operation of the form \( (W, o) \), this may be caused by an inappropriate choice of origin. For example, the operation \((-I, (1/2, 1/2, 1/2))\) is turned into the inversion \((-I, (0, 0, 0))\) 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 \( T \) contains an operation of the form \( (W, o) \).

**Definition**

Let \( \mathcal{G} \) be a space group with translation subgroup \( T \). If it is possible to choose the coordinate system such that every coset of \( \mathcal{G} \) with respect to \( T \) contains an operation \( (W, o) \) 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 \( \mathcal{G} = \{ (W, w) | W \in \mathcal{P}, w \in \mathbf{L} \} \) is a space group in which the coset representatives can be chosen as \( (W, o) \).

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 \( T \) and these are obtained by choosing for each operation \( W \in \mathcal{P} \) a translation part \( w \). Owing to the translations, it is sufficient to consider vectors \( w \) 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 \( (W, w^k) \) has to be a translation \( (I, t) \) with \( t \in \mathbf{L} \). Working this out, this imposes the restriction that \( (W^{k-1} + \ldots + W + I)w \in \mathbf{L} \).

### 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.

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**References**