Fundamental types of lattices and crystal symmetry

Crystal symmetry:

What is a symmetry operation?

It is a physical operation that changes the positions of the lattice points at exactly the same places after and before the operation. In other words, it is an operation when applied to an object leaves it apparently unchanged.

e.g. A translational symmetry is occurred, for example, when the function $\sin x$ has a translation through an interval $x = 2\pi$ leaves it apparently unchanged.

Otherwise a non-symmetric operation can be foreseen by the rotation of a rectangle through $\pi/2$.

There are two groups of symmetry operations represented by:

a) The point groups.

b) The space groups (these are a combination of point groups with translation symmetry elements). There are 230 space groups exhibited by crystals.

a) When the symmetry operations in crystal lattice are applied about a lattice point, the point groups must be used.

b) When the symmetry operations are performed about a point or a line in addition to symmetry operations performed by translations, these are called space group symmetry operations.

Types of symmetry operations:

There are five types of symmetry operations and their corresponding elements.

Note: The operation and its corresponding element are denoted by the same symbol.

1) The identity $\Rightarrow E$:

   It consists of doing nothing.

2) Rotation $\Rightarrow C_n$:

   It is the rotation about an axis of symmetry (which is called "element"). If the rotation through $2\pi/n$ (where n is integer), and the lattice remains unchanged by this rotation, then it has an n-fold axis. However the translational symmetry of a lattice limits the values of n to 1, 2, 3, 4 and 6 where the angle of rotation must be of 2π, π , $2\pi/3$, $\pi/2$and $\pi/3$ and it cannot be any other value.

Exercise: Show that 5-fold and 7-fold rotation axes are not compatible with a lattice and only 1, 2, 3, 4 and 6-fold rotation axes do exist.

The elements of rotation can be summarized as:

Element (n)	Angle of rotation	Name of rotation group	symbol
1	2π	E	
2	π	C_2 (Diads)	O
3	$2\pi/3$	C_3 (Triads)	Δ
4	$\pi/2$	C_4 (Tetrads)	□
6	$\pi/3$	C_6 (Hexads)	⬡

3) Mirror symmetry (σ):

   It is a reflection (operation) in a mirror plane (element). A single mirror symmetry plane is perpendicular to the page and its intersection of a plane of lattice points is represented by "I", and shown as heavy lines in Figure 49. Two orthogonal symmetry planes is represented by "+", as shown in figure 50, and four mirror planes with 45° is represented by "∗", as shown in figure 52.

Three types of mirror symmetry planes are named as:

a. Vertical mirror plane σ_v.

b. Horizontal mirror plane σ_h.

c. Dihedral plane σ_d.

4) Inversion symmetry i:

An inversion through a center of symmetry. The inversion operation is the imaginary operation of taking each point of the object through its center and out to an equal distance on the other side. However the net effect is to replace $\vec{r}$ by $-\vec{r}$ and the crystal appears exactly the same.

5) An improper rotation (or rotary-reflection) about an axis of improper rotation S_n:

This is an operation consists of an n-fold rotation followed by a horizontal reflection. e.g. CH_4 has three S_4 axes.

6) Other compound operations:

a) Glide (= Reflection + Translation)

b) Screw (= Rotation + Translation).

Two-dimensional types of Bravais lattices:

There are five Bravais lattices in two dimensions.

1. Oblique lattice: $|\vec{a}_1| \neq |\vec{a}_2|$ and $\gamma \neq \pi/2$

It is the least symmetric 2-D lattice type.

The existing symmetries: C_2 (2-fold rotations) and E (C_1).

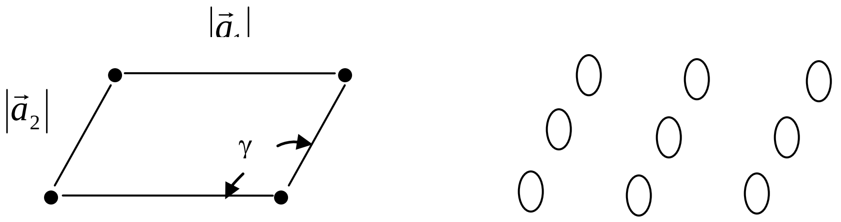

Figure 48: Oblique unit cell with its symmetry elements

a) oblique unit cell

b) Two-fold rotations at each corner, mid side and the center.

2. Rectangular lattice: $|\vec{a}_1| \neq |\vec{a}_2|$ and $\gamma = \pi/2$

It is a primitive rectangular form.

Symmetry requirements:

i) 2-fold rotations

ii) Mirror symmetry (mirror lines) or reflection. i.e. two perpendicular sets of mirror lines.

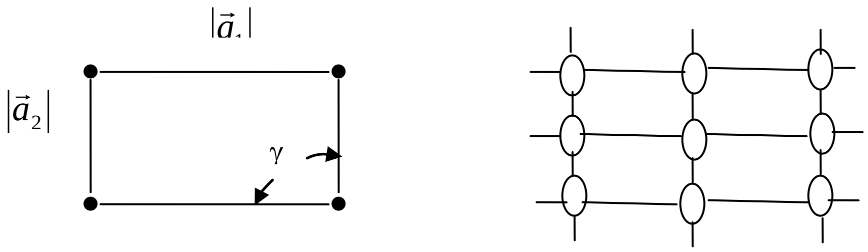

Figure 49: Rectangular unit cell with its symmetry elements

a) Rectangular unit cell

b) Symmetry elements for a rectangular unit cell

Notes:

1) Distribution of diads (2-fold axes) is the same for oblique and rectangular lattices.

2) The only difference between oblique and rectangular lattices is the absence of mirror lines in the oblique lattices.

3. Centered rectangular lattice: $|\vec{a}_1| \neq |\vec{a}_2|$ and $\gamma = \pi/2$

It is a non-primitive form.

[Note: The primitive unit cell is an oblique parallelogram with $|\vec{a}_1| \neq |\vec{a}_2|$.

Symmetry requirements:

i) 2-fold rotations

ii) Mirror symmetry (mirror lines).

iii) Additional 2-fold rotations for lattice points at center of rectangles.

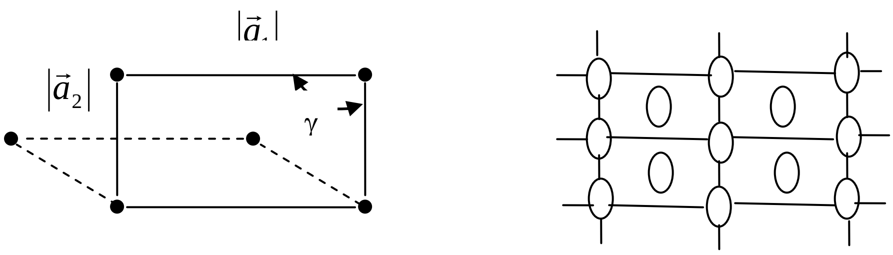

Figure 50: Centered rectangular unit cell with its symmetry elements

a) Centered rectangular unit cell.

b) Symmetry elements for centered rectangular unit cell.

[Note: Two primitive lattice points are associated with each rectangular unit cell. So the rectangle cannot be primitive.

4. Square lattice: $|\vec{a}_1| = |\vec{a}_2|$ and $\gamma = \pi/2$

Symmetry requirements:

i) 4-fold symmetry axis through lattice points at the corners and through the cell center.

ii) Mirror planes every 45° at the same lattice points in *(i)*. (Four mirror planes).

iii) 2-fold rotation symmetry at the mid point of the edges.

iv) Orthogonal mirror plane at same points of (*iii*).

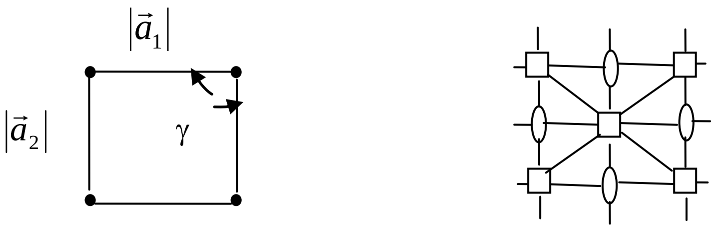

Figure 51: Square unit cell with its symmetry elements

a) square unit cell.

b) Symmetry elements for square unit cell.

5. Hexagonal lattice: $|\vec{a}_1| = |\vec{a}_2|$ and $\gamma = \pi/3$

This contains three primitive cells where each primitive cell consists of two identical equivalent triangles inverted with respect to each other. This lattice can be thought as special case of centered rectangular lattice with $|\vec{a}_1| = |\vec{a}_2|$ and $\gamma = \pi/3$ or $2\pi/3$.

Symmetry requirements for a primitive cell:

i) 3-fold axes pass through the centers of the triangles.

ii) 2-fold axes pass through the edge centers of the triangles.

iii) Mirror lines join each cell corner to the mid point of the opposite edge.

Symmetry requirements for a conventional hexagonal cell:

i) 6-fold axes.

ii) Six mirror lines.

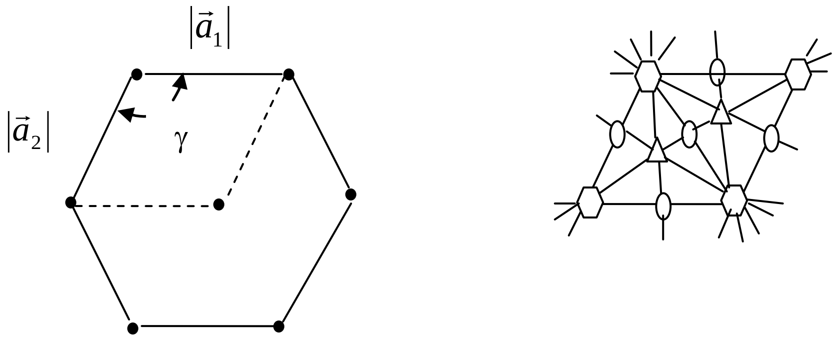

Figure 52: Hexagonal unit cell with its symmetry elements

a) Hexagonal unit cell.

b) Symmetry elements for a hexagonal unit cell.