

## UNIT – I

### CRYSTAL PHYSICS

Many of the properties of solid materials depend mainly on their crystal structures. Based on the arrangement of atoms and molecules, the solid material classified as follows

#### Crystalline Material

*The periodic arrangement of atoms in all three dimensions space is called crystal.* It has regular shape and when it is broken, all broken pieces have the same regular shape. It has sharp melting point. The physical properties of the crystal vary with direction and therefore they are called *anisotropic* substances. It may be made up of metallic crystals or non-metallic crystals.

**Examples:** Cu, Al, W, Mg, Carbon, crystalized polymer and plastics.

#### Non-Crystalline Material

*Random arrangement of atoms in all three dimensions space is called non-crystalline material or amorphous.* They have no directional properties and therefore they are called *isotropic* substances. They do not possess any regular shape and they have a wide range of melting points.

**Examples:** Glass and Rubber.

#### Fundamental Definitions

##### Space Lattice

A regular and periodic arrangement of infinite number of points in three



Lattice

dimensions space is known as space lattice. Every point in this arrangement is identical to that of every other point.

##### Basis (Motif)

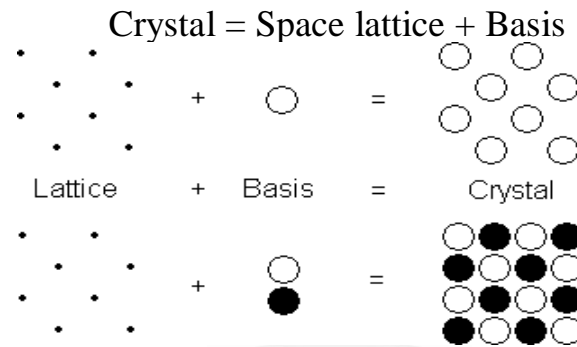
*A group of atoms in every lattice point is called basis or motif.*



Basis

##### Crystal

*A crystal is defined as regular and periodic arrangements of atoms or molecule in three dimensional spaces.*



It can be classified into two types. They are,

1. Single Crystal
2. Polycrystalline Material

### 1. Single Crystal

The entire crystalline material consists of only one crystal is known as single crystal.

*Example:* KDP, ADP.

### 2. Polycrystalline Material

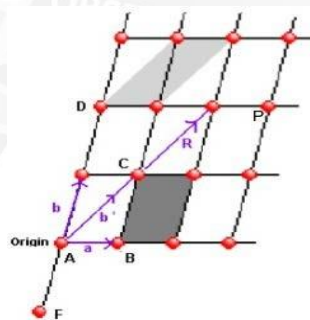
A collection of many small crystals are separated by well-defined boundaries is called polycrystalline materials.

*Example:* GaP, GaAs, ZnO and ZnS.

### Fundamental translation vector

*Mathematical representation of position vector in the space lattice is called fundamental translation vector.*

In two dimension  $R = n_1a + n_2b$



In three dimension  $R = n_1a + n_2b + n_3c$

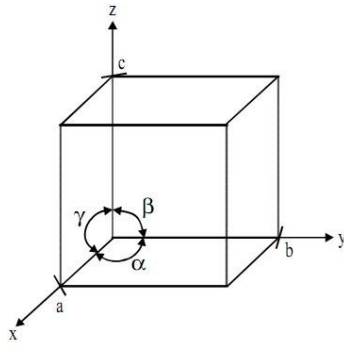
Where,  $a$ ,  $b$  and  $c$  are the fundamental translation vectors and  $n_1$ ,  $n_2$  and  $n_3$  are the integers.

### Interfacial angle

*The angles between the three crystallographic axes are known as interfacial*

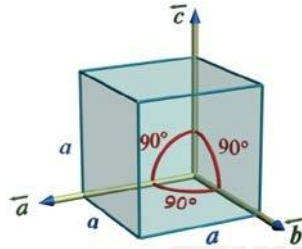
*angles.*

*Generally it's are represented as  $\alpha$ ,  $\beta$  and  $\gamma$  respectively.*



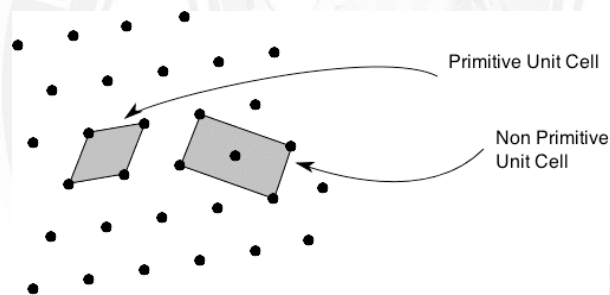
## Unit Cell

*The unit cell is a smallest geometric volume containing one or more atoms arranged in three dimension.* And also, it is called fundamental building block of a crystal structure.



## Primitive cell

*Primitive cell is the smallest volume unit cell which contains the lattice points at the corner*



only.

## Lattice Constant

The distance between any two successive lattice points along any three dimensional directions is called lattice constant.

### 1. MILLER INDICES

**Miller indices** are set of integers used to designate a plane in a crystal. They are the reciprocals of the intercepts made by the plane on the three crystallographic axes which are reduced to smallest whole numbers. They are represented as (h k l).

#### Procedure for finding Miller Indices

**Step 1:** The intercepts made by the plane along the axes X, Y and Z are noted.

**Step 2:** The coefficients of the intercepts are noted separately.

**Step 3:** Inverse is to be taken

**Step 4:** Find the least common multiple (*LCM*) and multiply each by this LCM to get the smallest whole number.

**Step 5:** The result is written in parenthesis.

This is called the 'Miller Indices' of the plane in the form (h k l).

### Important Features of Miller Indices

- A plane which is parallel to any one of the co-ordinate axes has an intercept at infinity ( $\infty$ ). Therefore the Miller index for that axis is zero; i.e. for an intercept at infinity, the corresponding index is zero.
- A plane passing through the origin is defined in terms of a parallel plane having non zero intercepts.
- All equally spaced parallel planes have same 'Miller indices'.
- If a normal to a plane (hkl), the direction of the normal is [hkl].
- If a plane cuts an axis on the negative side of the origin, corresponding index is negative.
- For a cubic system, the relation between interplanar distance and interatomic distance is given by  $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$
- The angle between any two crystallographic directions [h k l] and [h'k'l'] can be calculated as

$$\cos \theta = \frac{hh' + kk' + ll'}{(h^2 + k^2 + l^2)^{1/2} (h'^2 + k'^2 + l'^2)^{1/2}}$$

**Note:** while writing miller indices comma or dot between any two numbers may be avoided.

### 'd' Spacing (or) Interplanar Distance

'd' spacing or interplanar distance is the distance between two successive parallel planes in a crystal.

Consider a cubic crystal of side 'a', and a plane ABC as shown in figure. Let  $d_1$  be the distance between the origin and the first plane ABC. Let (h k l) be the Miller indices for the plane ABC. Let ON be the perpendicular distance drawn from the origin to the plane ABC. Let  $\alpha$ ,  $\beta$  and  $\gamma$  be the interfacial angles between co-ordinate axes X, Y, Z and ON respectively.

The intercepts of the plane on the three axes are  $OA = \frac{a}{h}$   $OB = \frac{a}{k}$   $OC = \frac{a}{l}$

From fig  $ON=d_1$  (for the plane ABC)

$$\Delta ONA \quad \cos \alpha' = \frac{ON}{OA} = \frac{d_1}{a/h} = \frac{d_1 h}{a}$$

$$\Delta ONB \quad \cos \beta' = \frac{ON}{OB} = \frac{d_1}{a/k} = \frac{d_1 k}{a}$$

$$\Delta ONC \quad \cos \gamma' = \frac{ON}{OC} = \frac{d_1}{a/l} = \frac{d_1 l}{a}$$

From the law of direction of cosines of any line,

$$\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1$$

$$\left(\frac{d_1 h}{a}\right)^2 + \left(\frac{d_1 k}{a}\right)^2 + \left(\frac{d_1 l}{a}\right)^2 = 1$$

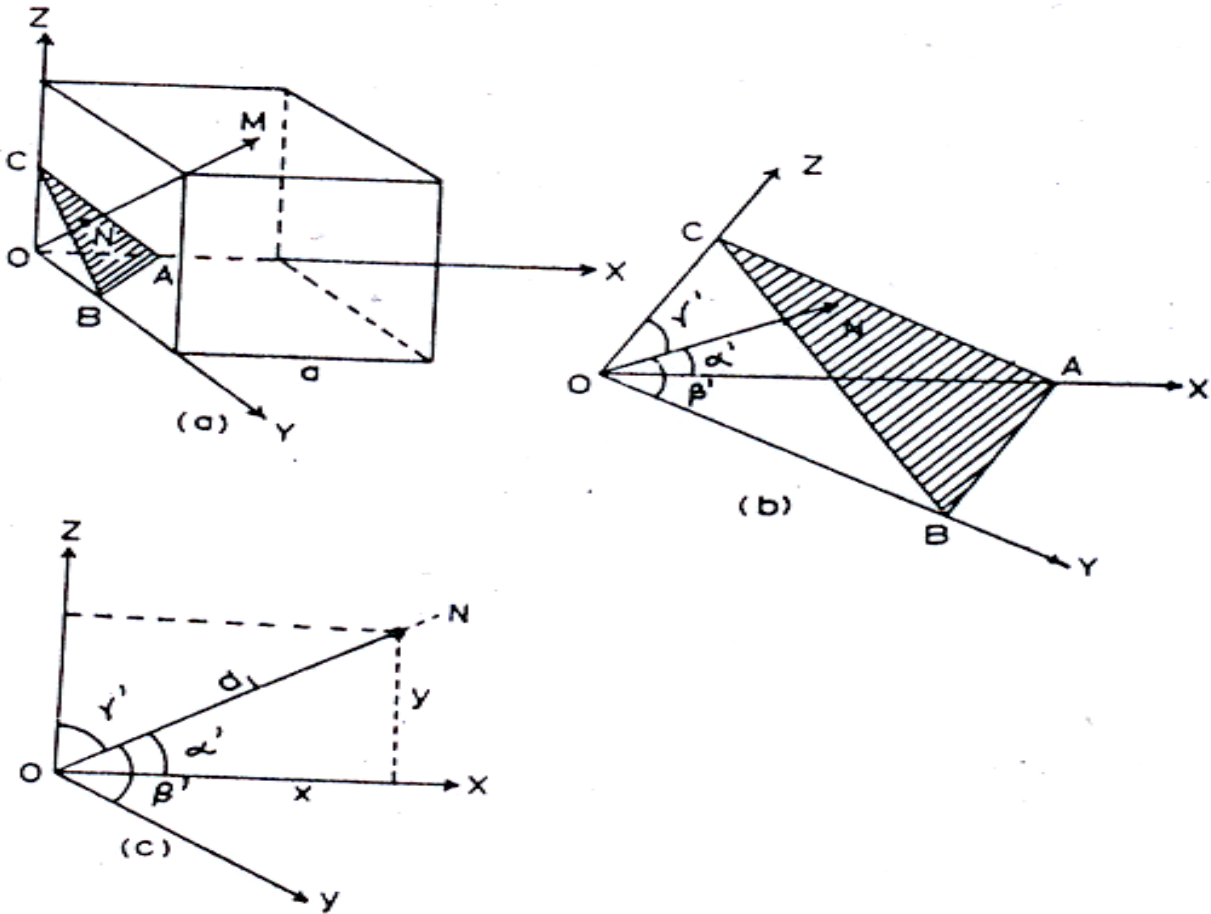
$$\frac{d_1^2}{a^2} [h^2 + k^2 + l^2] = 1$$

$$d_1^2 = \frac{a^2}{[h^2 + k^2 + l^2]}$$

$$d_1 = \frac{a}{[h^2 + k^2 + l^2]^{1/2}}$$

Similarly for the plane A'B'C'

$$d_2 = \frac{2a}{[h^2 + k^2 + l^2]^{1/2}}$$



The interplanar distance of planes with miller indices  $(hkl)$  is

$$d = d_2 - d_1$$

$$d = \frac{2a}{[h^2 + k^2 + l^2]^{1/2}} - \frac{a}{[h^2 + k^2 + l^2]^{1/2}} = \frac{a}{[h^2 + k^2 + l^2]^{1/2}}$$

$$d = \frac{a}{[h^2 + k^2 + l^2]^{1/2}} \dots\dots\dots (1)$$

This gives the relation between interplanar distance and interatomic distance.