Mathematical description of a crystal

Definition
A **Bravais lattice** is an infinite array of points generated by integer combinations of 3 independent primitive vectors:

\[ \{ n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \mid n_1, n_2, n_3 \in \mathbb{Z} \}. \]

Crystal structures are described by attaching a **basis** consisting of one or more atoms to each lattice point.
Symmetries of a crystalline solid

By definition a crystal is invariant under translation by a lattice vector

\[ \mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \quad n_1, n_2, n_3 \in \mathbb{Z}. \]

In general there will be other symmetries, such as rotation, which leave one point fixed. These form the **point group** of the crystal. The group of all symmetry operations is called the **space group** of the crystal.

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<tr>
<td>( \mathbf{a}_1 \neq</td>
<td>\mathbf{a}_2</td>
<td>, \phi \neq 90^\circ )</td>
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**Figure**: Oblique and hexagonal lattices
Isometries and the Euclidean group

Definition
An isometry is a distance-preserving map. The isometries mapping \( \mathbb{R}^n \) to itself form a group under function composition, called the Euclidean group \( E_n \).

Theorem
The group of translations \( T_n = \{ \mathbf{x} \rightarrow \mathbf{x} + \mathbf{a} \mid \mathbf{a} \in \mathbb{R}^n \} \) is an invariant subgroup of \( E_n \)

\[ E_n / T_n \cong O(n) \]

\[ E_n \cong T_n \rtimes O(n) \]

Every element of \( E_n \) can be uniquely written as the product of a translation and a rotation or reflection.
Definition
A space group in $n$ dimensions is a subgroup of $E_n$.

Definition
The point group of a given space group is the subgroup of symmetry operations that leave one point fixed (i.e. proper and improper rotations). In other words, the point group of a space group is its intersection with $O(n)$.
Crystallographic restriction theorem

**Theorem**

*The rotational symmetries of a discrete lattice are limited to 2-, 3-, 4-, and 6-fold.*

**Proof.**

Suppose $R$ is a rotational symmetry of the lattice, i.e. $r' = Rr$ for lattice points $r, r'$. Then the matrix elements of $R$ with respect to the basis of lattice vectors are integers, so

$$
\text{Tr } R \in \mathbb{Z}.
$$

Because the trace is invariant under a change of basis,

$$
\text{Tr } \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix} = 1 + 2 \cos \theta \in \mathbb{Z}.
$$
Shrinking argument

Shrinking argument eliminates rotational symmetries greater than 6-fold as well as 5-fold.
Lattice systems in 2D

There are 4 distinct point groups that a Bravais lattice can have in two dimensions. The 5 fundamental lattices are grouped into 4 lattice systems based on their point group symmetry.
Crystallographic point groups in 2D

When a basis is added, there are 10 possible point groups in two dimensions:

\[ C_n \text{ and } D_n \text{ for } n = 1, 2, 3, 4, 6. \]

(a) \( D_6 \)  
(b) \( C_6 \)  
(c) \( C_2 \)  
(d) \( C_1 \)

**Figure:** Lattice symmetry is restricted by the basis
Space groups in 2D: Wallpaper groups

- Subgroups of $E_2$ compatible with translational symmetry (i.e. space groups whose associated point group is one of the 10 crystallographic point groups in 2D).
- There are 17 possible wallpaper groups.
- Prove by construction or using topology (Euler characteristic zero)

(a) p2  (b) p4m  (c) cm
The 17 wallpaper groups

Figure: http://thinkzone.wlonk.com/Symmetry/Symmetry.htm.
Subscripts are Hermann-Mauguin (international) notation
Lattice systems in 3D

There are 14 fundamental lattices in 3D, grouped into 7 lattice systems based on their point group symmetry.
General crystal structures, constructed by adding bases to the 14 Bravais lattices, can have

- 32 distinct point groups (10 in 2D)
- 230 distinct space groups (17 in 2D)

http://en.wikipedia.org/wiki/Space_group#Table_of_space_groups_in_3_dimensions
Summary of crystal symmetries

- 5 rotations (order 1, 2, 3, 4, 6)
- 14 Bravais lattices
- 32 point groups
- 230 space groups

But x-ray diffraction patterns that don't correspond to any of the space groups have been observed. In the 1980s crystal structures with apparent 5-fold symmetry were discovered...
Quasicrystals

- First observation by D. Shechtman in Al-Mn alloy
- Correspond to aperiodic tilings (lack translational symmetry)
- Can display rotational symmetry of orders other than 2, 3, 4, and 6

(a) Penrose tiling

(b) Ho-Mg-Zn icosahedral quasicrystal and x-ray diffraction pattern
References