

Polarization by

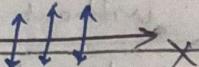
Scattering -

(Vibrations in all possible directions)

Scattered

(size of the scatterer will be comparable with λ)

Polarized light along Y-axis



(Polarized light along X-axis)

Observing light \perp to X-axis & \parallel to Y-axis

\Rightarrow
(Observing light \perp to Y-axis &
 \parallel to X-axis)

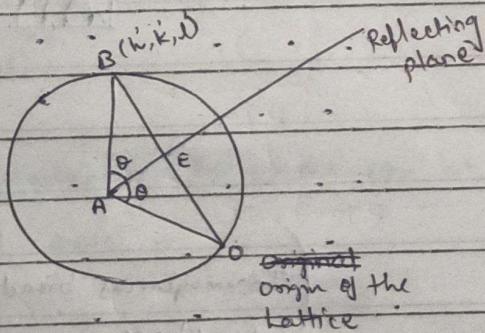
$$I \propto F^2 \text{ for simple cubic}$$

$$I \propto 14F^2 \text{ for FCC}$$

$$I \propto 12F^2 \text{ for BCC}$$

} But requires Lorentz correction factor
and Polarization correction factor.

Geometrical Interpretation of the Bragg condition



$$\vec{AO} = \frac{1}{\lambda}$$

$$\angle EAO = \theta \text{ and}$$

$$OB = \frac{n}{d}$$

$$\text{Now, } \vec{OB} = \frac{2 \sin \theta}{\lambda}$$

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

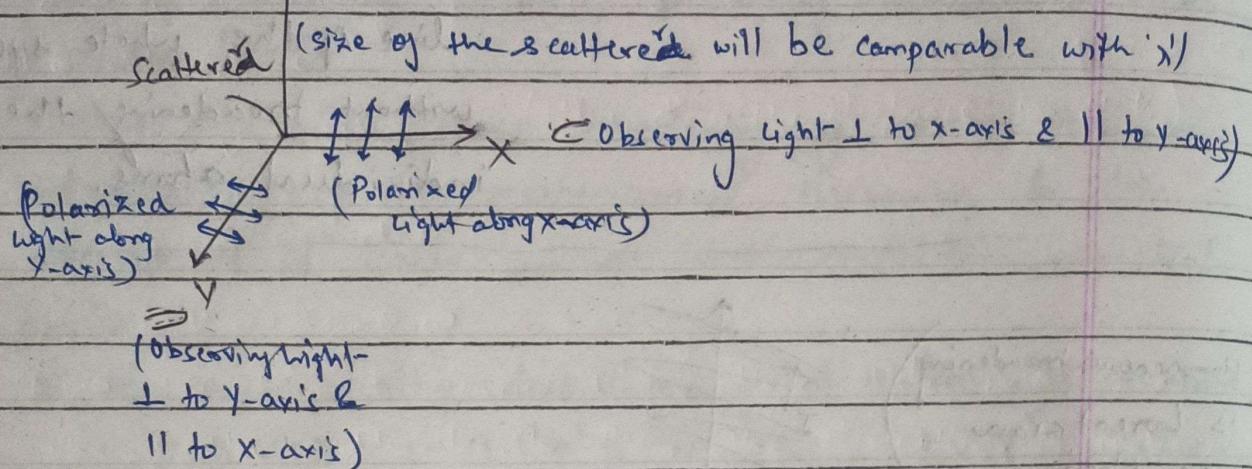
$$\Rightarrow 2d \sin \theta = n\lambda$$

(λ = radius)
circle \rightarrow evolved sphere/
evolved construction.

Polarization by Scattering -

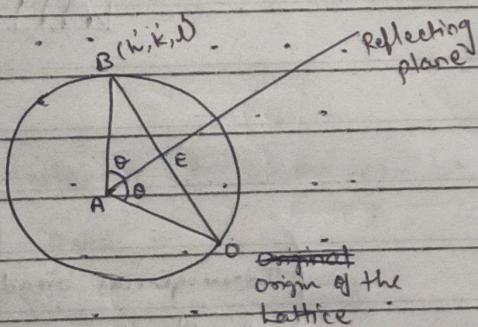


(Vibrations in all possible directions)



$$\left. \begin{array}{l} I \propto F^2 \text{ for simple cubic} \\ I \propto 1/4F^2 \text{ for FCC} \\ I \propto 1/2F^2 \text{ for BCC} \end{array} \right\} \begin{array}{l} \text{But requires Lorentz correction factor} \\ \text{and Polarization correction factor.} \end{array}$$

Geometrical Interpretation of the Bragg condition -



$$AO = \frac{1}{\lambda}$$

$$\angle EAO = \theta \quad \text{and}$$

$$OB = \frac{n}{d}$$

$$\text{Now, } OB = \frac{2 \sin \theta}{\lambda}$$

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

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

$(\frac{1}{\lambda} = \text{radius})$
circle \rightarrow evoked sphere/
evoked construction.

Lorentz Correction Factor → Time taken by the X-ray to reach the evolved sphere.

Lorentz and Polarization Correction

We know,

$$|F_{hkl}| \propto \sqrt{I_{hkl}}$$

Modulus of structure factor is called the structure amplitude.

It is used to calculate $\rho(x, y, z)$

Hence to calculate (x_i, y_i, z_i)

I_{hkl} value to the observed structure factor amplitude

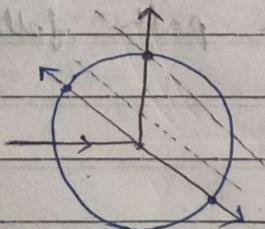
$$I_{\text{obs}(hkl)} = |F_{hkl}|^2$$

$$\Rightarrow |F_{\text{obs}(hkl)}| = \sqrt{\frac{K I_{\text{obs}(hkl)}}{L b}} \quad \text{where } L \text{ is the Lorentz factor}$$

b is the polarization factor

K depends on crystal size, the beam intensity and few fundamental constants.

$$|F_{\text{rel.}}(hkl)| = K' |F_{\text{obs.}}(hkl)| = \sqrt{\frac{I_{\text{obs.}}(hkl)}{L b}}$$



Lorentz factor arises from the time required of a reciprocal lattice (rl) point to pass ~~through~~ the Ewald sphere. This time is not constant for all the rl points. This depends on the location of individual reciprocal lattice (rl) points and the speed and the direction from which it ^(rl point) approaches the ~~out~~ Ewald sphere.

As the crystal is rotated about ϕ or ω at a given angular velocity ω , the rl points also rotate at the same

angular velocity.

Therefore the linear velocity of a g.l. point located at d^* g.l. unit away from origin as it approaches to the Ewald ~~sphere~~ sphere.

$$v = d^* \omega \quad (\text{Here, } d^* \text{ is the distance in g.l.})$$

$$d^* = \left(\frac{\lambda}{d} \right)$$

$$v = 2 \sin \theta \omega$$

Now, the time 't' required for this g.l. point pass through the path length P in the direction of motion is given by

$$\Rightarrow t = \frac{P}{v} = \frac{P}{2 \sin \theta \omega}$$

Now, 'p' depends on the angle θ between the surface of the sphere of reflection and the path followed by the g.l. point.

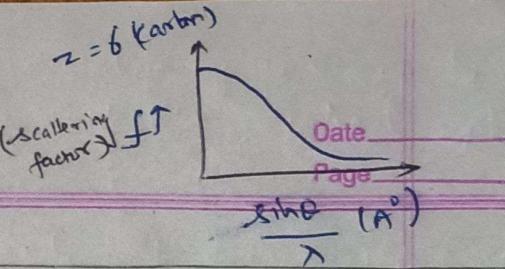
$$\text{Now, } p \propto \frac{1}{\cos \theta}$$

$$\Rightarrow t \propto \frac{1}{2 \sin \theta \cos \theta}$$

$$\Rightarrow t \propto \frac{1}{\sin 2\theta}$$

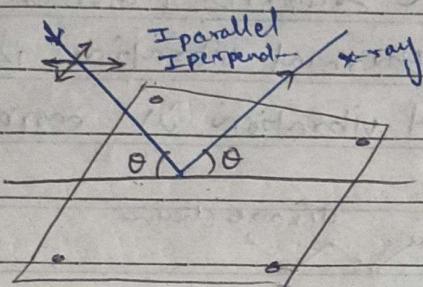
$$\Rightarrow L = \frac{1}{\sin 2\theta}$$

Lorentz correction factor.



Polarization correction factor

$$P = \frac{1}{2} (1 + \cos^2 \theta) \rightarrow \text{Polarization factor.}$$



$(\pi \text{ beam}) I_{\parallel} \rightarrow f(x, y, z)$ and independent of θ

$(\sigma \text{ beam}) I_{\perp} \rightarrow f(x, y, z)$ and dependent on θ

Note:- PCF is a very small value, and so for the practical determination of intensity, PCF can be neglected.

In case we are using crystal monochromator, the effect is important. The incident beam itself will be polarised.

Secondary polarization will influence the diffraction data.

$$P = \frac{1 + K \cos^2 \theta}{1 + K}$$

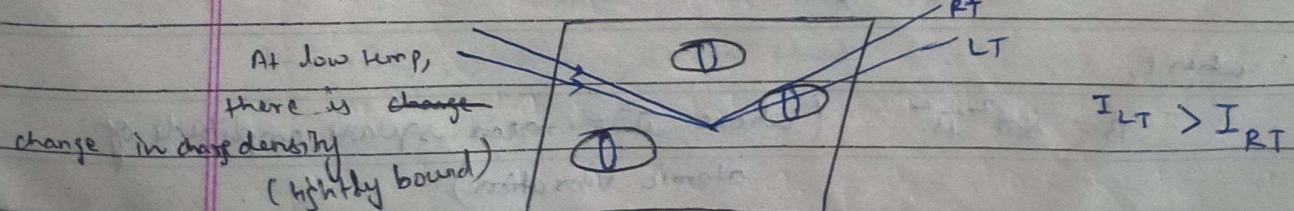
where K is the ratio of power of π beam w.r.t σ beam from the crystal monochromator.

If ~~the~~

~~the~~

Temperature factor on the intensity of the diffracted beam -

Absolute scaling and the effect of temperature factor

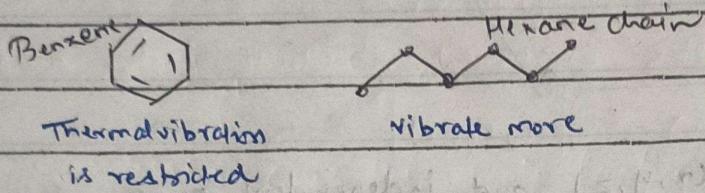


sinθ

sinθ

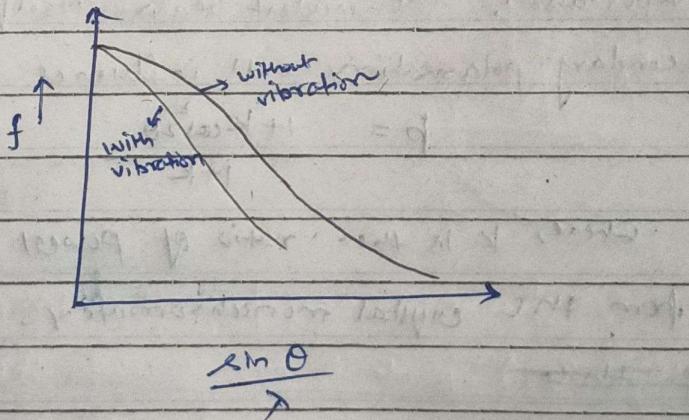
sinθ

At high temperature, these vibrations will be made significant and hence will influence the diffracted intensity more
 m = mass of the scatterer (atom)
 for heavier elements, thermal vibration is less and for lighter, the thermal vibration is more.



The ~~eff~~ effect of thermal vibration is to reduce the scattering power of an element, mostly lighter elements, and hence the diffracted intensity is weak.

Result \rightarrow Thermal vibration will lower the scattering factor (f)



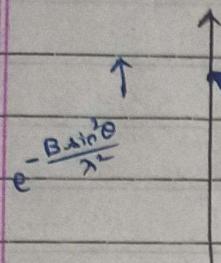
The variation in the atomic scattering factor is given by-

$$e^{-\frac{B \sin^2 \theta}{\lambda^2}}$$

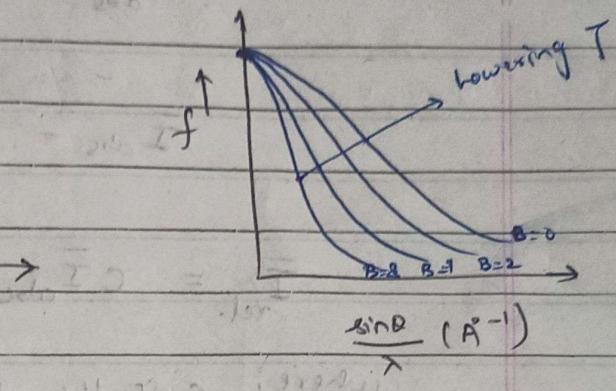
where,

$$B = 8\pi^2 \bar{m}^2 \quad (\text{where } \bar{m}^2 = \text{mean square amplitude of atomic vibration})$$

$$f = f_0 e^{-\frac{B \sin^2 \theta}{\lambda^2}}$$



$$\frac{\sin \theta}{\lambda} (\text{A}^{-1})$$



$$\frac{\sin \theta}{\lambda} (\text{A}^{-1})$$

The avg. observed intensity corrected for Lorentz and polarization factor.

$$\overline{I}_{\text{relative}} = \langle |F_{\text{rel.}}|^2 \rangle_{\text{avg.}}$$

If we have a unit cell with 'N' atoms then

~~$$\overline{I}_{\text{abs}} = \sum_{i=1}^N f_i^2$$~~
$$\overline{I}_{\text{abs}} = \sum_{i=1}^N f_i^2 \quad (\overline{I}_{\text{abs}} = \text{Theoretical avg. intensity})$$

Now, the ratio of $\frac{\overline{I}_{\text{abs}}}{I_{\text{rel}}}$ should be defined as the scale

factor to place the I_{rel} values on an absolute scale.

since f_i is not same over the range of $\frac{\sin \theta}{\lambda}$.

$\therefore I_{\text{abs}}$ also varies with ~~$\frac{\sin \theta}{\lambda}$~~ $\frac{\sin \theta}{\lambda}$

To avoid this, we divide the Ewald's sphere into small infinite shells such that the value of f_i do not change within the shell.

f_i are all influenced by the thermal motion

$$\bar{I}_{\text{abs}} = \sum_{i=1}^N f_{\text{c}}(i) e^{-\frac{2B_i \sin^2 \theta}{\lambda^2}}$$

$$\bar{I}_{\text{abs.}} = e^{-\frac{2B \sin^2 \theta}{\lambda^2}} \sum_{i=1}^N f_{\text{c}}^2(i)$$

$$\bar{I}_{\text{rel.}} = C \bar{I}_{\text{abs.}}$$

where, C is the scale factor

$$\bar{I}_{\text{rel.}} = C e^{-\frac{2B \sin^2 \theta}{\lambda^2}}$$

$$= C e^{-\frac{\pi^2 k T}{\lambda^2}}$$

JANUARY 2016						
S	M	T	W	T	F	S
31				1	2	
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30

2015

DECEMBER 31
ThursdayDate _____
Page _____XRC

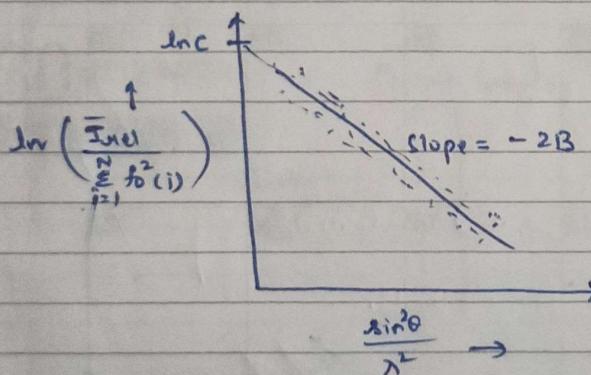
$$\frac{\bar{I}_{\text{rel}}}{\sum_{i=1}^N f_0^2(i)} = C e^{-\frac{2B \sin^2 \theta}{\lambda^2}}$$

↓
scale factor

Now,

$$\ln \left(\frac{\bar{I}_{\text{rel}}}{\sum_{i=1}^N f_0^2(i)} \right) = \ln C - \frac{2B \sin^2 \theta}{\lambda^2}$$

\underbrace{y} \underbrace{x}



Now,

$$\bar{I}_{\text{rel}} = C \bar{I}_{\text{abs}}$$

$$|F_{\text{rel}}|^2 = C |F_{\text{abs}}|^2$$

$$|F_{\text{abs}}| = \frac{1}{\sqrt{C}} |F_{\text{rel}}|$$

29 DECEMBER

2015

Tuesday

NOVEMBER 2015

S	M	T	W	T	F	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					

$$|F_{abs}| = k |F_{rel}|$$

↓
scale
comparat
constant

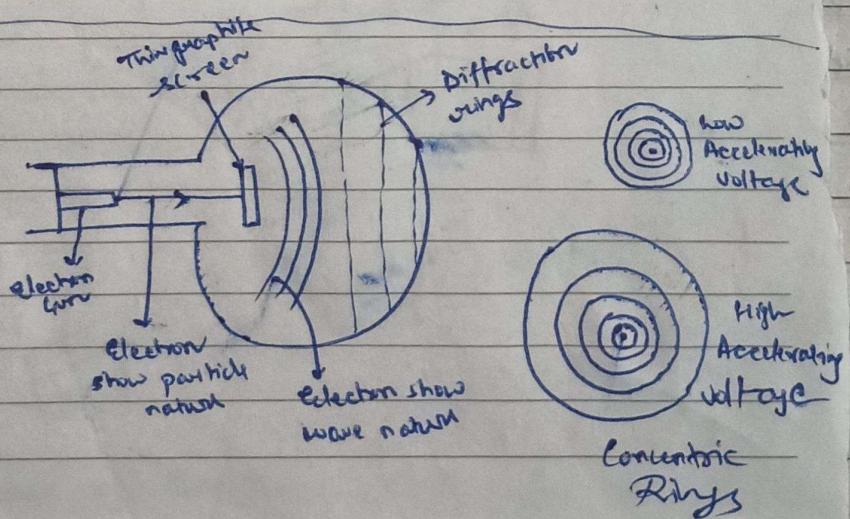
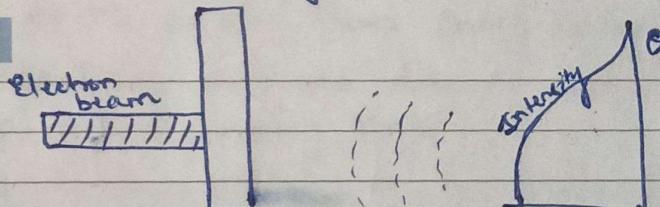
Electron Diffraction

If the e^- behave as a particle, the distribution of e^- will vary continuously as a function of angle. This distribution will vary only slightly with change in e^- energy.

30 DECEMBER

Wednesday

Carbon target



27
Sunday

25 DECEMBER

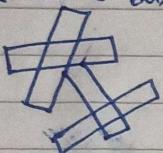
2015

Friday

NOVEMBER 2015						
S	M	T	W	T	F	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					

Selected Area Electron Diffraction (SAED)

- ① single crystalline - diffraction of a single crystal gives

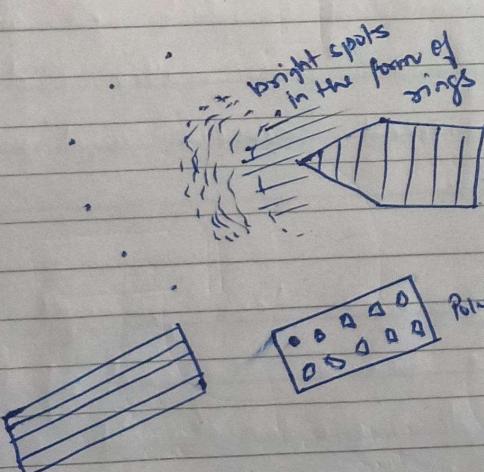


a discrete
or discrete spot

- ② Polycrystalline (consisting of many crystalline or single crystals), small spots making up

26 DECEMBER rings. Individual crystalline gives these spots arising from Bragg reflection resulting numerous discrete spots

and line up and forming rings.



and in case of Amorphous, (diffused rings)

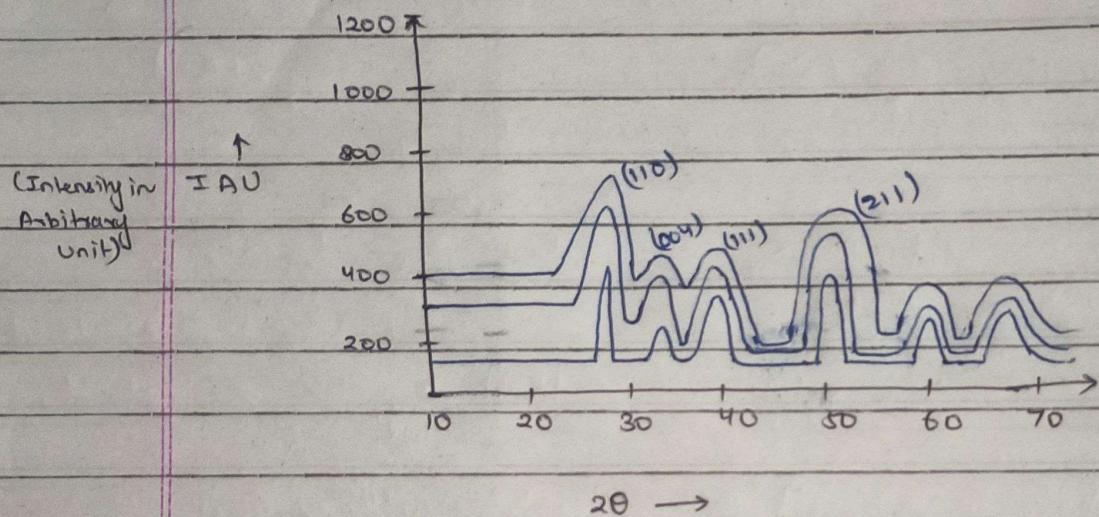
Date _____
Page _____

SAED

Amorphous - Diffuse Rings

Single crystal - Bright spots

Polycrystalline - Bright Rings

The same information we can achieve by XRD Analysis -Transmission Electron Microscope (TEM)

TEM is a very imp. tool in nanotechnology in which e⁻ are made to fall on sample. These e⁻ interact with matter and get transmitted and strike a fluorescent screen and produces high resolution complete images.

Principle - TEM works on the same basic principle as the light microscope but uses e⁻ beam instead of light beam to produce an image. As de-Broglie wavelength is much smaller than that of photons TEM is capable of producing high resolution images of sample. TEM can reveal the finest details of images.

Construction -