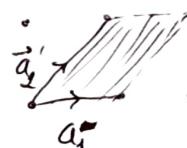
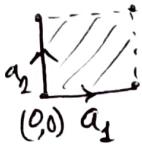


The ~~unit~~ primitive cell

The primitive cell is a volume (or area in 2D) of space, that, when translated through all the basis vectors in a Bravais lattice, fills all of the space without either overlapping itself or leaving voids. The primitive cell usually has the smallest volume (area) which produces this coverage of the whole lattice.

The choice of a unit cell is not unique for a particular Bravais lattice, for the same reason the choice of the basis vector is not unique. The ~~two~~^{three} possible choice of such primitive cell in a 2D lattice is shown below.



As one can see, if one translates the primitive cells shown in the figure through the basis vectors \vec{a}_1' and \vec{a}_2' , for all the possible choices of \vec{a}_1' and \vec{a}_2' , these unit cells will individually cover the whole Bravais lattice.

For example, in fig. (a), moving from $(0,0)$ to $(1,1)$ covers the

rightward cell. Then, going from $(0,0)$ to $(1,1)$ will cover the diagonally upper cell and so on so forth. The idea is that, if you translate your primitive cell for all choices of ~~(n_1, n_2)~~ (n_1, n_2) where $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2$, you cover the whole cell exactly once.

We can talk about two fundamental properties of the primitive cells.

of a particular Bravais lattice

(i) All primitive cells have the same area (volume), since this is the smallest area (volume) covering the whole lattice. You can easily prove this for specific cases, for example for ① and ⑥. The area of the primitive cell is unique, although the particular shape is not.

(ii) A primitive cell must contain precisely one lattice point. For example, ① precisely contains one lattice point. Although ① and ⑥ have four lattice points at the four corners, they are really shared by other cells. Each of the points is shared by four adjacent cells. Hence, each cell contains $4 \times \frac{1}{4} = 1$ lattice point again. It follows that if n is the density of the lattice points, ~~$\frac{n}{A}$~~ and A is the area of the

2

primitive cell, then, $nA=1$, or $A = \frac{1}{n}$. Since this result holds for any primitive cell, the area of a primitive cell is indeed independent of the choice of the cell - for a particular lattice.

All the previous statements can be extended to three dimensions in a straight forward manner. If \vec{a}_1, \vec{a}_2 and \vec{a}_3 are the basis vectors of the 3D Bravais lattice, then one can create a unit cell by forming a parallelepiped ~~cube~~ having its sides defined by \vec{a}_1, \vec{a}_2 and \vec{a}_3 . Here again, the primitive cell contains exactly one lattice point. If the cube with \vec{a}_1, \vec{a}_2 and \vec{a}_3 showing the basis vectors, then the no. of lattice points $= 8 \times \frac{1}{8} = 1$.

If n is the density of lattice points and V is the volume of the primitive cell, then $nV=1$ and $V = \frac{1}{n}$. Again, for a particular lattice n is the same and so all primitive cells must have the same volume, although the choice of the primitive cell is not unique.

If the primitive cell is defined by rectangles in 2D (parallelogram) and parallelepiped in 3D, then the area and volume of primitive cells are given by $|\vec{a}_1 \times \vec{a}_2|$ and $|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$ respectively.

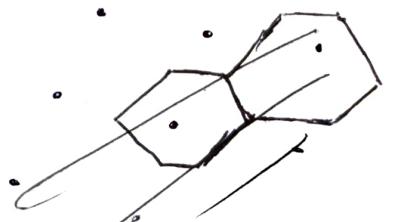
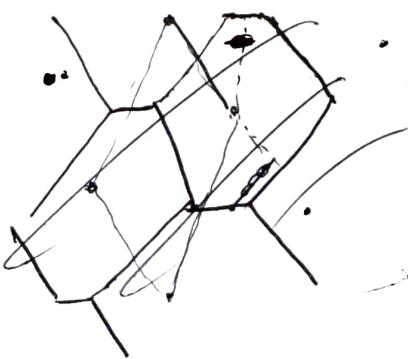
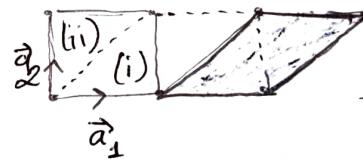
It also follows from the definition of primitive cells that, given any two primitive cells of arbitrary shapes, it is possible to cut the first into pieces, and translate them through appropriate basis vectors, can be assembled to give the second primitive cell. This is so, since by translating both primitive cells one can cover the whole lattice.

For example, one can translate

both part (i) and (ii) of the

primitive cell by just translating

them in the direction of \vec{a}_1 appropriately to find the shaded primitive cell.



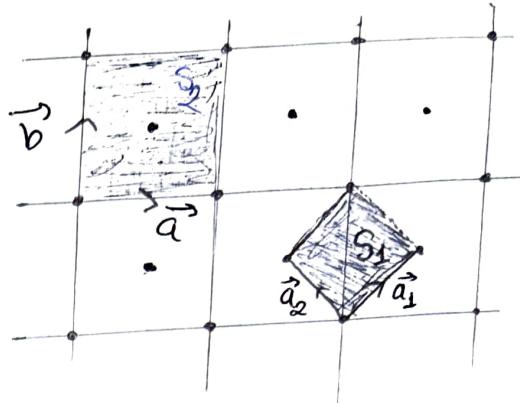
Here, we have the dark shaded hexagonal unit cell and the rectangular primitive unit cell. We break up the rectangular cell in four pieces. Then translate I in the \vec{c} direction, II in \vec{b} direction, III in \vec{a} direction and IV right where it is. This gives you the hexagonal primitive cell. If you define $\vec{a}_1 = \vec{a}$, $\vec{a}_2 = \vec{b}$ and $\vec{a}_3 = \vec{c}$ as basis vectors, then $\vec{a} = \vec{a}_1$, $\vec{b} = \vec{a}_1 + \vec{a}_2$ and $\vec{c} = \vec{a}_1 + \vec{a}_3$. So, all the translations are through basis vectors, as required.

Non-primitive unit cell

It is sometimes convenient to deal with unit cells which are larger than the primitive unit cell, and exhibit some particular symmetry more clearly. The non-primitive unit cell is also described by some basis vectors, however not satisfying the $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ with n_1, n_2 and n_3 being integer property. The non-primitive unit cell also fills the lattice without any overlapping when translated through those vectors.

Consider the Bravais lattice shown in the figure in the next page.

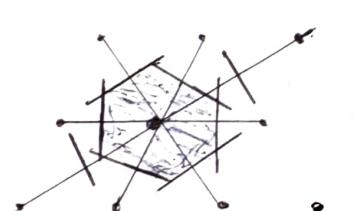
Here, S_1 created by the basis vectors \vec{a}_1 and \vec{a}_2 is a primitive unit cell. One can visualize the fact that the whole lattice can be covered by translating S_1 through all a_1 and a_2 , however this being a bit obscure. The unit cell S_2 made by $2\vec{a}_1$ and \vec{b} has nice and visible property such that if translated through \vec{a}_1 and \vec{b} it covers the whole lattice. This is a non-primitive unit cell. For, first, it contains two lattice points. Also, this is not the smallest unit cell, being twice as large as S_1 , which you can easily verify. One could also consider the ^{rectangle}_{parallelogram} made by $2\vec{a}_1$ and \vec{b} , which would also serve as a non-primitive unit cell. This would have four lattice points, also being four times larger than S_1 . (Argue why it should contain four lattice points).



Wigner-Seitz primitive cell

One can choose a primitive cell that has the same symmetry as of the Bravais lattice (we will

talk about this later). Such a choice is the Wigner-Seitz primitive cell, named after Eugene Wigner and Frederick Seitz. The Wigner-Seitz cell about a lattice point is the region of space that is closer to that lattice point than to any other lattice point. Since the Bravais lattice has translational symmetry, lattice point WS cell about a lattice point must be taken to WS cell about another lattice point, when the WS cell is translated by a basis vector that connects two lattice points. The construction of the WS primitive cell is as follows. You chose a lattice point. Then draw straight lines connecting the lattice point with its neighboring lattice points. In 2D, you draw a perpendicular bisector (line) and in 3D you draw a plane. Then you take the smallest polygon bounded by the bisecting lines (smallest polyhedron bounded by the bisecting planes) containing the lattice point. This smallest region is the WS primitive cell. An example of the WS cell in 2D is shown in the figure. As you can see, WS cell contains only one point. Also, you can translate the cell to ~~the~~ neighbouring lattice points by just translating by a vector connecting that



particular lattice point. In this way, you can cover the whole lattice without any overlapping. Although the WS primitive cell is not of any particular interest while describing crystal structure, it will become very important when we will talk about reciprocal lattice and something called the Bravais Zone.

Fundamental types of lattices

The problem of classifying all possible crystal structures is too complex to approach directly. It is the subject of crystallography to make such classification systematic and precise. We will only discuss about the classification of Bravais lattices and a few other aspects of symmetry briefly.

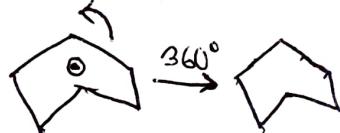
From the point of symmetry, a Bravais lattice is characterized by the specification of all rigid operations (meaning distance between lattice points remains ~~the same~~) that takes the lattice into itself. The set of operations are known as ^{the} symmetry group of the Bravais lattice.

The Bravais lattices can be mapped into themselves by the obvious translation $T_{\vec{R}}$ through a lattice vector \vec{R} . Since the lattice is made up of the primitive ^{unit} cells, considering the symmetry operations of the unit cells should be enough.

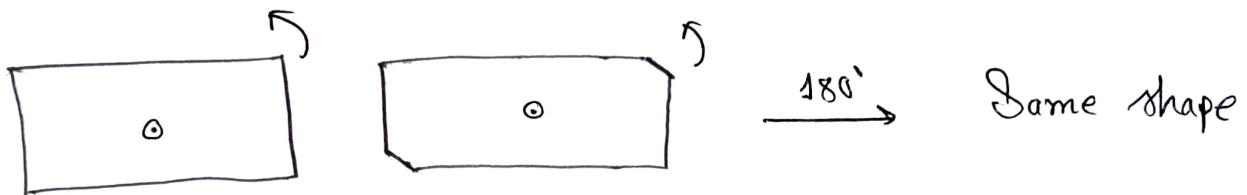
The translation of a cell by lattice vector \vec{R} obviously take the lattice to itself and hence is a symmetry operation. However, there are various other symmetry operations.

1. Rotational symmetry: A typical symmetry operation is that of rotation about an axis that passes through a point. If an object/cell is rotated about the axis by some particular angle and looks the same, then the object/cell is called rotationally symmetric. The rotation axis is called n-fold if the angle of such rotation is $\frac{2\pi}{n}$. For example,

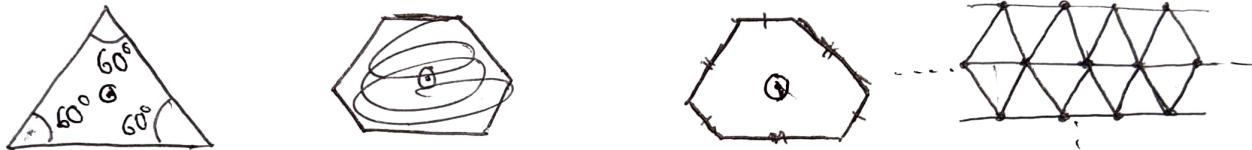
(i) 1-fold rotation: This is trivial. The object/cell takes it into itself after 2π rotation about an axis.



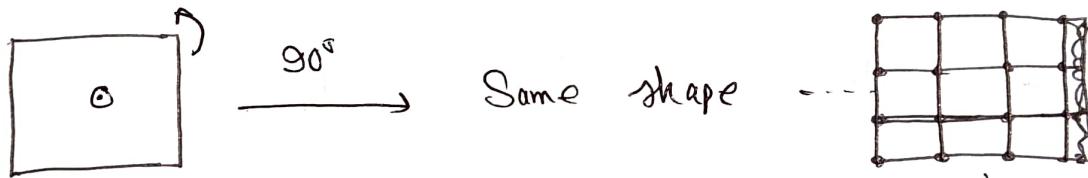
(ii) Two-fold rotation: Object/cell takes it into itself after 180° rotation.



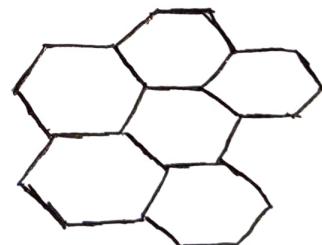
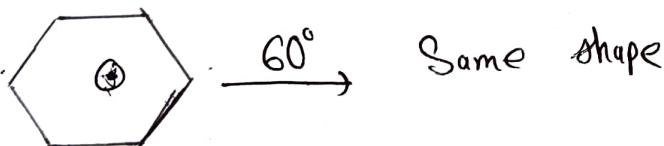
(iii) Three-fold rotation: ... after 120° rotation



(iv) Four-fold rotation: ... after 90° rotation



✓ Six fold rotation: ... after 60° rotation.



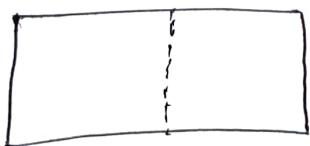
Although there are five fold and seven fold rotationally symmetric objects, these are not possible in lattice structures. If we try to produce a crystal structure on higher fold

ture with objects having 5-fold and 7-fold rotational symmetry, we will fail to construct a lattice, since we can't fill the area of a plane with connected pentagons or heptagons.

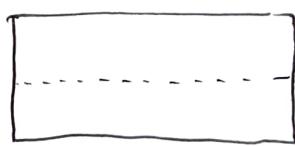


Trying with pentagon (with terrible drawing skill)

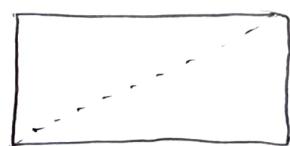
2. Reflection plane (mirror symmetry): The operation is done by imagining that you cut the object(cell) into half and place a mirror next to one of the halves along the cut. If the ~~refl~~ reflection produces the other half, then the object (cell) have mirror symmetry. Reflection plane is such a plane that, when a mirror reflection is performed in this plane, the cell remains invariant.



Mirror symmetry



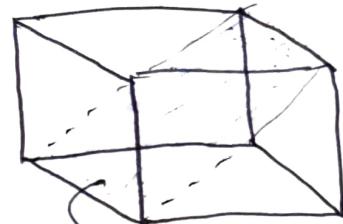
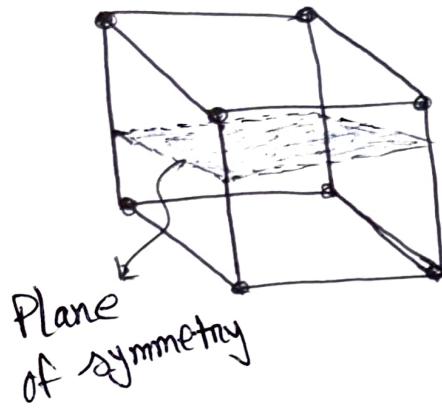
Mirror symmetry



Not a mirror symmetry



Reflection



Plane of symmetry

3. Inversion operation: A cell has an inversion center if there is a point at which the cell remains invariant when the transformation $\vec{R} \rightarrow -\vec{R}$ is performed on the cell with respect to the inversion center. All Bravais lattices are inversion symmetric, for, with every lattice vector $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$, there is an associated inverse lattice vector $\vec{R}_{-n} = -\vec{R}_n = -n_1 \vec{a}_1 - n_2 \vec{a}_2 - n_3 \vec{a}_3$.

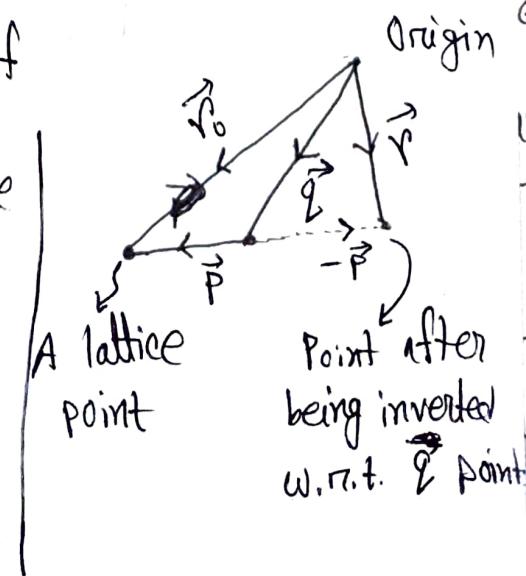
All Bravais lattice should have inversion centers.

To illustrate this, consider a point which has a position of \vec{q} with respect to some lattice point origin. We will invert the point w.r.t.

\vec{q} , so that if the position of the lattice point w.r.t. \vec{q} is \vec{P} , the

inverted point will be given by $-\vec{P}$ w.r.t. \vec{q} . Say, the lattice point

has a position vector \vec{r}_0 from the



origin and the inverted point has a position of \vec{r}^o from the origin.

$$\text{Now, } \vec{q} + \vec{P} = \vec{r}_o \Rightarrow \vec{P} = \vec{r}_o - \vec{q}$$

$$\text{and, } \vec{q} - \vec{P} = \vec{r}^o$$

$$\Rightarrow \vec{q} - (\vec{r}_o - \vec{q}) = \vec{r}^o$$

$$\therefore \vec{r}^o = 2\vec{q} - \vec{r}_o$$

Now, if $2\vec{q}$ is a point in the lattice, then \vec{r}^o must be another point in the lattice (this is so, since, if $2\vec{q}$ is a lattice point, this must be of the form $\vec{r}' = n'_1 \vec{a}_1 + n'_2 \vec{a}_2 + n'_3 \vec{a}_3$, and so is \vec{r}_o . So, \vec{r}^o must also be of the same form, and hence a lattice point). So, the inversion of a lattice point w.r.t. $2\vec{q}$ maps it to another lattice point, and hence $2\vec{q}$ is an inversion center. For example, in the previous example, taking $2\vec{q} = \vec{a}_1 + \vec{a}_2 + \vec{a}_3$ guarantees a lattice point, and so $\vec{r}^o = \frac{1}{2}(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)$ is an inversion center. Also, if $\vec{q} = \vec{r}$, which is the position of any lattice point, $2\vec{q} = 2\vec{r}$ must also be a lattice point, and hence the point can serve as the inversion center.