Lecture 4
Crystal Structure

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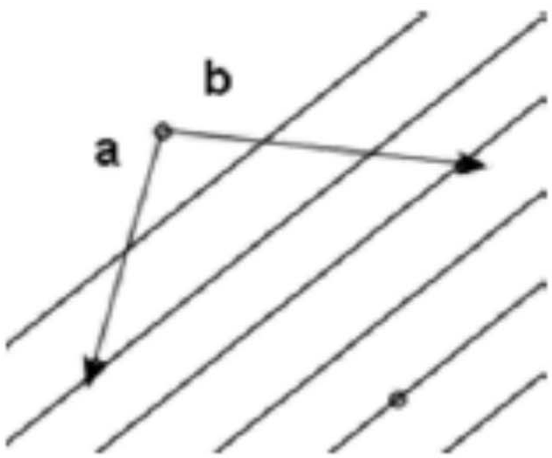
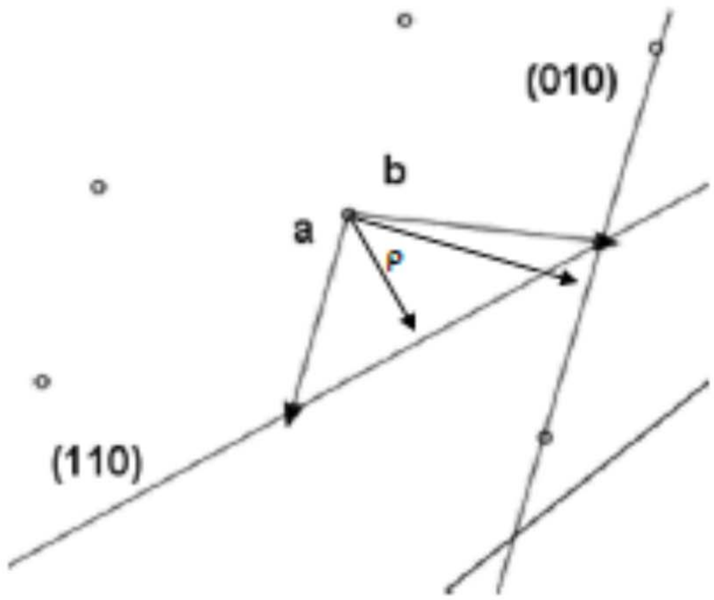
Chapter 4
OR Solid state physics, Kittel (Wiley)

Interplanar distances and angles

The **interplanar** distance d_{hkl} is defined to be the distance from the origin of the unit cell to the (hkl) plane nearest the origin along the normal to the plane, *i.e.* the perpendicular distance from the origin to the plane.

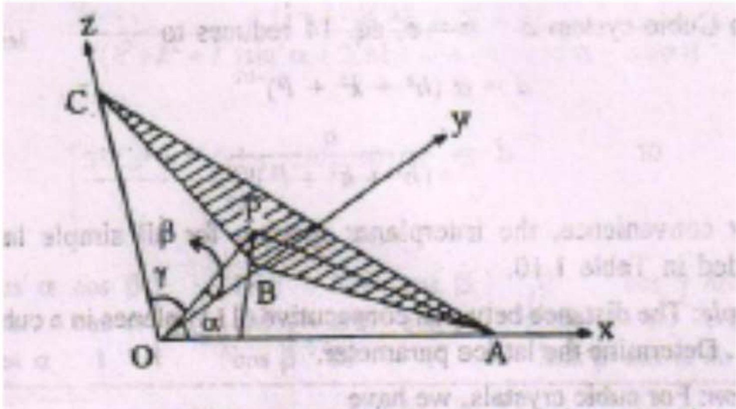




Interplanar Spacing

Assume that a plane (h k l) parallel to the plane passing through the origin makes intercepts on three axes are given by

OA=a / h
OB=b / k
OC=c / l



(hkl) plane intercepting *x*, *y*, and *z* axes at *A*, *B* and *C*, respectively

$$\cos\alpha = \frac{OP}{OA} = \frac{d}{(a/h)}, \quad \cos\beta = \frac{OP}{OB} = \frac{d}{(b/k)}$$

$$\cos\gamma = \frac{OP}{OC} = \frac{d}{(c/l)}$$

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

$$\frac{d^2}{(a/h)^2} + \frac{d^2}{(b/k)^2} + \frac{d^2}{(c/l)^2} = 1$$

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

So that
$$d = \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]^{-1/2}$$

(i) Tetragonal system : $a = b \neq c$,

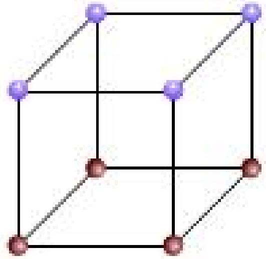
$$d = \left[\frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}\right]^{-1/2}$$

(ii) Cubic system $a = b = c$,

$$d = a\,(h^2 + k^2 + l^2)^{-1/2}$$

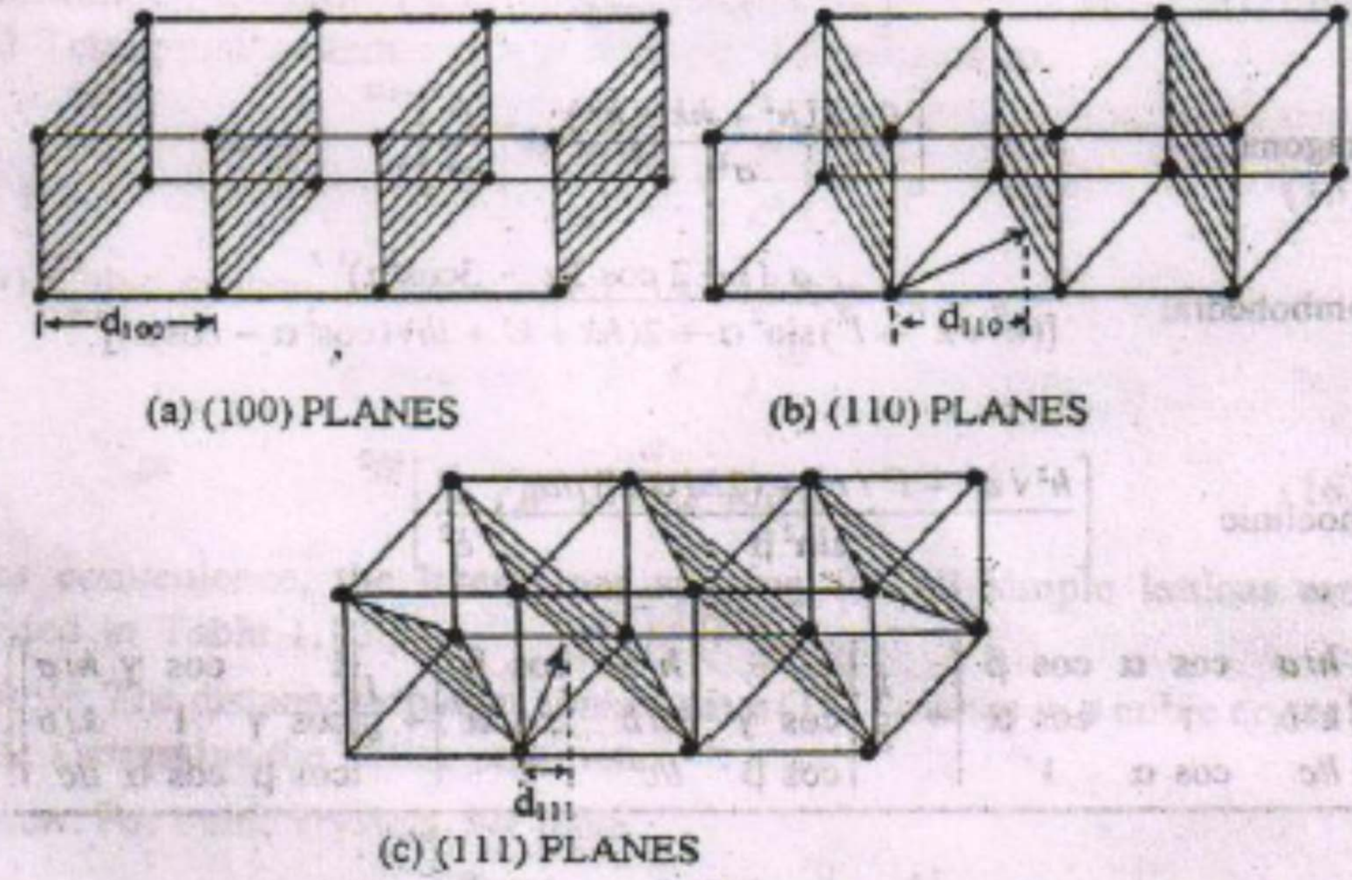
or
$$d = \frac{a}{(h^2 + k^2 + l^2)^{1/2}}$$

Interplanar Spacing in Simple Cubic Lattice



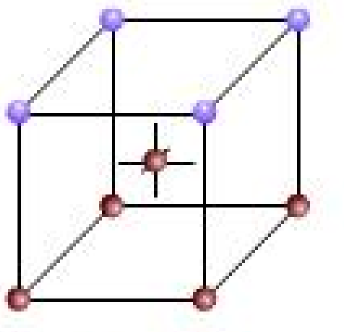
$$d_{100} = a,\ d_{110} = \frac{a}{\sqrt{2}} \text{ and } d_{111} = \frac{a}{\sqrt{3}}$$

Hence their ratio is



Low index planes in simple cubic crystal: (a) (100) planes (b) (110) planes (c) (111) planes

Interplanar Spacing in Body Centred Cubic Lattice

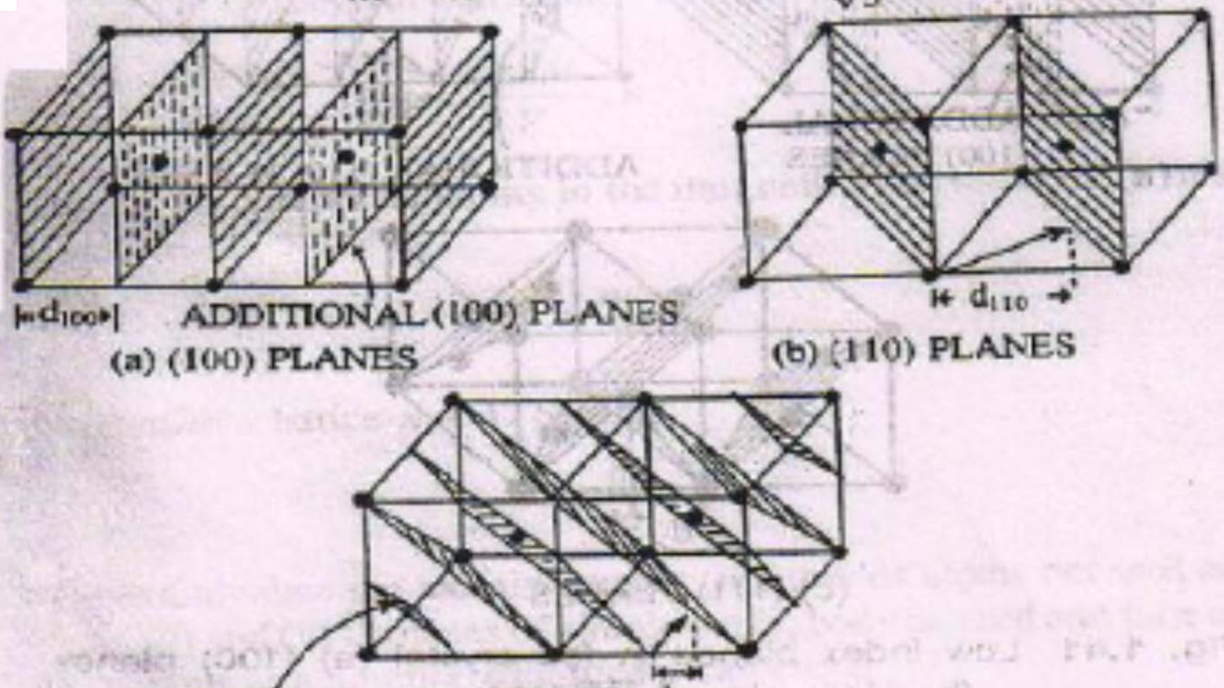


$$d_{100} = \frac{1}{2}\,(d_{100})\ \text{simple cubic lattice} = \frac{a}{2}$$

$$d_{110} = (d_{100})\ \text{simple cubic lattice} = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{1}{2}\,(d_{111})\ \text{simple cubic lattice} = \frac{a}{2\sqrt{3}}$$

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



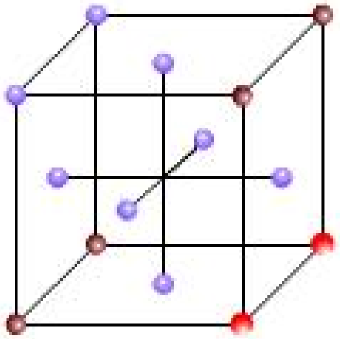
(a) (100) PLANES

(b) (110) PLANES

(c) (111) PLANES

Low index planes in bcc crystal: (a) (100) planes (b) (110) planes (c) (111) planes

Interplanar Spacing in Face Centred Cubic Lattice

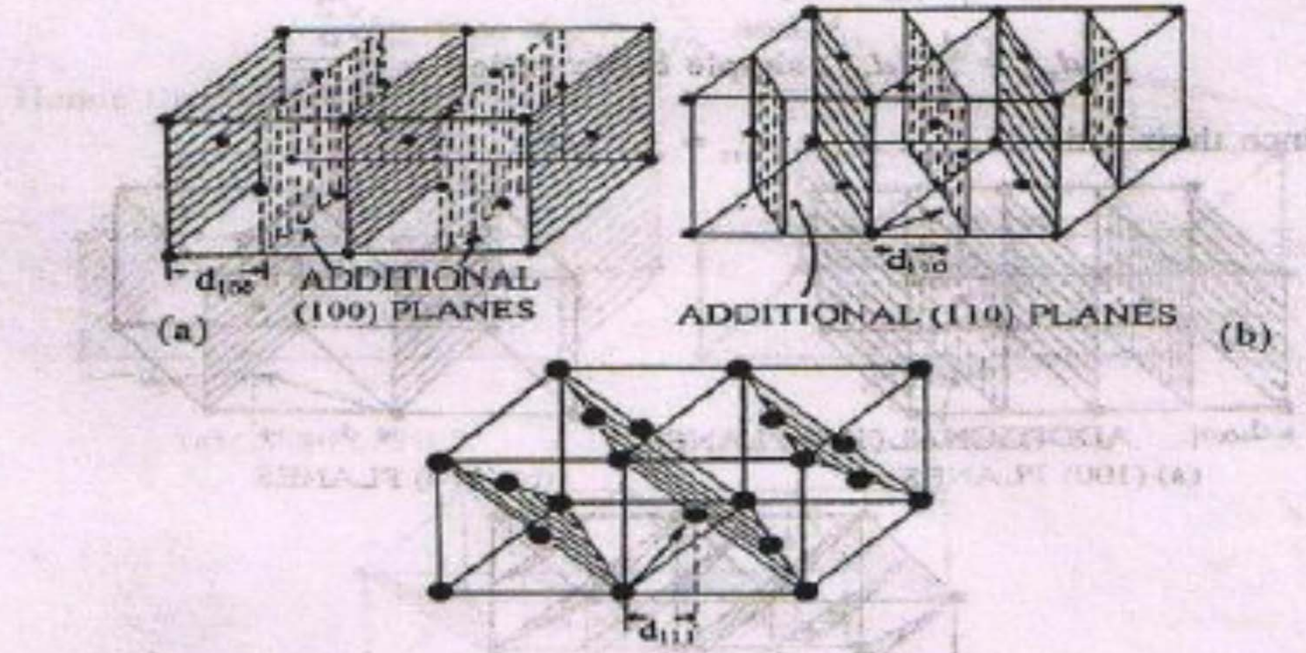


$$d_{100} = \frac{1}{2}\,(d_{100})\text{ simple cubic lattice} = \frac{a}{2}$$

$$d_{110} = \frac{1}{2}\,(d_{110})\text{ simple cubic lattice} = \frac{a}{2\sqrt{2}}$$

$$d_{111} = (d_{111})\text{ simple cubic lattice} = \frac{a}{\sqrt{3}}$$

Hence their ratio is $d_{100} : d_{110} : d_{111} = 1 : \frac{1}{\sqrt{2}} : \frac{2}{\sqrt{3}}$

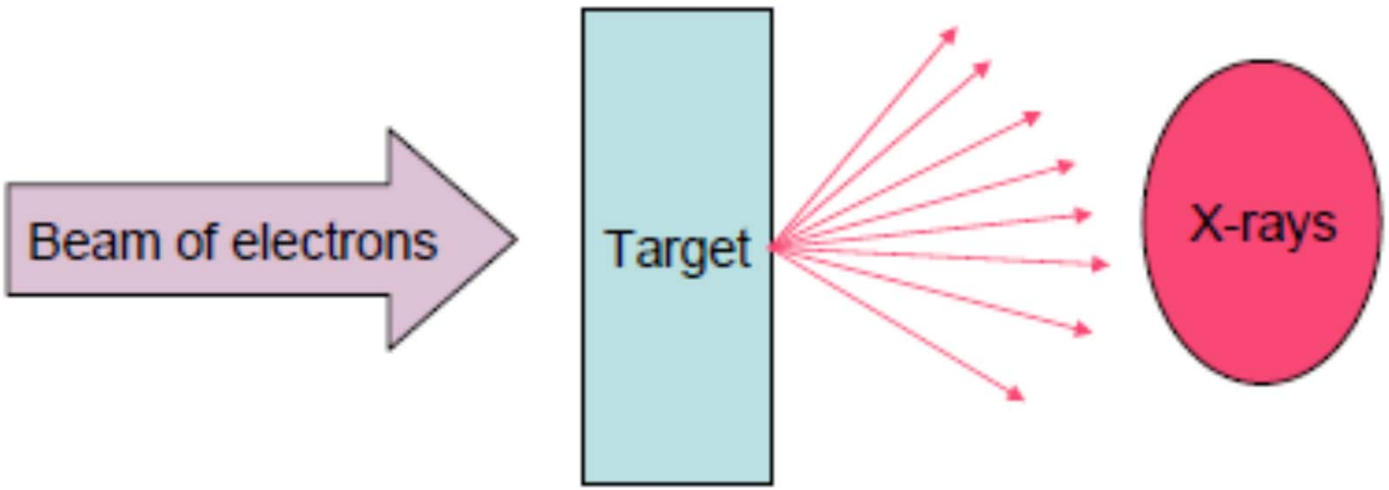


(c) (111) PLANES

Low index planes in fcc crystal (a) (100) planes (b) (110) planes (c) (111) planes

X-RAY DIFFRACTION

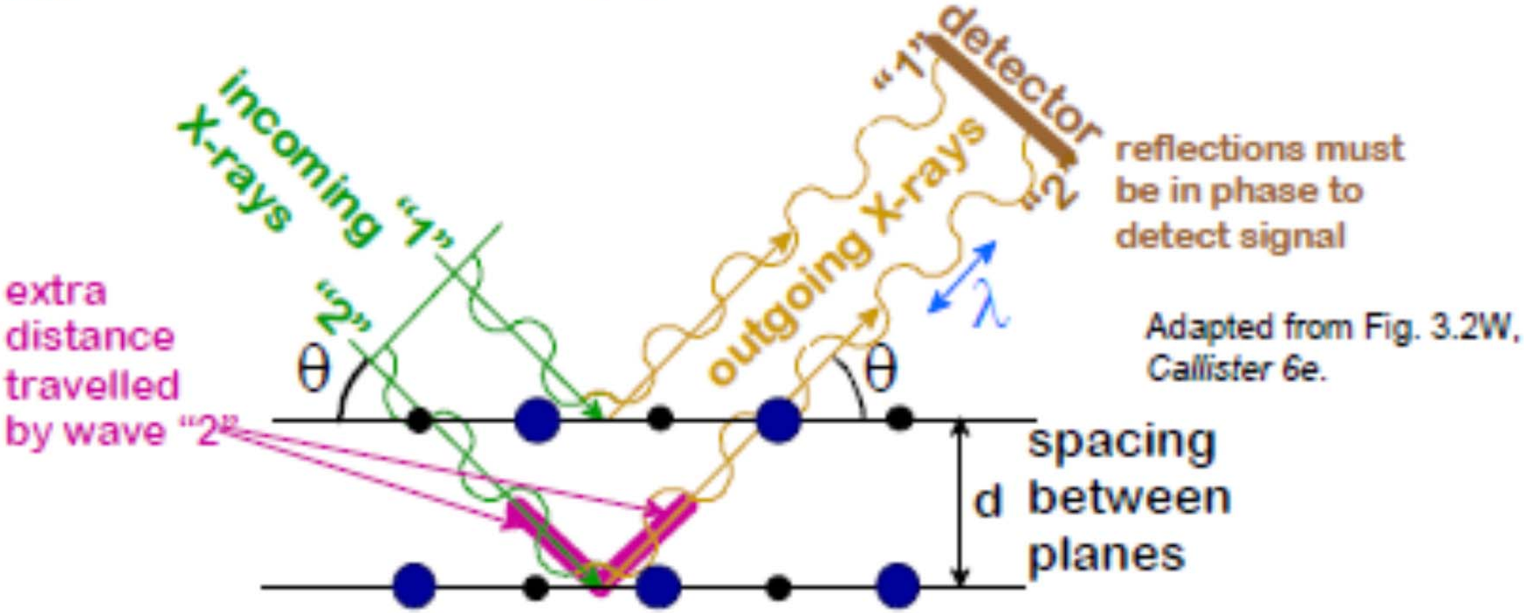
- For electromagnetic radiation to be diffracted the spacing in the grating should be of the same order as the wavelength
- In crystals the typical interatomic spacing ~ 2-3 Å so the suitable radiation is X-rays
- Hence, X-rays can be used for the study of crystal structures



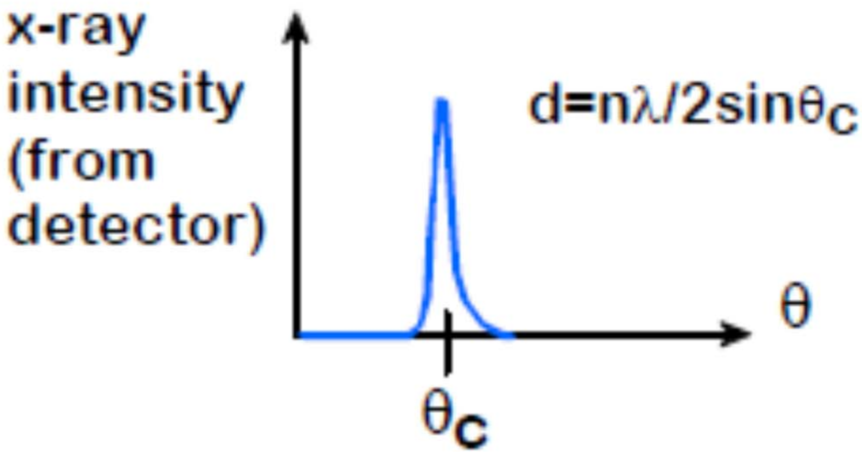
An accelerating (/decelerating) charge radiates electromagnetic radiation

X-RAYS TO CONFIRM CRYSTAL STRUCTURE

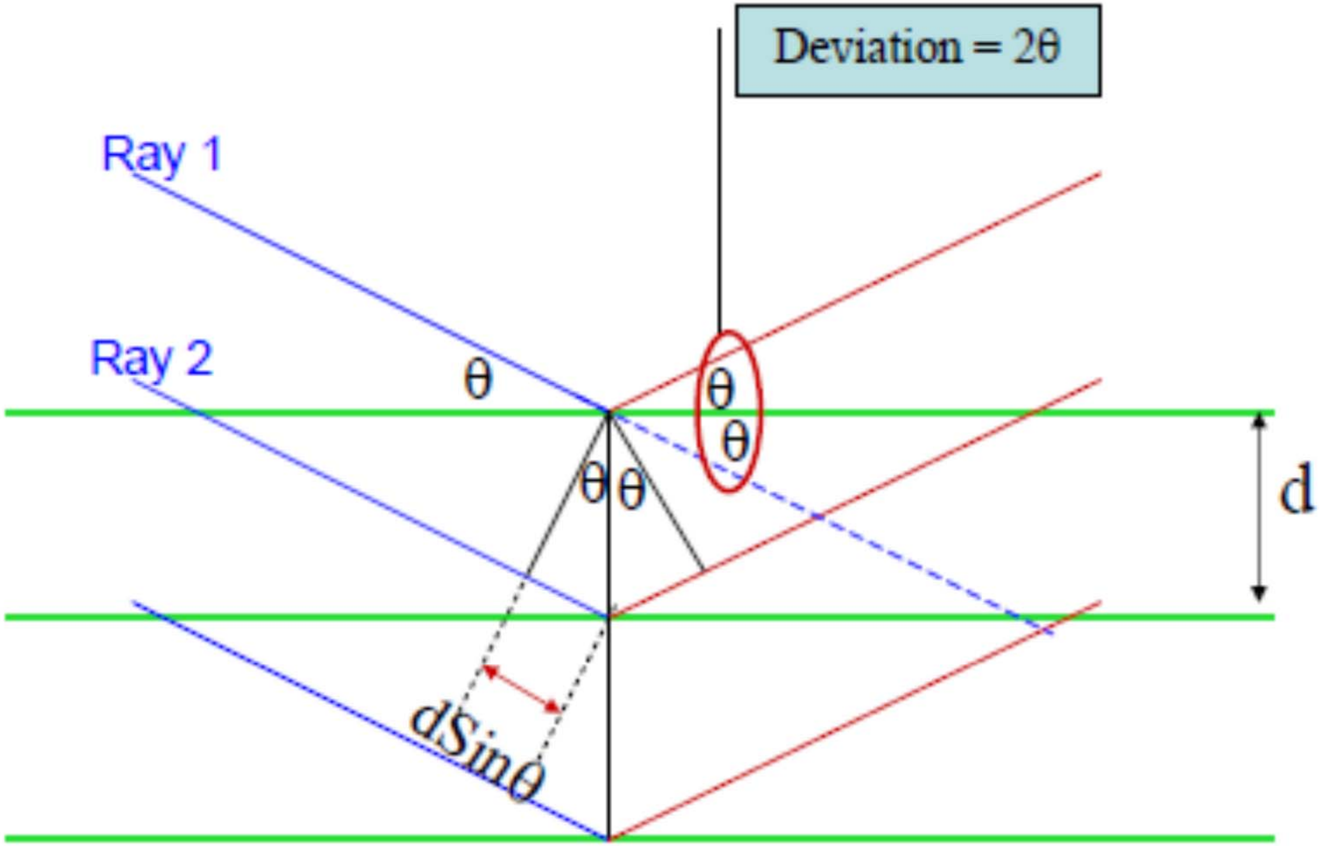
- Incoming X-rays diffract from crystal planes, following Braggs law: $n \lambda = 2d \sin(\theta)$



- Measurement of:
  Critical angles, θ_c, for X-rays provide atomic spacing, d.



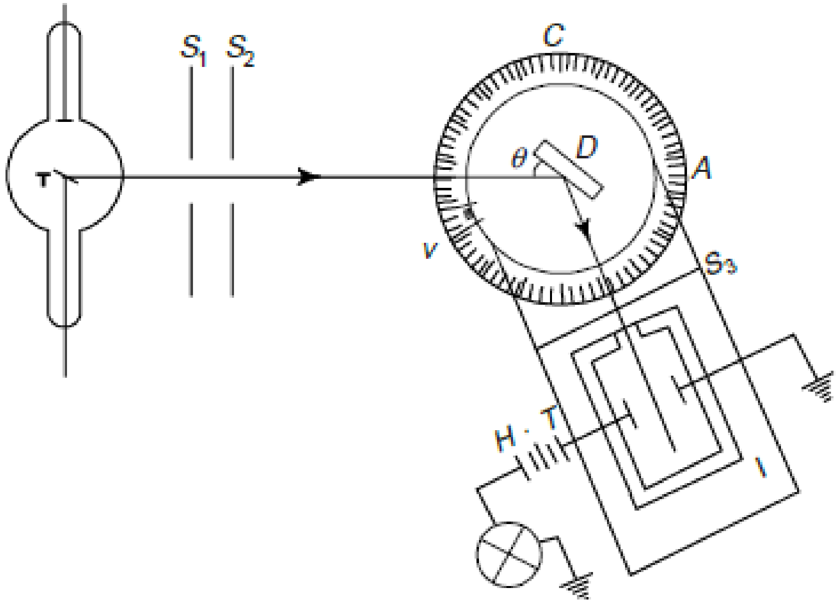
BRAGG's EQUATION



- The path difference between ray 1 and ray 2 = 2d Sinθ
- For constructive interference: $n\lambda = 2d \sin\theta$

BRAGG'S X-RAY SPECTROMETER

The experimental results have shown that the first order reflection maxima occurred at 5.9° , 8.4° and 5.2° for (100), (110) and (111) planes respectively.



For first order reflection, $n = 1$ and hence

$$d = \frac{\lambda}{2\sin\theta}$$

$$d \propto \frac{1}{\sin\theta}$$

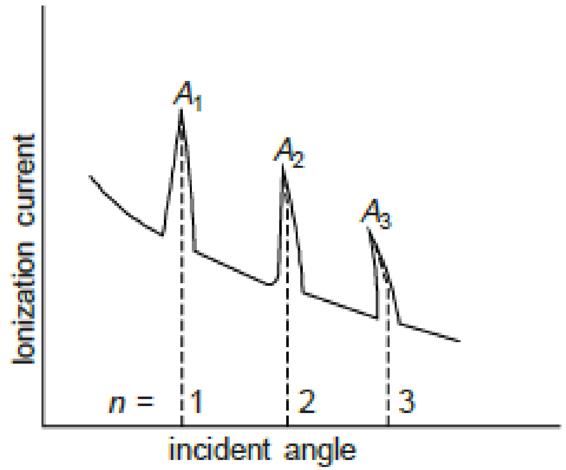
$$d_{100} : d_{110} : d_{111} = \frac{1}{\sin\theta_1} : \frac{1}{\sin\theta_2} : \frac{1}{\sin\theta_3}$$

$$d_{100} : d_{110} : d_{111} = \frac{1}{\sin 5.9^\circ} : \frac{1}{\sin 8.4^\circ} : \frac{1}{\sin 5.2^\circ}$$

$$= 9.73 : 6.84 : 11.04$$

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

This corresponds to the value for FCC system. Hence NaCl have FCC structure.



The variation of ionization current for a crystal of NaCl.