

Crystallography

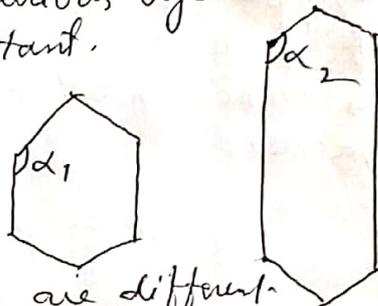
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6th sem.

Crystal is the intermediate state in between solid and liquid. Crystals are bounded by surfaces which are usually planar and arranged on a definite shape and structure. The definite shape of external are the rearrangement of internal shape.

Laws of crystallography

1. Steno's law: It states that the angles between the corresponding faces on various crystals of the same substances are constant.

$\alpha_1 = \alpha_2$
although shape of the crystals are not exactly same. That means shapes are different but angles remain the same.



2. Second law (Haüy's law): According to this law the crystals are made up of innumerable smaller crystals. If a crystal is suitably and continuously divided, we shall obtain smaller and smaller crystals. In this type of crystal we can draw a picture of definite concept regarding the geometrical shape.

The distance of the points where the standard face cuts are called intercepts.

$$x : y : z = pa : qb : rc$$

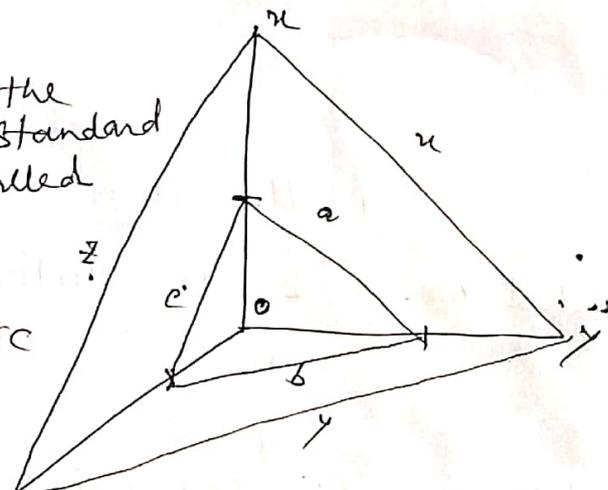
where p, q and

r the coefficients

which have integral numbers like 0, 1, 2, 3 etc. Suppose $p=1, q=2, r=3$

then $x : y : z = a : 2b : 3c$

$$\therefore x : y : z = 1 : 2 : 3$$



(2)

These ratios characterise and represent any plane of the crystal. The coefficients are called Weiss indices of the plane.

Suppose $x : y : z = 2a : b : 2c$.

In such cases the we Weiss indices have now been universally replaced by Miller indices. Miller indices are obtained by taking the reciprocal of the coefficients of a , b and c and when necessary the ratio is to be multiplied by the least common factor.

$$x : y : z = a : 2b : c$$

The coefficients are 1, 2, 1

$$\text{Miller indices } 1 : \frac{1}{2} : 1$$

$$2 : 1 : 2$$

Again suppose

$$x : y : z = a : 3b : 2c$$

$$\text{Miller indices} = 1, 3, 2 \text{ (coefficients)}$$

$$= \frac{1}{1} : \frac{1}{3} : \frac{1}{2}$$

$$= 1 : \frac{1}{3} : 0$$

$$\underline{\text{Miller indices}} = 3 : 1 : 0$$

What would be the Miller indices of

$$1 : 2 : 2 \text{ (Weiss)}$$

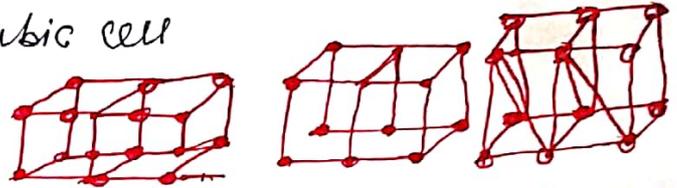
$$1 : 0 : 0 \text{ (Miller)}$$

We can thus say that if a face of a crystal makes intercepts OA , OB and OC where a , b and c are cutting points.

Crystallography and determination of structure:-

The structure of crystal can be determined with the known value of angle θ and distance between the successive lattice planes. When λ is known or unknown the pace of the crystal planes can be determined.

Suppose a simple cubic lattice having each corner of the cubic cell



The axes are x, y and z

The distance between two successive planes is d
we know

$$d = \frac{a}{\sqrt{h^2 + l^2 + k^2}}$$

$$d_{100} = \frac{a}{\sqrt{(1)^2 + (0)^2 + (0)^2}} = a$$

$$d_{110} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (0)^2}} = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{a}{\sqrt{(1)^2 + (1)^2 + (1)^2}} = \frac{a}{\sqrt{3}}$$

Hence ratio of distances

$$d_{100} : d_{110} : d_{111} = a : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}}$$

$$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \sqrt{2} : \sqrt{3}$$

Knowing the values of distances in between the crystal planes and from the known values edges and wavelength, the structure can be calculated.

Similarly calculations can be carried out of face centred cubic lattice and body centred cubic lattice at all.

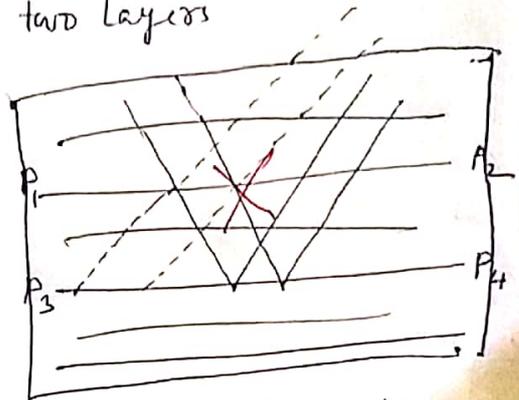
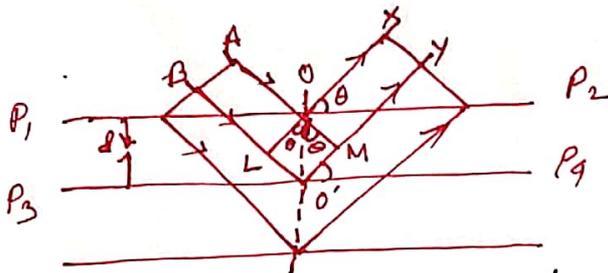
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Bragg's equation:-

Through the construction of crystal arrangement we can explain the distribution of atoms in regards to the reflection of beam. A beam of homogenous rays are allowed to pass through the plane where it diffracted, the surface may be different layers but for our's simplicity we shall consider two layers.

Suppose $P_1 P_2$ and $P_3 P_4$ are two layers



A and B are incident rays
 OX and $O'y$ are refracted rays which make angle θ with the normal drawn on the paper.
 here $\angle LO' = MO'$, $\angle MO'O = \theta$, $\angle LO'O = \theta$

$$\angle LO'O = 90^\circ - \theta$$

$$LO' + MO' = n\lambda \quad \text{where } \lambda \rightarrow \text{wave length} \quad \text{--- (1)}$$

$$LO' = MO' = OO' \sin \theta = d \sin \theta$$

Substituting in eqⁿ (1)

$$d \sin \theta + d \sin \theta = n\lambda$$

$$\boxed{2d \sin \theta = n\lambda}$$

For a given set of planes, d is a fixed value
 If homogenous X rays are diffracted having wave length λ and number of positions corresponding to $n = 1, 2, 3$ then

$$\theta = \sin^{-1} \left(\frac{\lambda}{2d} \right) \quad \text{--- 1st order reflection}$$

$$\theta = \sin^{-1} \left(\frac{\lambda}{2d} \right) \quad \text{--- 2nd " "}$$

$$\theta = \sin^{-1} \left(\frac{\lambda}{2d} \right) \quad \text{--- 3rd " "}$$

These equations are known as Bragg's eqⁿ.