If both θ and -θ are symmetry operators, the green and orange points must also be lattice points of the same Bravais lattice, and thus the distance between a green and orange points (marked as $m\,a$) must be an integer times the lattice constant a. Two sides of the triangle has length a. The third side is $m\,a$. The top angle is $2\,\pi - 2\,\theta$. Thus geometry tells us that

$$m\,a = \sqrt{a^2 + a^2 - 2\,a^2\cos(2\,\pi - 2\,\theta)} = 2\,a\sqrt{\frac{1 - \cos(\pi - 2\,\theta)}{2}} = 2\,a\sqrt{\frac{1 + \cos(2\,\theta)}{2}} = 2\,a\cos(\theta) \tag{5.4}$$

$$\cos\theta = \frac{m}{2} \tag{5.5}$$

Because m is an integer and $-1 \le |\cos\theta| \le +1$, m can only take the following values: $-2, -1, 0, +1, +2$. So θ can only be $\pi, 2\,\pi/3, \pi/2, \pi/3, 0$.

5.3. Lattice systems

There are multiple ways to classify crystals. In earlier chapters, we introduced the idea of **crystal families**. There are 6 crystal families. Each family contains 1,2, 3 or 4 Bravais lattices, and there are 14 Bravais lattice in total.

After we understand the ideas of point groups, we can introduce a new classification, known as **lattice system**. There 7 lattice systems, one more than crystal families. Lattice systems **are very close** to crystal families. The only modification is to split hexagonal crystal family into two lattice systems: **hexagonal and rhombohedral**.

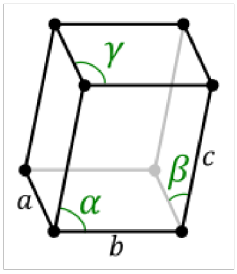
NOTE: there is an hexagonal crystal family and there is a hexagonal lattice system. They are both called "hexagonal", but they are not the same thing. Th hexagonal lattice system is a subset of the hexagonal crystal family.

The idea of **lattice system**s is as the following: assume that we draw all possible Bravais lattice and we put a sphere at each Bravais lattice point (ignoring details inside each primitive unit). Then we can ask what is the point group for all these lattices? It turns out that there are only 7 possible point groups here. They give us the 7 lattice systems.

NOTE: in a crystal, the degeneracy is often higher than the prediction below for 2 reasons (1) many crystal has additional symmetries, e.g. the time-reversal symmetry and (2) when we consider spin-1/2 particles, like electrons, there are additional representations, known as double-group representations. This extra representations are from quantum physics.

5.3.1. Triclinic lattice system with C_i symmetry

Triclinic lattice system coincides with the triclinic crystal family. Lattices in this lattice systems has C_i symmetry, identity and inversion.

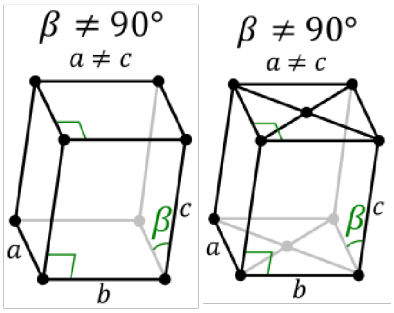


C_i contains 2 elements, and thus 2 1D representations. Because only has 1D representations, no degeneracy is in general expected in this type of crystals.

5.3.2. Monoclinic lattice system with $C_{2\,h}$ symmetry

Monoclinic lattice system coincides with the monoclinic crystal family. Lattices in this lattice systems has $C_{2\,h}$ symmetry.

$C_{2\,h}$ contains identity, a 2-fold rotation (perpendicular to the non-rectangular surface), a mirror plane (parallel to the non-rectangular surface), and inversion.

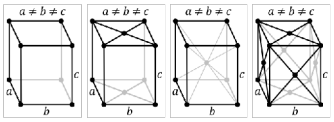


C_{2h} contains 4 elements, and thus 4 1D representations. Because only has 1D representations, no degeneracy is in general expected in this type of crystals.

5.3.3. Orthorhombic lattice system with D_{2h} symmetry

Orthorhombic lattice system coincides with the orthorhombic crystal family. Lattices in this lattice systems has D_{2h} symmetry, like a **cuboid**.

The D_{2h} group contains 8 elements: Identity, 2-fold rotations along x, y and z, inversion I, and three mirror planes xy, yz xz.

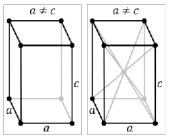


D_{2h} contains 8 elements, and 8 1D representations. Because only has 1D representations, no degeneracy is in general expected in this type of crystals.

5.3.4. tetragonal lattice system with D_{4h} symmetry

Orthorhombic lattice system coincides with the orthorhombic crystal family. Lattices in this lattice systems has D_{4h} symmetry, like a **square prism**

The D_{4h} group contains 16 elements: Identity, 90 and 180 and 270 degree rotations along z, 2-fold rotations along x or y, 2-fold rotations along x+y or x-y, inversion I, mirror planes xy, yz, xz, (x+y)z and (x-y)z, 90 and 270 degree improper rotation along z.



D_{2h} contains 16 elements, and 8 1D representations and 2 2D representations.

$$16 = 8\times 1^1 + 2\times 2^2 \tag{5.6}$$

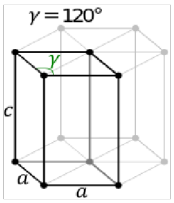
This lattice support 2-fold degeneracy

5.3.5. Hexagonal lattice system with D_{6h} symmetry

Hexagonal lattice system is a sub-set of the hexagonal crystal family. Lattices in this lattice systems has D_{6h} symmetry, like a **hexagonal prism**

The D_{6h} group contains 24 elements:

- Identity (one)
- $\frac{2\pi}{6}\times n$-degree rotations along z (five),
- 2-fold rotations six axes in the xy-plane (six)
- Inversion (one)
- six mirror planes perpendicular to the xy plane (six)
- xy mirror plane (one)
- two 6-fold improper rotations S_6 along z (two)
- two 3-fold improper rotations S_3 along z (two)



D_{6h} contains 24 elements, and 8 1D representations and 4 2D representations.

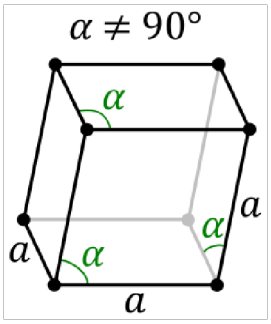
$$24 = 8 \times 1^1 + 4 \times 2^2 \tag{5.7}$$

This lattice support 2-fold degeneracy.

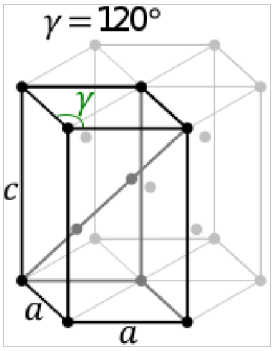
Note: graphene is a 2D material. Its point group symmetry is D_{6h}. The key physics is in graphene is the Dirac points, at which two energy bands meet together with the same energy. The reason this is possible in graphene is because the symmetry group allow two-fold degeneracy. If we break the symmetry (make the x-y plan not perfect hexagonal, by stretching along one direction), the degeneracy will be lifted and the Dirac point will be gapped.

5.3.6. Rhombohedral lattice system with D_{3d} symmetry

rhombohedral lattice system is a sub-set of the hexagonal crystal family. Lattices in this lattice systems has D_{3d} symmetry, like a rhombohedron



For a lattice made of rhombohedrons, if we look along a diagonal line, we see stacks of equilateral triangle. In that sense the rhombohedral lattice system is very similar to the hexagonal lattice system. This is why in crystal family classifications, we don't even distinguish them. To see this connection, we can draw a (bigger) conventional unit cell, which contains three primitive cells. This conventional cell is identical to the primitive cell of a hexagonal lattice.



These lattices are similar to hexagonal, but they have a different rotational symmetry. The key difference is, now along the z-axis, we only have 3-fold rotational symmetry, instead of 6-fold.

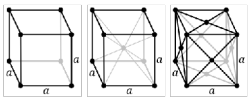
The D_{3d} group contains 12 elements. It has 4 1D representations and 2 2D representations.

$$12 = 4 \times 1^1 + 2 \times 2^2 \tag{5.8}$$

This lattice support 2-fold degeneracy.

5.3.7. Cubic lattice system with O_h symmetry

Cubic lattice system is the same as the cubic crystal family. Lattices in this lattice systems has O_h symmetry, like a cube



The O_h group contains 48 elements. It has two 1D representations, one 2D representation, and two 3D representations

$$48 = 4\times 1^1 + 2\times 2^2 + 4\times 3^2 \tag{5.9}$$

This lattice support 2-fold and 3-fold degeneracy.

5.4. Beyond lattice systems

Crystal classification: in general two types (1) classify the Bravais lattices and (2) classify based on the real symmetry of the crystal.

Q: Are these two types of classifications mathematically compatible?

A: Almost, but no.

5.4.1. Bravais lattices vs real material

Lattice systems only classifies Bravais lattice. It doesn't care about structures inside a unit cell. This cause two problems

1. It doesn't contain all the information about a lattice. A lot important details are ignored.

2. The symmetry of a real material may be lower than the symmetry of its Bravais lattice (i.e. the symmetry we talked about here is the symmetry of Bravais lattice, but it may not be the symmetry of the material).

This is because we ignored anything inside a unit cell when we draw the Bravais lattice. What is inside a unit cell may be very crucial.

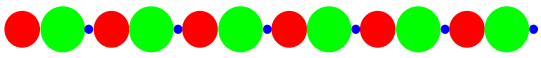
5.4.2. Point group symmetry of a crystal

As we discussed in earlier chapters, Bravais lattices only care about the periodicity. It doesn't carry information about what is inside each unit. In the lattice system classification, we also ignored information inside each unit cell, i.e. we put a sphere at each lattice site of the Bravais lattice. Because these spheres are invariant under any rotations, mirror reflections, inversions, improper rotations, we ignored information about the rotations inside each unit.

In general, a real solid is NOT like this. It is NOT made of perfect spheres at each Bravais lattice site. As a result, the symmetry of a real solid may be lower than that of the Bravais lattice. For example,

Here is the figure of a 1D Bravais lattice. If we put one atom at each lattice site (i.e. a sphere at each site), we can rotate the chain by 180 degree (along an axis perpendicular to the chain), and the crystal is invariant.

However, if each unit cell is composed by more than one atom, e.g. 3 atoms as shown in the figure below



The Bravais lattice is still the same, but for this crystal, we cannot rotate 180 degree, and thus it has lower symmetry.

If we consider the structure inside a unit cell, the point group symmetry may be lower than the point group symmetry of the Bravais lattices.

In group theory language, this means: the point group of a real solid is the subgroup of the point group of the Bravais lattices (i.e. the sub-group of one of the 7 point groups discussed above).

Bottom line:

Without considering the structure inside each unit cell, there are 7 possible point groups, and they give us the seven lattice systems.

If we consider the structure inside a cell, there are 32 possible point groups. These 32 groups are the 7 groups above + their subgroups.

These 32 point groups classifies crystals into 32 classes, known as crystal classes.

5.4.3. Classifying Bravais lattices vs Classifying the symmetry of the crystal

Q: Are the 32 crystal classes compatible with the 7 lattice systems?

A: Almost, but no.

Problems about the rhombohedral and hexagonal lattice systems

Both lattice systems and crystal classes are based on point groups. The former ignore information about structure inside a cell, so we may expect the latter is a finer classification. Maybe crystal classes are sub-classes of lattice systems? This is true for 5 of the lattice systems, but not the rhombohedral and hexagonal lattice systems.

- triclinic lattice system = $C_1 + C_i$
- monoclinice lattice system = $C_2 + C_S + C_{2h}$
- orthorhombic lattice system= $D_2 + C_{2v} + D_{2h}$
- tetragonal lattice system = $C_4 + S_4 + C_{4h} + D_4 + C_{4v} + D_{2d} + D_{4h}$
- rhombohedral + hexagonal lattice systems = $C_3 + S_6 + D_3 + C_{3v} + D_{3d} + C_6 + C_{3h} + C_{6h} + D_6 + C_{6v} + D_{3h} + D_{6h}$
- cubic lattice system= $T + T_d + T_h + O + O_h$

Once we take into consideration of things inside a unit cell, the rhombohedral and hexagonal lattice systems are not fully compatible with point group classifications. Knowing the point group of a material doesn't uniquely determine the lattice systems. We can resolve this incompatibility using one of the following two methods: (1) merge rhombohedral + hexagonal lattice systems into one and (2) regroup crystals in these two lattice systems into two classes, which are compatible with point groups.

- **6 crystal families:** Similar to lattice systems, but rhombohedral and hexagonal lattice systems are merged into 1 crystal family, known as the hexagonal crystal family.
- **7 crystal systems**: similar to lattice systems, but regroup rhombohedral and hexagonal lattice systems into trigonal and hexagonal crystal systems.

trigonal crystal systems= $C_3 + S_6 + D_3 + C_{3v} + D_{3d}$

hexagonal crystal systems = $C_6 + C_{3h} + C_{6h} + D_6 + C_{6v} + D_{3h} + D_{6h}$

The trigonal crystal system is slightly larger than the rhombohedral lattice system. The hexagonal crystal system is slightly smaller than the hexagonal lattice systems.

5.4.4. Space groups

Space group taken into account both translations and point group symmetries, as well as their combinations. There are 230 space groups, and they gives 230 different classes of crystals, known as 230 **space group types**.

The space groups contains lattice translations, point group symmetries, their combinations, and more.

More here means: translations that is a fraction of a lattice vector, combined with a rotation/mirror/inversion/...

- Translations:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \Delta_x \\ \Delta_y \\ \Delta_z \end{pmatrix} \tag{5.10}$$

For a lattice, $\vec{\Delta}$ must be lattice vector

- Point group symmetries: (operations that fix one point, fix the length of any vectors, and fix the angle between any two vectors)

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = M \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{5.11}$$

where $M\,M^T = M^T\,M = E$

- General formula for a space group element

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = M \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \Delta_x \\ \Delta_y \\ \Delta_z \end{pmatrix} \tag{5.12}$$

If M is an element in the point group of the lattice, and $\vec{\Delta}$ is a lattice vector, their combination is an elements of the space group. **But space group has more elements then them: Glide planes and Screw axes**

Glide planes: A glide plane is a reflection in a plane, followed by a translation parallel with that plane

Example: a row of arrows with up-down-up-down patterns.

Screw Axes: A screw axis is a rotation about an axis, followed by a translation along the direction of the axis.