

# X-ray diffraction

→ X-rays

→ Diffraction → rays are diffracted  
↓

When there will be any obstacle.

→ atoms

↓  
arranged in lattice plane.

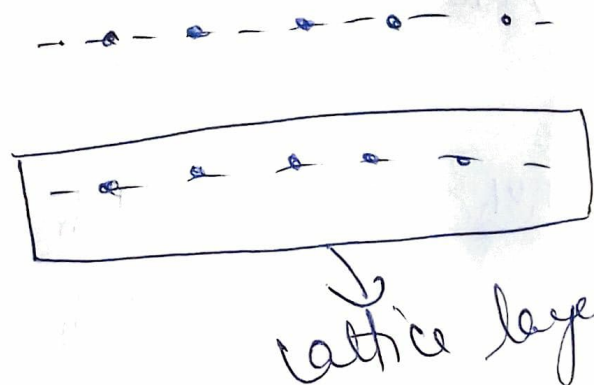
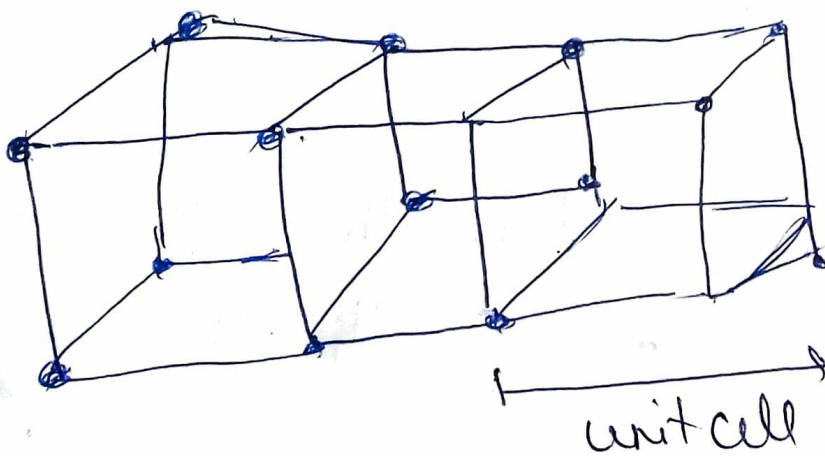
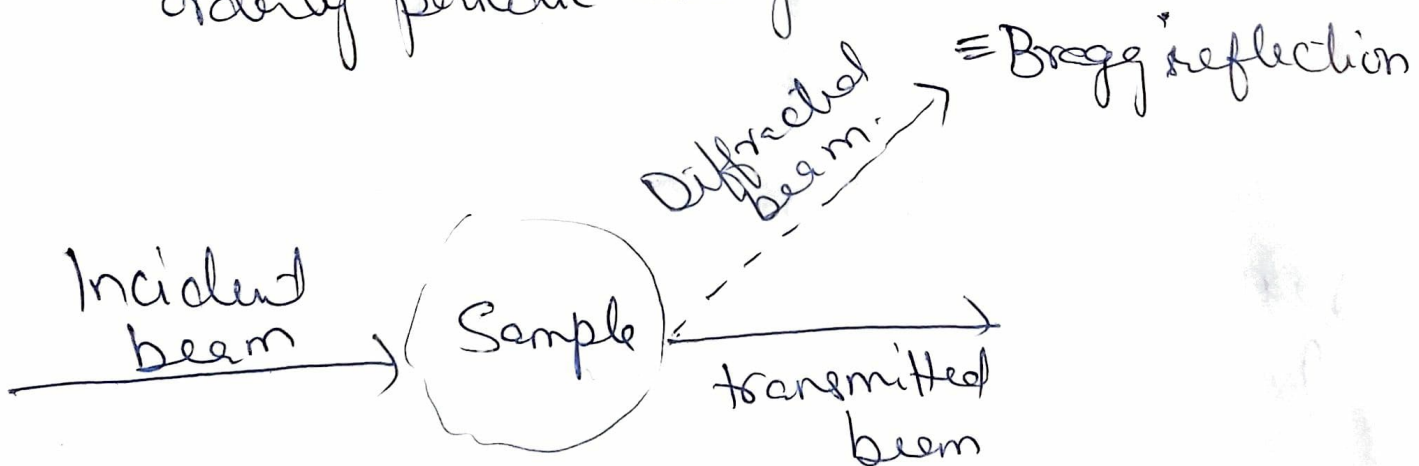
→ solid

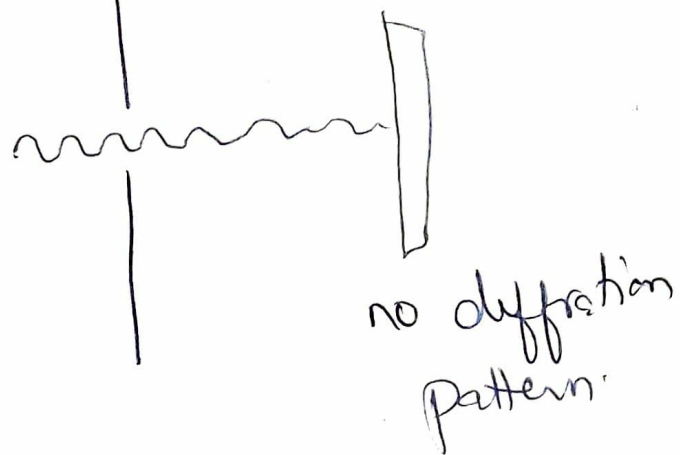
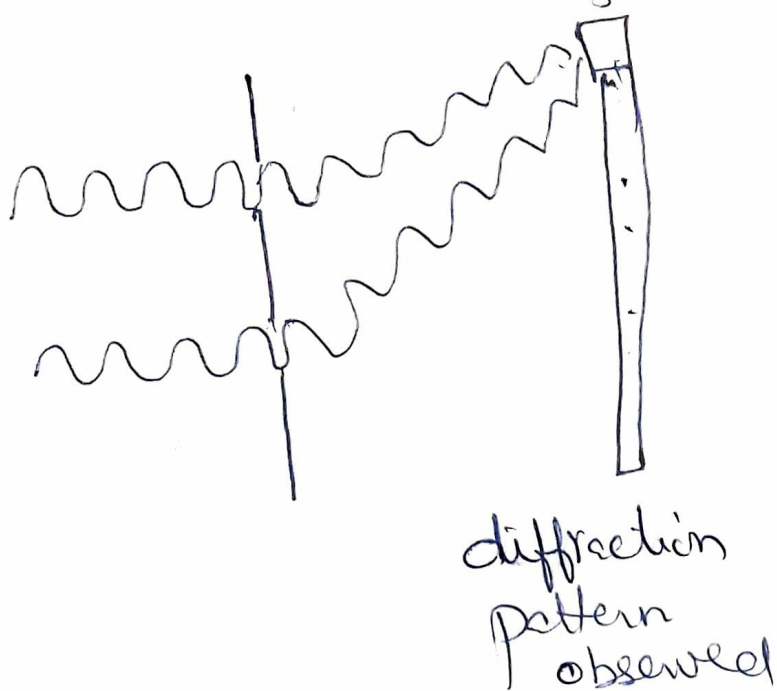
↓

crystal

↓

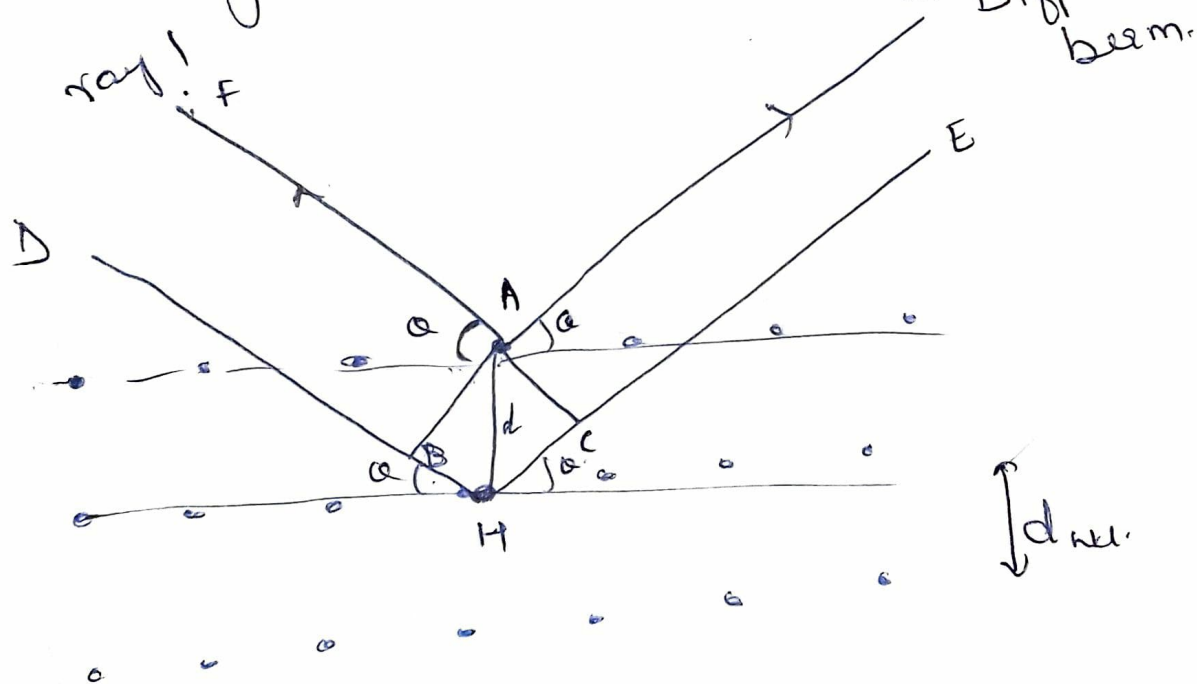
atoms are arranged in orderly periodic arrangement





Visible light  $\rightarrow 10^{-6} \text{ m}$

X-ray  $\rightarrow 10^{-10} \text{ m}$   $\rightarrow$  no pattern

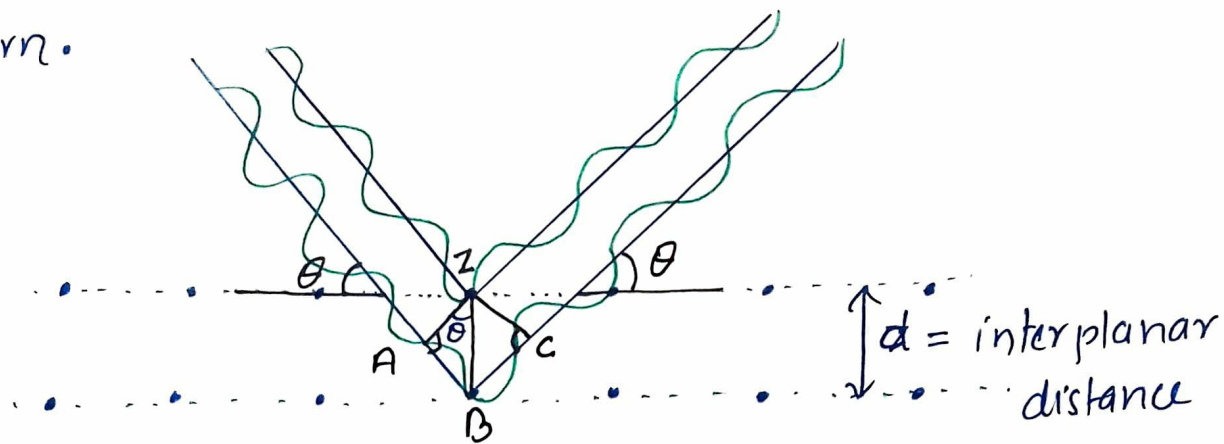


Bragg's  
 $\rightarrow$   
 Path difference =  $n\lambda$   
 $\downarrow$   
 constructive interference

$\theta$  = Glancing angle



produces constructive interference pattern.

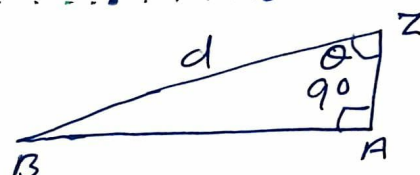


$\theta$  = Angle of incidence

$d$  =  $BZ$  interplanar distance

$AZ$  &  $CZ$  are perpendicular on  $AB$  and  $AC$  respectively

$\lambda$  = wavelength of X-ray.



—  $AB + BC$  distance will be travelled by whole number multiple of wavelength  $\lambda$ .

$$n\lambda = AB + BC$$

$$n\lambda = 2AB \quad \text{--- (i) (Since } AB = BC \text{)}$$

From triangle  $ABZ$ ;  $\sin \theta = \frac{AB}{BZ} = \frac{AB}{d}$

$$AB = d \sin \theta \quad \text{--- (ii)}$$

From equation (i) & (ii)

$$\boxed{n\lambda = 2d \sin \theta} \Rightarrow \text{Bragg's equation}$$

$$n = 1, 2, 3, 4, \text{ etc.}$$

— Constructive interference of wave 1 & 2 occurs only when, their path difference is  $n$  (whole no.) multiple of the wave length occurs.

# Miller Indices



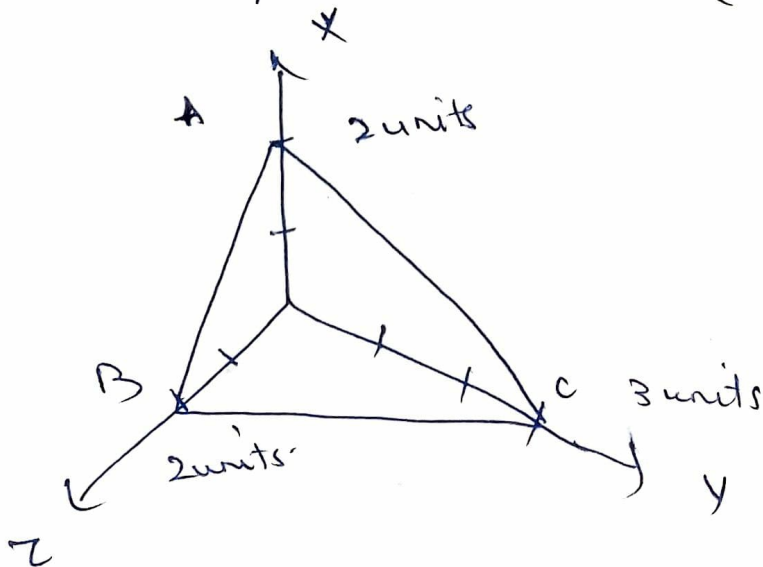
Indication of crystal planes  
Specify direction & planes

$(hkl) \rightarrow$  plane at  $x, y, z$  axis

reciprocals of the intercepts made  
by the plane.

## Steps

- ① Intercepts along  $x, y, z \rightarrow a, b \& c$  lattice constant
- ② Reciprocal
- ③ LCM & multiply each
- ④ Result in parenthesis  $\rightarrow$  miller indices  $(hkl)$



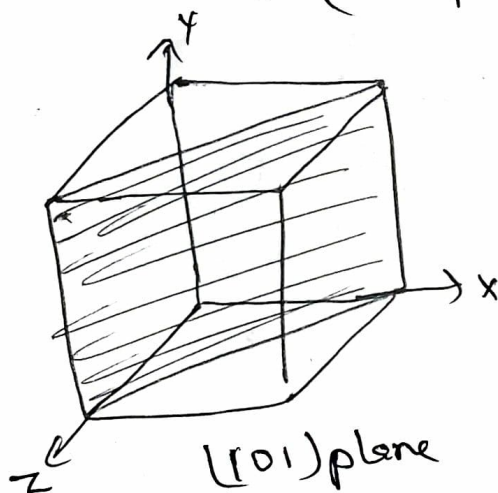
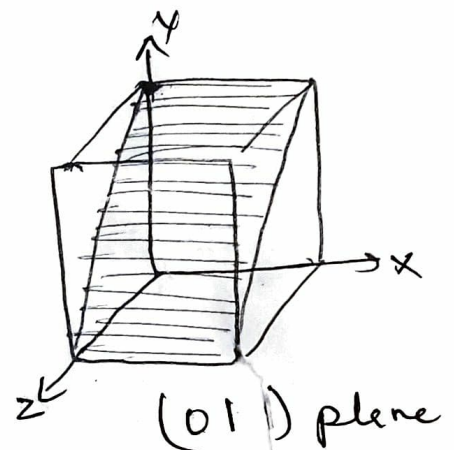
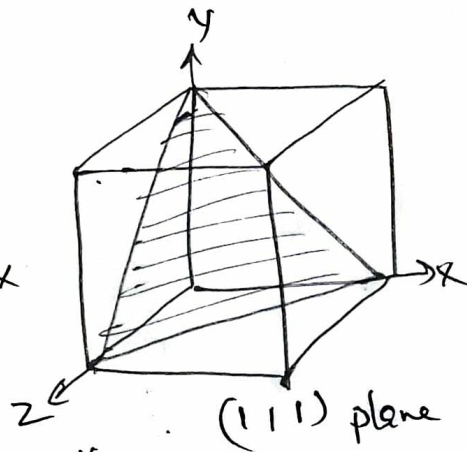
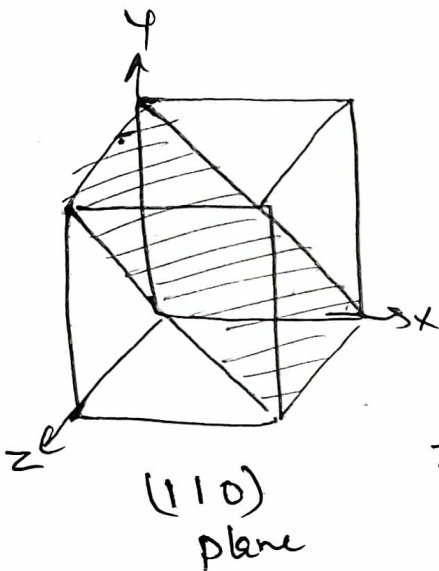
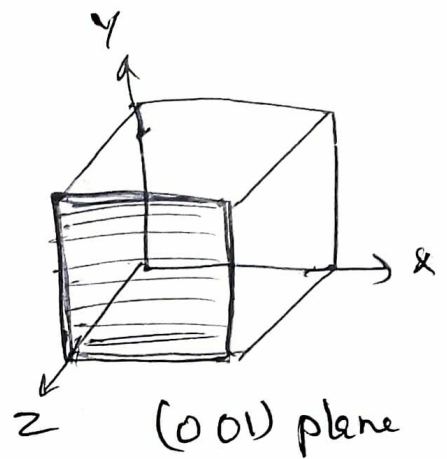
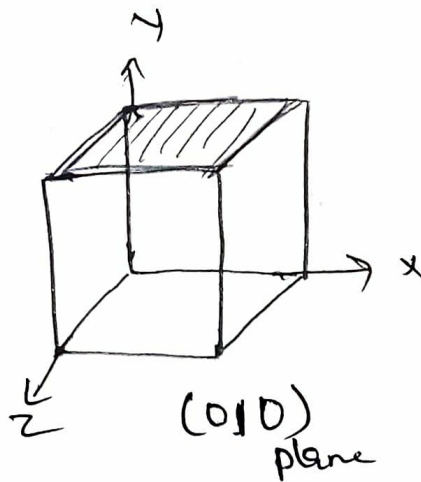
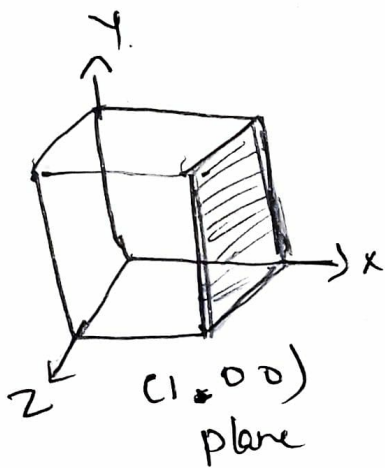
<u>Miller Indices</u>				
	<u>Intercept</u>	<u>Reciprocal</u>		M.I
x axis	2	$\frac{1}{2}$	$\frac{6}{2}$	3
y axis	3	$\frac{1}{3}$	$\frac{6}{3}$	2
z axis	2	$\frac{1}{2}$	$\frac{6}{2}$	3

Miller Indices for plane ABC  
is (323)

Imp pt ① → plane || to any coordinate  
↓  
intercept  $\infty$   
↓  
M.I = 0 for that axis

② plane cut on -ve side of the origin  
↓  
M. Index will be -ve  
↓  
( $\bar{1}00$ )





Example Calculate miller indices for the plane intersecting  
at  $x = \frac{1}{4}$ ,  $y = 1$ ,  $z = \frac{1}{2}$

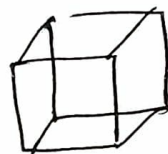
	<u>Intercept</u>	<u>Reciprocal</u>
x	$\frac{1}{4}$	4
y	1	1
z	$\frac{1}{2}$	2

$\therefore$  Miller Indices  
(4  $\bar{1}$  2)

Interplanar Spacing ( $d_{hkl}$ ): is the sep<sup>n</sup> b/w sets of parallel planes formed by the individual cells in a lattice structure, depends on the radii of the atoms forming the structure as well as on the shape of the structure.

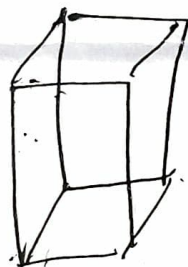
Interplanar spacing,  $d$  for a cubic structure of lattice parameter  $a$ , is given by:

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



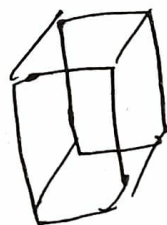
$a = b = c$   
 $\alpha = \beta = \gamma = 90^\circ$   
 cubic

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2}} + \frac{c}{\sqrt{l^2}}$$



$a = b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
 tetragonal

$$d_{hkl} = \frac{a}{\sqrt{h^2}} + \frac{b}{\sqrt{k^2}} + \frac{c}{\sqrt{l^2}}$$



$a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$   
 orthorhombic