

## CRYSTAL LATTICE

How to form a crystal?

1. Define the structure of the lattice
2. Define the lattice constant
3. Define the basis

Defining lattice: Mathematical construct; ideally infinite arrangement of points in space.

Bravais lattice: Array of an infinite number of discrete points that look *exactly* the same from any point.

Mathematically; arrangement of points with position vectors given by

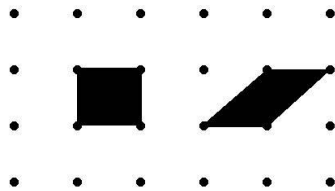
$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

where  $\mathbf{a}_i$  are three vectors all not on one plane and  $n_i$  cover all integer values.

Associate with Bravais lattice are one or more sets of primitive vectors  $\mathbf{a}_i$  that can translate any point in the lattice to any other point with a suitable set of integers  $n_i$

$$\hat{\mathbf{r}} = \mathbf{r} + n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

this implies that the Bravais lattice has translational symmetry. Note that the primitive vectors need not be unique!



**Figure 1: Non-universality of primitive vectors**

The volume defined by the primitive vectors is called the primitive cell/unit cell – smallest volume that can be constructed using the lattice points. Each such cell contains exactly one lattice point.

Defining Basis: Basis is whatever we put physically at the abstract lattice points – can be single atom/ion or groups of them. Each lattice point will have identical basis – this makes up the crystal structure.

**Lattice + Basis = crystal structure**

Co-ordination number: Number of nearest neighbours in a lattice. E.g. for simple cubic structure it is 6.

Examples of some important crystal structures:

Simple cubic: Co-ordination number 6; extremely rare in nature, only one element crystallizes in this form.

Body-centered cubic (BCC): Co-ordination number 8; quite common in nature e.g. alkali metals – can treat as simple cubic with a 2 atom basis or a lattice with a single atom basis with the primitive lattice vectors defined as  $\mathbf{a}_1 = \frac{a}{2}(\mathbf{y} + \mathbf{z} - \mathbf{x})$  and so on.

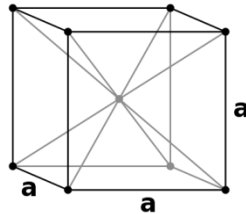


Figure 2: BCC structure

Face-centered cubic (FCC): Co-ordination number 12; again quite common in nature e.g. noble metals, Ni – can treat as simple cubic with a 4 atom basis or a lattice with a single atom basis with the primitive lattice vectors defined as  $\mathbf{a}_1 = \frac{a}{2}(\mathbf{y} + \mathbf{z})$  and so on.

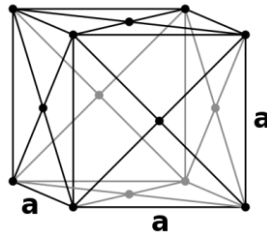


Figure 3: FCC structure

Hexagonal close-packed (HCP): *Not* a Bravais lattice – many elements (~ 30) crystallize in this form.

Think of stacking balls on top of each other – in some sense the most natural arrangement. In a-b plane forms close packed triangular lattice – stack them up along the c-axis by placing atoms on the alternate voids formed in the lower layer. If the arrangement is ABAB... then we get HCP; the arrangement ABCABC... gives FCC!

Both FCC and HCP are close packed structures – they can achieve the highest packing density of  $\frac{\pi}{3\sqrt{2}} \sim 0.74$  both have co-ordination number 12 - if the energy of the crystal depended only on the number of nearest neighbours then FCC and HCP would have had the same energy with no way to distinguish one over the other.

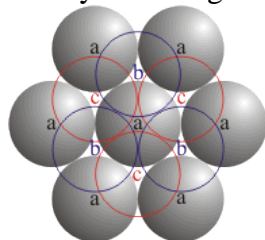


Figure 4: FCC closed-packed structure

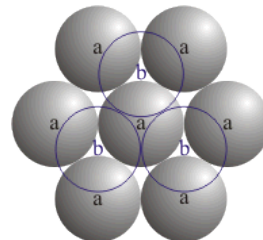
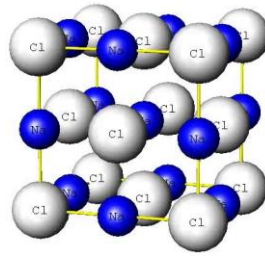


Figure 5: HCP structure

NaCl structure: Till now dealt with basis having same types of atoms. NaCl crystallizes with  $\text{Na}^+$  and  $\text{Cl}^-$  place at alternate sites in a simple cubic lattice – each ion has six ions of the other

species as its nearest neighbours. Describe the structure as FCC with a two point basis –  $\text{Na}^+$  at the origin and  $\text{Cl}^-$  at  $a/2(x + y + z)$  (at the center of the conventional cube).

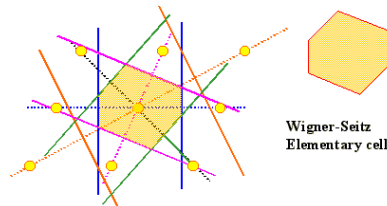


**Figure 6: NaCl structure**

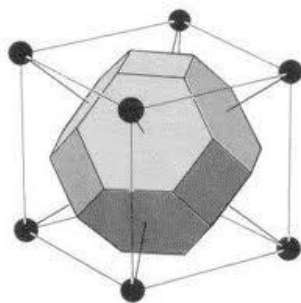
### Wigner-Seitz cell

The choice of unit cell depends on convenience – can however always choose one that reflects the full symmetry of the underlying lattice. A common choice is Wigner-Seitz cell.

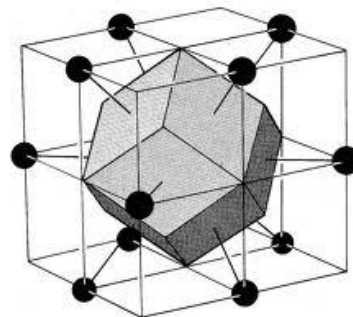
- Choose a zero point of the lattice
- Draw lines from your zero point to all neighbouring lattice points; take as many as you want - nearest neighbours, second-nearest neighbours, etc.
- Draw a plane (two-dimensional a line) that exactly bisects all of your lines at a right angle.
- A subset of all your planes will form some closed body, and that is your Wigner Seitz elementary cell.



**Figure 7: Wigner Seitz cell**



**Figure 8: Wigner-Seitz cell for BCC structure**



**Figure 9: Wigner-Seitz cell for FCC structure**

## Reciprocal Lattice

Consider a Bravais lattice formed by a set of points  $\mathbf{R}$ . A wave of any arbitrary wave-vector  $\mathbf{K}$  will not have the full periodicity of the lattice. To be periodic

$$e^{i\mathbf{K}\cdot(\mathbf{R}+\mathbf{r})} = e^{i\mathbf{K}\cdot\mathbf{r}}$$

for any  $\mathbf{r}$  and all  $\mathbf{R}$  in the Bravais lattice

This condition gives

$$e^{i\mathbf{K}\cdot\mathbf{R}} = 1 \quad (1)$$

The set of all such vectors  $\mathbf{K}$  forms a lattice – Reciprocal lattice – conjugate lattice in the momentum space. Reciprocal lattice is the Fourier transform of the real space lattice.

### How to form Reciprocal lattice?

If the primitive lattice vectors are  $\mathbf{a}_i$ , then the primitive vectors of the reciprocal lattice are given by

$$\mathbf{b}_i = \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \mathbf{a}_j \times \mathbf{a}_k}$$

Proof: Given the vectors  $\mathbf{b}_i$  defined above, any vector  $\mathbf{K}$  can be written as their linear combination as  $\mathbf{K} = \sum_i k_i \mathbf{b}_i$ . If  $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$  for  $\mathbf{R} = \sum_i n_i \mathbf{a}_i$  then  $\sum_i k_i n_i = 2\pi(\text{integer})$  for any arbitrary  $n_i$ . This implies that  $k_i$  must all be integers. So all vectors that satisfy eqn. 1 can be written as linear combinations of  $\mathbf{b}_i$  with integer coefficients. This implies that the reciprocal lattice is a Bravais lattice and that  $\mathbf{b}_i$  are its primitive vectors.

### **The reciprocal lattice of the Reciprocal lattice is the Bravais lattice.**

Examples of reciprocal lattice:

1. Simple cubic: The reciprocal lattice of a SC lattice of lattice vectors  $\mathbf{a}_i$  is a SC lattice with lattice vectors  $\mathbf{b}_i = 2\pi/a \mathbf{i}$ .
2. FCC: Reciprocal lattice of FCC lattice with conventional cube sides of length  $a$  is a BCC with cube of side  $4\pi/a$  and *vice-versa*.

First Brillouin zone: The Wigner-Seitz cell of the reciprocal lattice is called the first Brillouin zone.

### Relation between lattice planes and reciprocal lattice points:

The direct lattice can be decomposed into a family of lattice planes - parallel equally spaced lattice planes that contain all the points in the direct lattice.

For every reciprocal lattice vector  $\mathbf{K}$  there is a family of lattice plains perpendicular to it with spacing  $d$ , where  $2\pi/d$  equals the length of the smallest reciprocal lattice vector parallel to  $\mathbf{K}$ . Conversely, for every family of lattice plains with a spacing  $d$  there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length  $2\pi/d$ .

Proof: Remember that for  $\mathbf{K}$  to be a reciprocal vector we should have  $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$  for all values of  $\mathbf{R}$ . Given a set of planes with separation  $d$  let  $\mathbf{K}$  be a wave vector  $\frac{2\pi}{d}\mathbf{n}$  where  $\mathbf{n}$  is the unit vector normal to the planes. The plane wave  $e^{i\mathbf{K}\cdot\mathbf{r}}$  should have the same value at all points  $\mathbf{r}$  which lies in planes perpendicular to  $\mathbf{K}$  and separated by a length  $\frac{2\pi}{K} = d$ . Since the origin lies in one such plane,  $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$  for all points in the Bravais lattice showing that  $\mathbf{K}$  is a reciprocal lattice vector. It is the smallest reciprocal lattice vector perpendicular to the planes being considered because any smaller vector will have a wavelength larger than  $d$  and hence cannot have the symmetry of the real lattice.

Miller indices: How to label family of planes? Take advantage of the fact that with each family of planes is associated a *unique* reciprocal lattice vector. If the shortest reciprocal lattice vector perpendicular to a family of planes is  $h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$  then the family of planes is labeled by the Miller indices  $(hkl)$ .

What does it mean physically? A plane with Miller indices  $(hkl)$  is perpendicular to a reciprocal lattice vector  $\mathbf{K} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ , so its equation is  $\mathbf{K}\cdot\mathbf{r} = C$  where  $C$  is a constant. Suppose that the plane intersects the real lattice axes at  $n_1\mathbf{a}_1$ ,  $n_2\mathbf{a}_2$  and  $n_3\mathbf{a}_3$ . Since these three points lie on the plane, we have  $\mathbf{K}\cdot n_1\mathbf{a}_1 = \mathbf{K}\cdot n_2\mathbf{a}_2 = \mathbf{K}\cdot n_3\mathbf{a}_3 = C$  implying that  $n_1 = C/2\pi h$  and so on. So the Miller indices are inversely proportional to the intercepts that the planes make on the real space lattice.