Crystallographic Point Groups and Space Groups

Physics 251 Spring 2011

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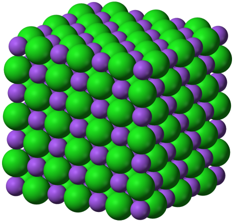
Mathematical description of a crystal

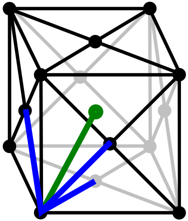
Definition

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

$$\mathbf{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3} \qquad n_1, n_2, n_3 \in \mathbb{Z}.$$

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.

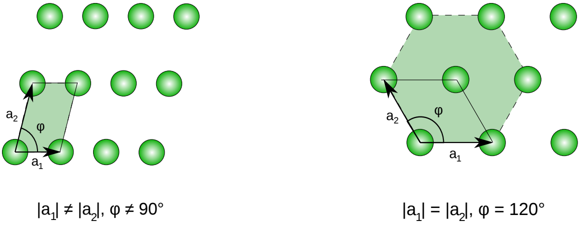


Figure: Oblique and hexagonal lattices

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 $T_n = \{\mathbf{x} \to \mathbf{x} + \mathbf{a} \mid \mathbf{a} \in \mathbb{R}^n\}$ *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.*

Point and space groups: formal definition

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

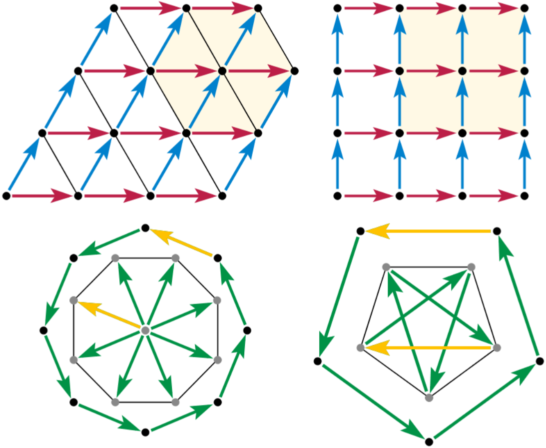
$$\operatorname{Tr} \mathbf{R} \in \mathbb{Z}.$$

Because the trace is invariant under a change of basis,

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

□

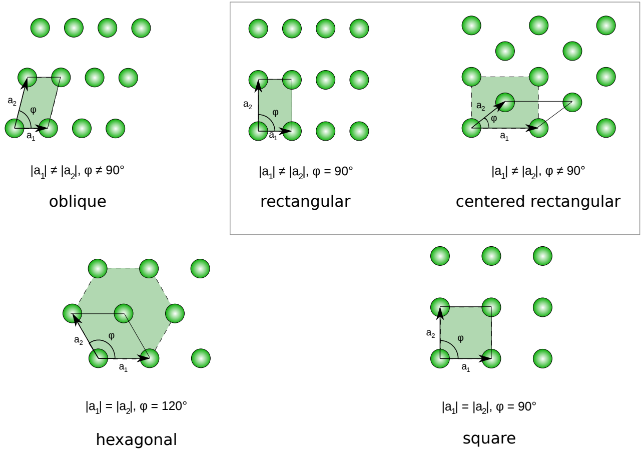
Shrinking argument



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:

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

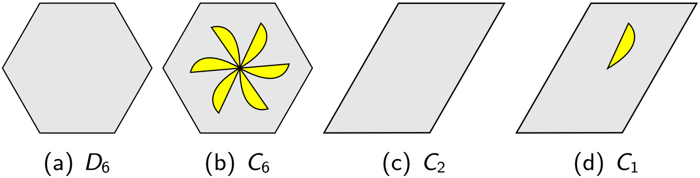
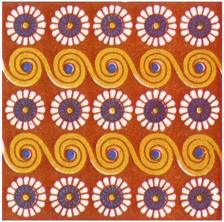


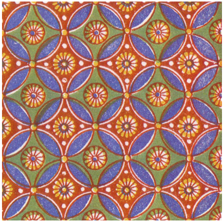
Figure: Lattice symmetry is restricted by the basis

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

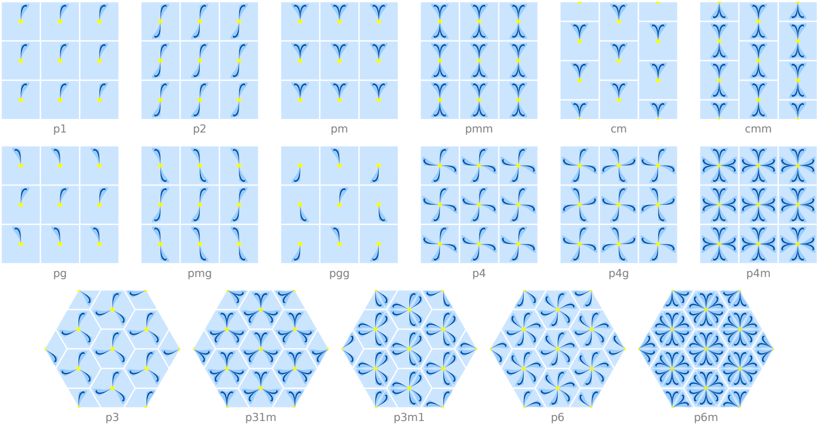
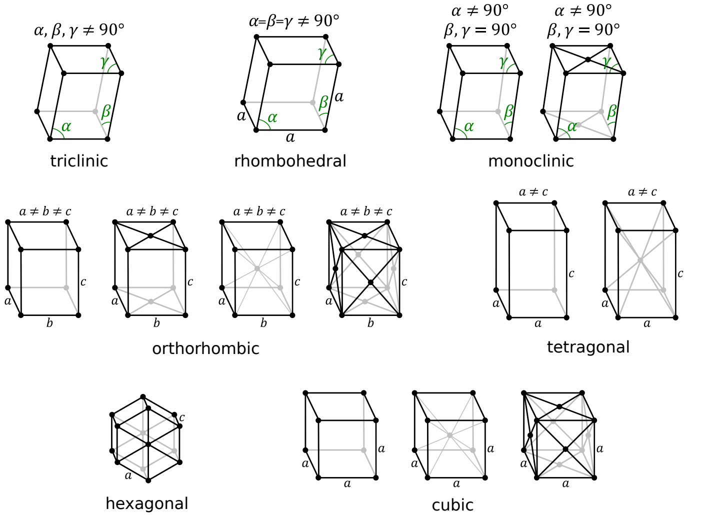


Figure: http://thinkzone.wlonk.com/Symmetry/Symmetry.htm.
Subscripts are Hermann-Mauguin (international) notation

Lattice systems in 3D

There are 14 fundamental lattices in 3D, grouped into 7 lattice systems based on their point group symmetry.



Crystallographic point groups and space groups in 3D

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

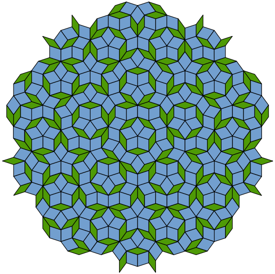
Summary of crystal symmetries

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

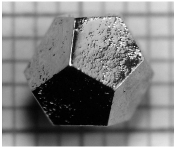
But x-ray diffraction patterns that don't correspond to any of the space groups have been observed. In the 1980s crystal structures with apparent 5-fold symmetry were discovered...

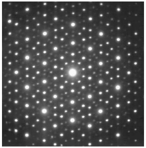
Quasicrystals

- First observation by D. Shechtman in Al-Mn alloy
- Correspond to aperiodic tilings (lack translational symmetry)
- Can dispay 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

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