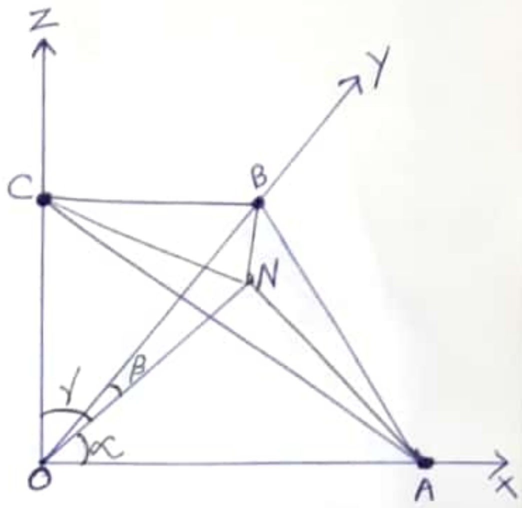
INTERPLANAR SPACING (d_{hkl})

The perpendicular distance between two successive parallel lattice planes is known as interplanar distance (d)

Consider a plane ABC with Miller Indices (hkl). To find the interplanar distance, consider a plane parallel to ABC and passing through the origin O. Then the length of the ⊥ normal from origin to plane ABC gives the distance 'd'. Let the normal makes an angle α, β, γ with X, Y, Z axes.



Then $ON = d$, x intercept(OA) = a/h
Y intercept(OB) = b/K
Z intercept(OC) = c/l

ΔONA, $\cos\alpha = \frac{ON}{OA} = \frac{d}{a/h}$

ΔONB, $\cos\beta = \frac{ON}{OB} = \frac{d}{b/K}$

ΔONC, $\cos\gamma = \frac{ON}{OC} = \frac{d}{c/l}$

The law of direction cosines is $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$

$$\therefore \left(\frac{d}{a/h}\right)^2 + \left(\frac{d}{b/K}\right)^2 + \left(\frac{d}{c/l}\right)^2 = 1$$

$$d^2\left[\frac{h^2}{a^2} + \frac{K^2}{b^2} + \frac{l^2}{c^2}\right] = 1$$

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{K^2}{b^2} + \frac{l^2}{c^2}}}$$

For cubic system $a = b = c$

$$\boxed{d_{hkl} = \frac{a}{\sqrt{h^2 + K^2 + l^2}}}$$

Note:
Relation b/w atomic radius (r) and lattice const (a)

SC: $r = \frac{a}{2}$

BCC: $r = \frac{\sqrt{3}\,a}{4}$

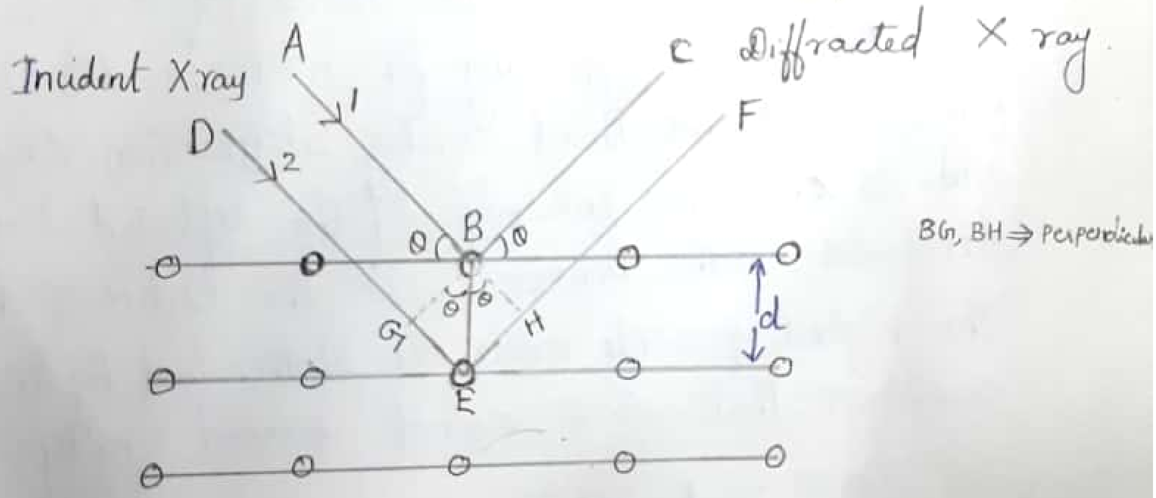
FCC: $r = \frac{\sqrt{2}\,a}{4}$

X Ray Diffraction (XRD)

The knowledge of crystal structure has been obtained from X ray diffraction experiment. X rays are high energy radiations of very short wavelength (~ 1A°). Diffraction of waves occur when the waves are scattered by a periodic arrays of scattering centres separated by a distance of the order of a wavelength. A plane grating is a device used to study diffraction of light. ~~which~~ It is made by ruling thousands of parallel lines on a piece of glass such that spacing between the lines ruled on the grating should be of the order of wavelength of light used. In a crystalline solid the atoms are very closely distributed in crystal planes. The dimension of atoms and the interatomic spacing in a crystal are of the order of 2 to 5A°, which is of the order of wavelength of X rays. In view of this the scientist Laue suggested that a crystal acts as a natural three dimension grating for X rays, where three dimensional array of regularly spaced atoms serve the role of parallel ruled lines.

BRAGG'S LAW

W.H. Bragg and W L Bragg explained the X-ray diffraction from a crystal. A crystal may be regarded as a set of parallel planes of atoms called Bragg Planes. These Bragg planes constitute the crystal grating. When X rays (have same order of wavelength as that of atomic dimensions) are incident on a crystal, X rays are reflected by the Bragg planes and they undergo interference. This is called Bragg diffraction or Bragg reflection. Braggs derived a mathematical relationship which serves as the condition for Bragg reflection to occur. This condition is called Bragg's Law



To obtain Bragg's law consider a set of parallel atomic planes with interplanar spacing 'd'. Let parallel beam of X rays of wavelength 'λ' be incident on these parallel planes at a glancing angle θ. Consider two such rays 1 and 2, which incident on the first two planes and get reflected at same angle θ. Diffraction is the consequence of constructive interference of these reflected rays.

For constructive interference of ray 1 and 2, their path difference must be an integral multiple of wavelength λ, i.e

$$\text{Path difference } \delta = n\lambda$$

$$GE + EH = n\lambda$$

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

$\Delta BGE \Rightarrow \sin\theta = \frac{GE}{BE}$

$\Delta BHE \Rightarrow \sin\theta = \frac{EH}{BE}$

$\Rightarrow 2BE\sin\theta = n\lambda$

$BE = d$ is the interplanar spacing

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

This is called Bragg's Law. The diffraction takes place for those values of θ, d, λ and n which satisfy the Bragg's condition

In Bragg's law 'n' represents order of reflection. For the given value of d and λ, higher order reflections appear for larger values of θ. The diffraction lines appearing for $n=1, 2,$ and 3 are called first, second, and third order diffraction respectively and so on. The intensity of the reflected lines decreases with increase in the value of n or θ.

The highest possible order is determined by the condition that $\sin\theta$ cannot exceed unity

$\sin\theta \leq 1$ $\therefore$ λ must be $\leq d$ for Bragg reflection

Taking $d \simeq 10^{-10}$ m, we obtain $\lambda \leq 10^{-10}$ m or 1Å.

X rays having wavelength in this range. Therefore, X rays are prefered for analysis of crystal structures.