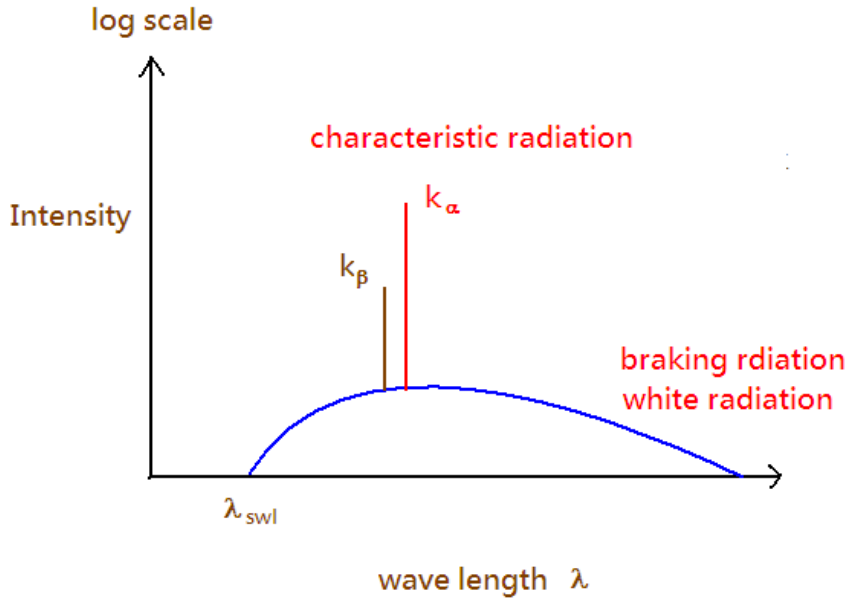
IX X-ray diffraction

9-1 production of X-ray

X-ray is usually generated by a high energy electron beam impinging onto the Cu target. This would generate characteristic peaks and a continuous white radiation.

A sketch of a typical X-ray spectrum is shown below.



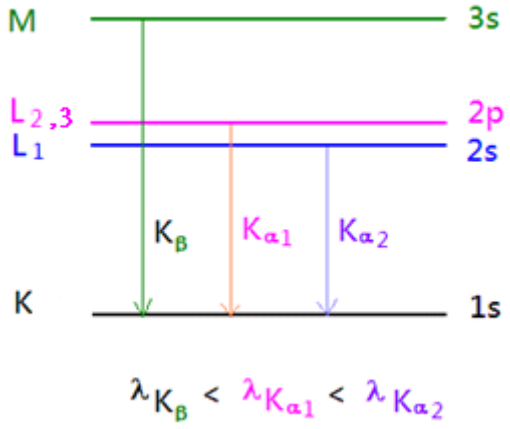
(i) $\lambda_{swl} \equiv$ short wavelength limit

$$E = h\nu$$

$$eV = h\frac{c}{\lambda_{swl}}$$

where V is the voltage applied to X-ray tube

(ii) characteristic radiation



(iii) CuK_α

$$\begin{cases} k_{\alpha_1} = 1.54050\text{Å} \\ k_{\alpha_2} = 1.54434\text{Å} \end{cases} \text{ for high angle line}$$

$$k_\alpha = 1.5418\text{Å} \quad \text{for low angle line}$$

Why we can resolve k_{α_1} and k_{α_2} double lines at high angle?

$$\lambda = 2d_{hkl}\sin\theta$$

$$\frac{d\lambda}{d\theta} = 2d_{hkl}\cos\theta = 2\frac{\lambda}{2\sin\theta}\cos\theta$$

$$\frac{d\lambda}{d\theta} = \lambda\cot\theta$$

$$d\theta = \frac{d\lambda}{\lambda}\tan\theta$$

Note that

$$\theta \uparrow \ \Rightarrow \ \tan\theta \uparrow \ \Rightarrow \ d\theta \uparrow$$

So, we can see k_{α_1} and k_{α_2} double lines at high angle.

9-2. X-ray diffraction

(i) Laue method λ variable, white radiation, θ fixed

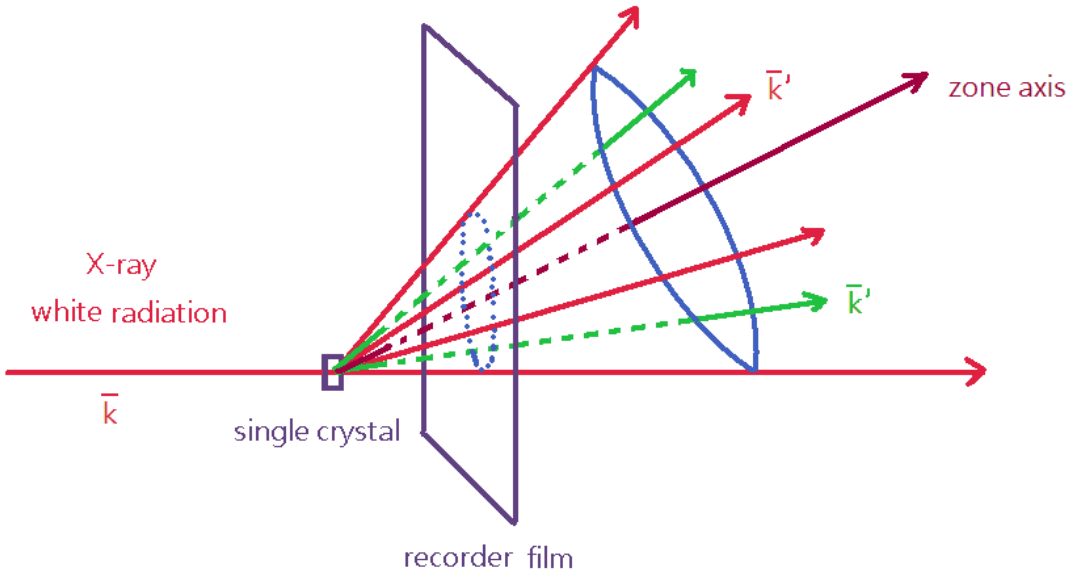
(ii) Diffractometer method λ fixed, characteristic

radiation, θ variable

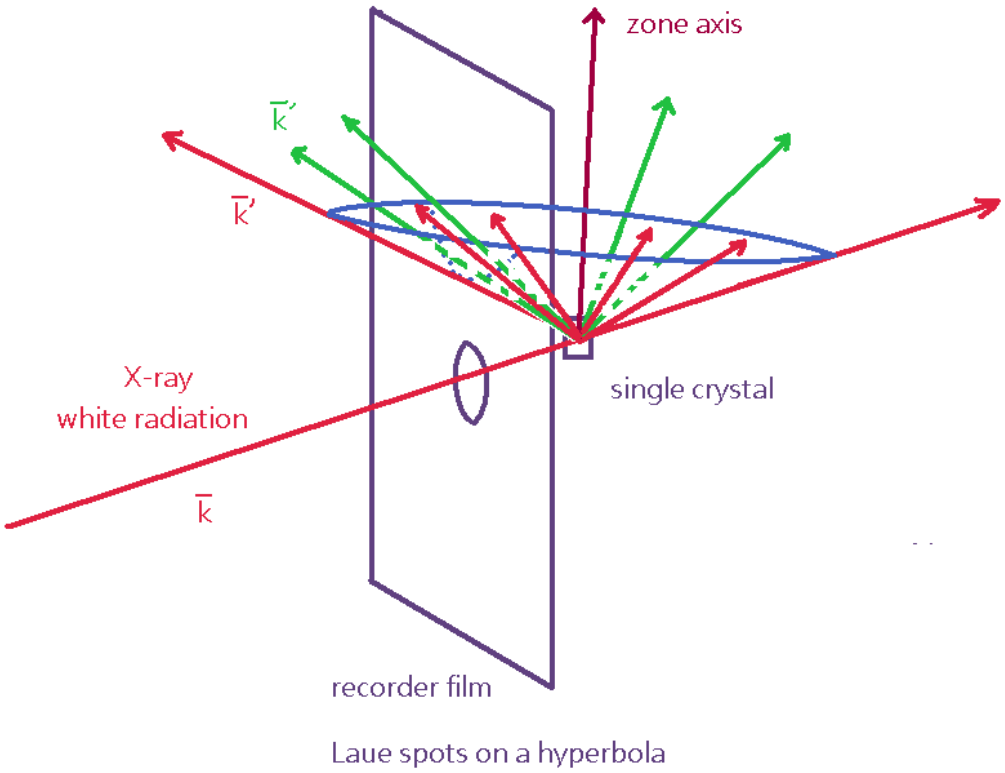
(iii) Powder method λ fixed, characteristic radiation, θ variable

(iv) Rotating crystal method λ fixed, characteristic radiation, θ variable (in part)

9-2-1 Laue method



Laue spots on an ellipse



(1) Laue condition

Von Laue derived the " Laue conditions " in 1912 to express the necessary conditions for diffraction.

Assume that $\vec{a}$, $\vec{b}$, $\vec{c}$ are three crystal lattice vectors in a crystal

$$\vec{a}\cdot\left(\vec{S}'-\vec{S}\right)=\vec{a}\cdot\vec{G}^{*}_{hkl}=\vec{a}\cdot\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)$$

$$\vec{a}\cdot\left(\vec{S}'-\vec{S}\right)=h$$

Similarly,

$$\vec{b}\cdot\left(\vec{S}'-\vec{S}\right)=k$$

$$\vec{c}\cdot\left(\vec{S}'-\vec{S}\right)=l$$

Very often , the Laue conditions are expressed as

$$\vec{a}\cdot\left(\hat{S}'-\hat{S}\right)=h\lambda$$

$$\vec{b}\cdot\left(\hat{S}'-\hat{S}\right)=k\lambda$$

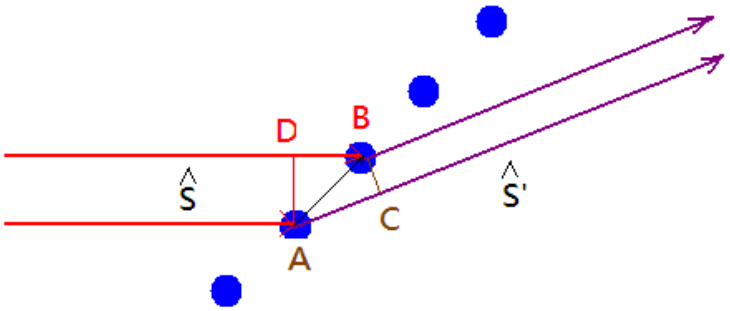
$$\vec{c}\cdot\left(\hat{S}'-\hat{S}\right)=l\lambda$$

where

$$\vec{S}' = \frac{\hat{S}'}{\lambda}$$
$$\vec{S} = \frac{\hat{S}}{\lambda}$$

The three Laue conditions must be satisfied simultaneously for diffraction to occur. The physical meaning of the 3 Laue conditions are illustrated below.

1st Laue conditions



The path difference between the waves equals to

$$AC - BD = \vec{a} \cdot (\hat{S}' - \hat{S})$$

where $\vec{a} = \overrightarrow{AB}$. The criterion for diffraction to occur is

$$\vec{a} \cdot (\hat{S}' - \hat{S}) = h\lambda$$

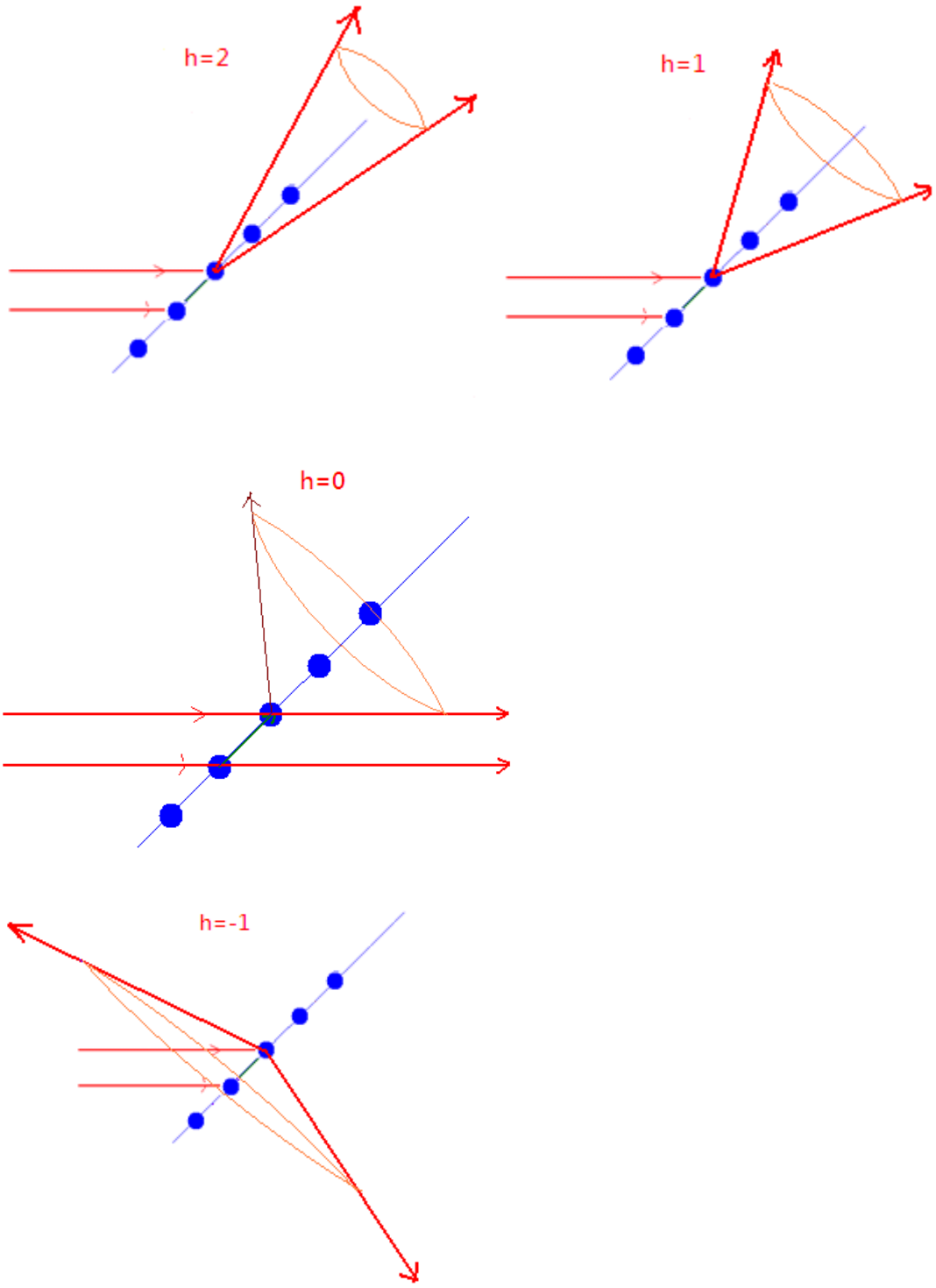
or

$$\vec{a} \cdot (\vec{S}' - \vec{S}) = h$$

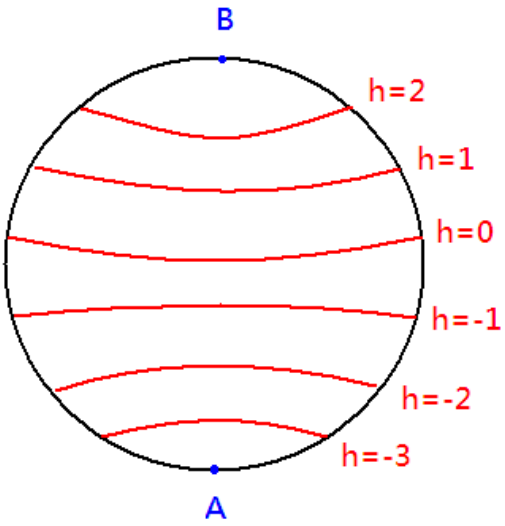
; h is an integer (1st Laue conditions)

For 1-dimensional crystal

Cones of diffracted beams for different h



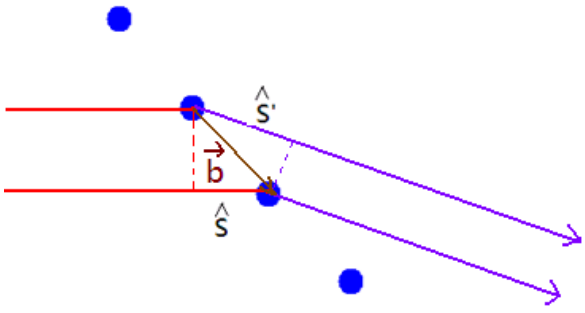
Stereographic projection representation for 1-D crystals



The projection of diffracted beams for h = 0 is a great circle if the incident beam direction is perpendicular, i.e. $\vec{S} \perp \vec{a}$.

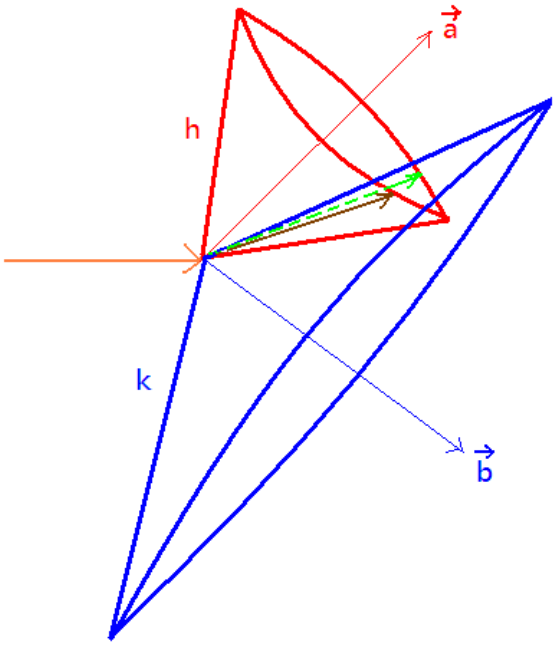
The projection of diffracted beams for h = 0 is a small circle if the incident beam direction is not perpendicular,

2nd Laue condition



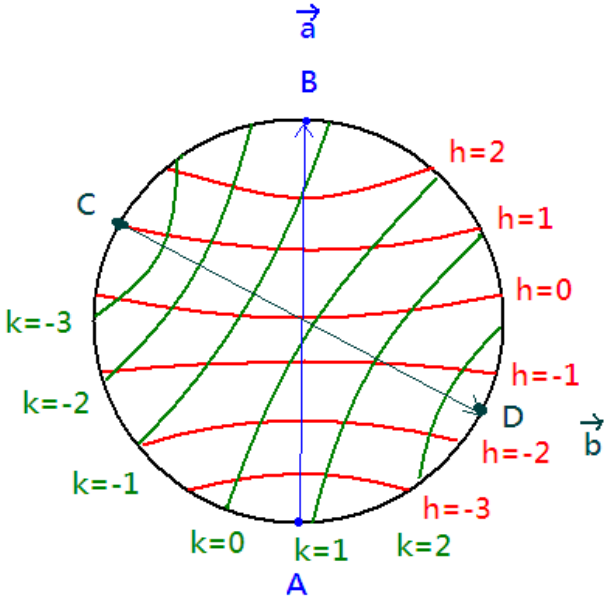
$\vec{b} \cdot (\vec{S}' - \vec{S}) = k$; k is an integer.

For a two-dimensional crystal



The 1st and 2nd conditions are simultaneously satisfied only along lines of intersection of cones.

Stereographic projection for 2-D crystals

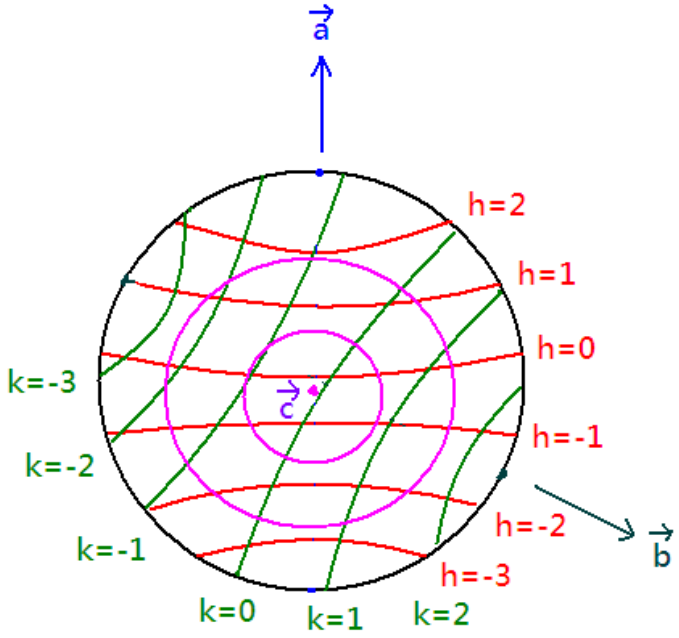


The lines of intersection of cones are labeled as (h , k)

3rd Laue condition

$\vec{c} \cdot (\vec{S}' - \vec{S}) = l$; l is an integer

For a 3-D crystal



For a single crystal and a monochromatic wavelength, it is usually no diffraction to occur.

(2) Laue photograph

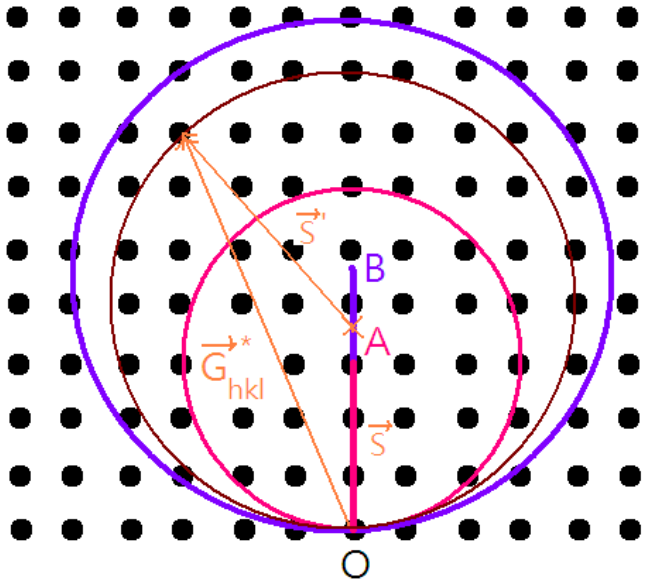
Laue photograph is performed at " single crystal and variable wavelength " .

(2-1) Ewald sphere construction

$$\vec{S}' - \vec{S} = \vec{G}^*_{hkl}$$

This is equivalent to

$$\frac{\vec{\kappa}' - \vec{\kappa}}{2\pi} = \vec{G}^*_{hkl}$$



Two Ewald spheres of radius OA and OB form, where

$$OA = \frac{1}{\lambda_{lwl}}$$

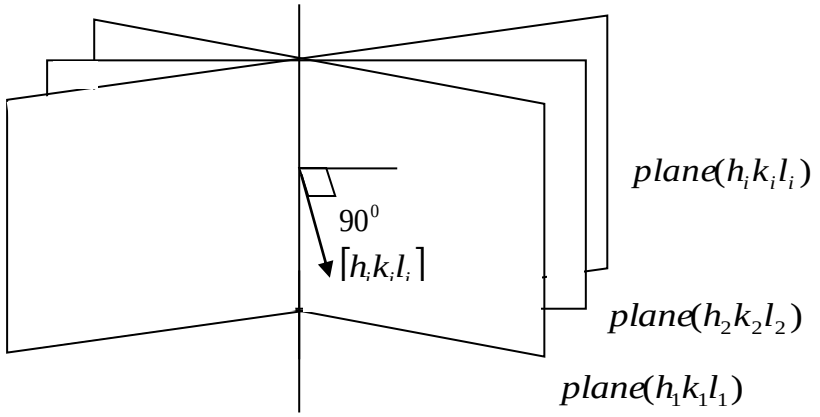
$$OB = \frac{1}{\lambda_{swl}}$$

where λ_{lwl} and λ_{swl} represent the longest and shortest wavelength in the white radiation.

$\vec{G}^*_{hkl}$ in between two spherical surface meets the diffraction condition since the wavelength is continuous in white radiation.

(2-2) zone axis

The planes belong to a zone



We define several planes belong to a zone [uvw], their plane normal $[\mathrm{h_i k_i l_i}]$ are perpendicular to the zone axis, In other words,

$$[\mathrm{uvw}] \cdot [\mathrm{h_i k_i l_i}] = 0$$
$$\mathrm{h_i u + k_i v + l_i w = 0}$$

In the Laue experiments, all the planes meet the diffraction criterion. Each plane meets the 3 Laue conditions.

$$\vec{\mathrm{a}} \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = \mathrm{h_i}\lambda$$
$$\vec{\mathrm{b}} \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = \mathrm{k_i}\lambda$$
$$\vec{\mathrm{c}} \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = \mathrm{l_i}\lambda$$
$$\left(\mathrm{u}\vec{\mathrm{a}} + \mathrm{v}\vec{\mathrm{b}} + \mathrm{w}\vec{\mathrm{c}}\right) \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = \mathrm{h_i u}\lambda + \mathrm{k_i v}\lambda + \mathrm{l_i w}\lambda = (\mathrm{h_i u + k_i v + l_i w})\lambda$$

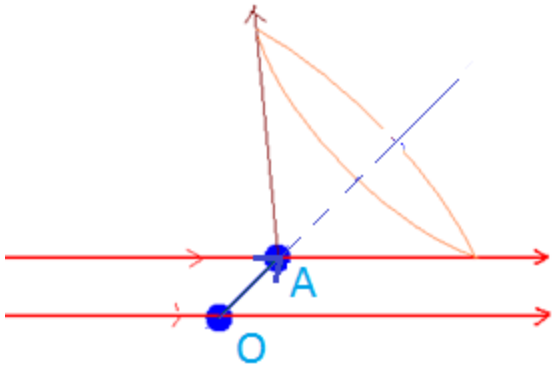
So

$$\left(\mathrm{u}\vec{\mathrm{a}} + \mathrm{v}\vec{\mathrm{b}} + \mathrm{w}\vec{\mathrm{c}}\right) \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = 0$$

for all the plane belonged to the zone [uvw].

If we define $\overrightarrow{\mathrm{OA}} = \mathrm{u}\vec{\mathrm{a}} + \mathrm{v}\vec{\mathrm{b}} + \mathrm{w}\vec{\mathrm{c}}$,

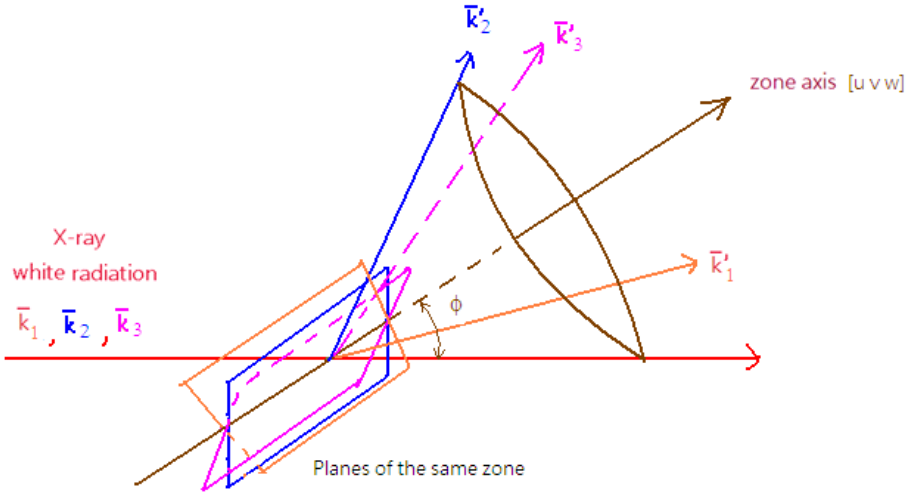
$$\left(\mathrm{u}\vec{\mathrm{a}} + \mathrm{v}\vec{\mathrm{b}} + \mathrm{w}\vec{\mathrm{c}}\right) \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = \overrightarrow{\mathrm{OA}} \cdot \left(\hat{\mathrm{S}}' - \hat{\mathrm{S}}\right) = 0$$



The path difference between the waves equals to

$$\overrightarrow{OA} \cdot (\hat{S}' - \hat{S}) = 0$$

A. for the condition $\phi < 45°$



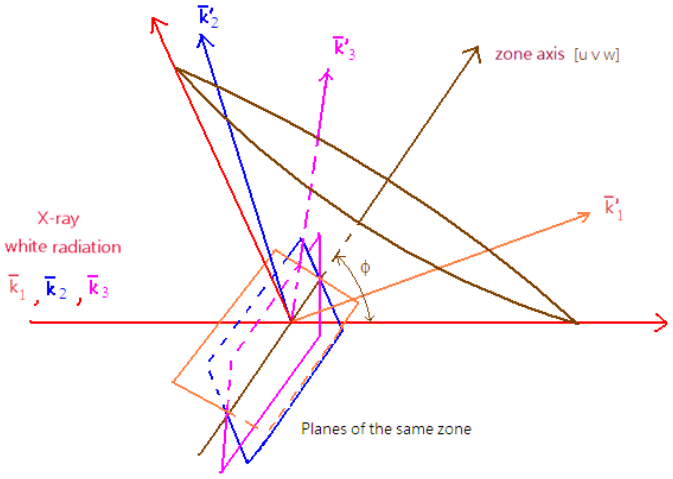
For all the planes $(h_i k_i l_i)$in the same zone [uvw],

$$h_i u + k_i v + l_i w = 0$$

$$\overrightarrow{OA} \cdot (\hat{S}' - \hat{S}) = (h_i u + k_i v + l_i w)\lambda = 0$$

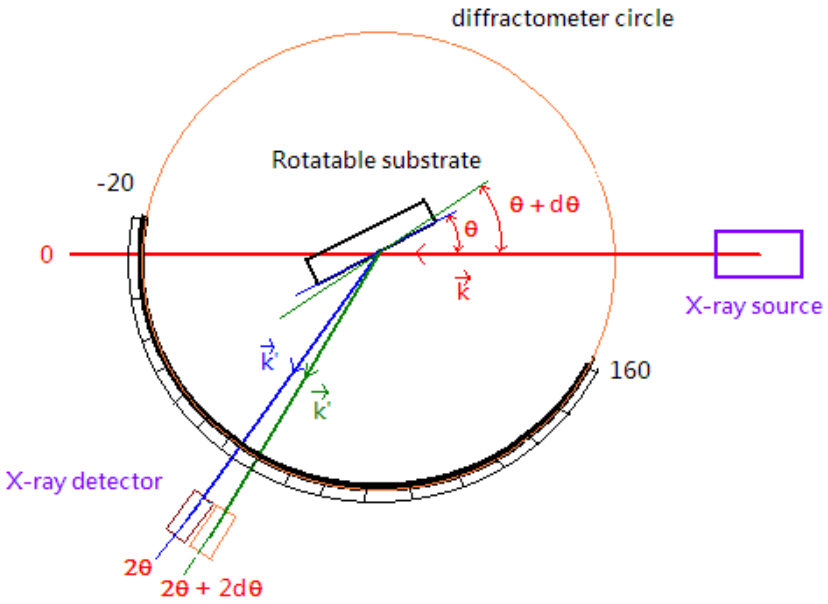
Therefore all the diffracted beam directions $\hat{S}'_1, \hat{S}'_2, \hat{S}'_3 \cdots \hat{S}'_i$ are on the same cone surface.

B. for the condition $\phi > 45°$

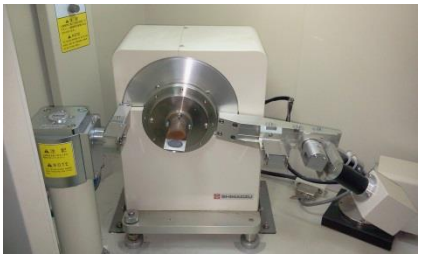
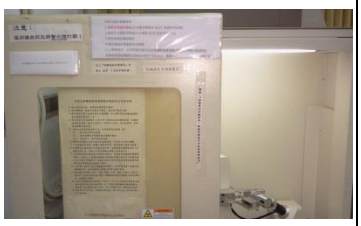
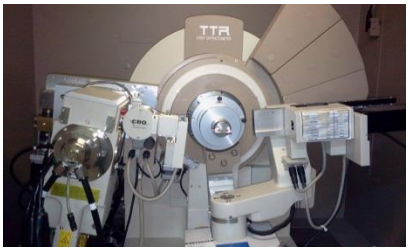
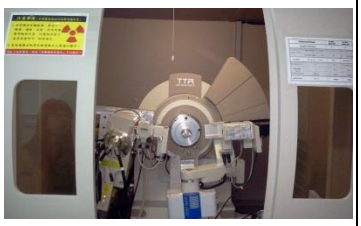
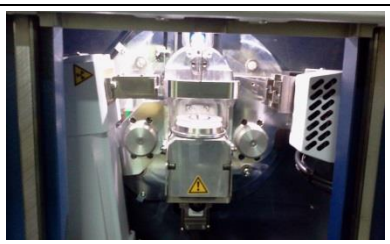


All the diffracted beam directions $\hat{S}'_1, \hat{S}'_2, \hat{S}'_3 \cdots \hat{S}'_i$ are on the same cone surface.

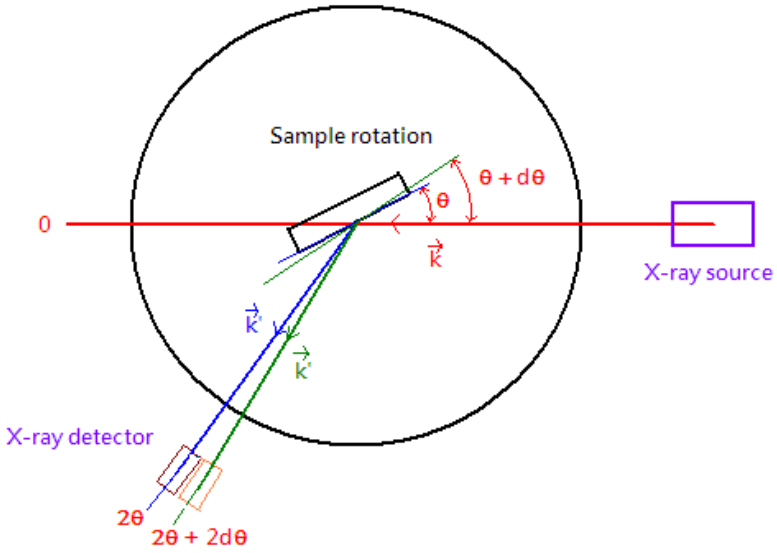
9-2-2 Diffractometer method



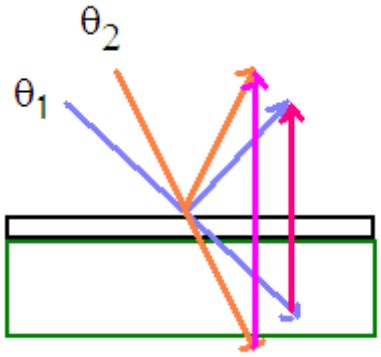
Instrumentation at MSE, NTHU

Model	Diffractometer	Outlook
XRD 6000 wide angle		
TTR wide angle grazing angle		
D2 phaser wide angle		

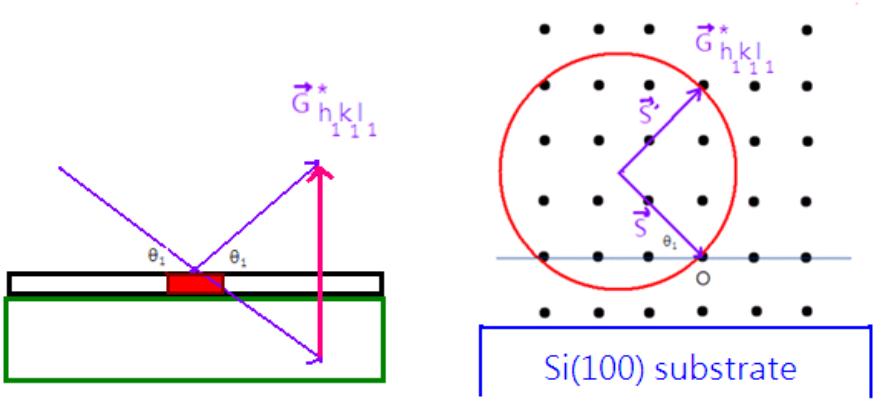
9-2-2-1 θ – 2θ scan



If a new material is deposited on Si(100) and put on the substrate holder in the diffractometer set-up, $\vec{k}' - \vec{k}$ is always parallel to the Si(100) surface normal.



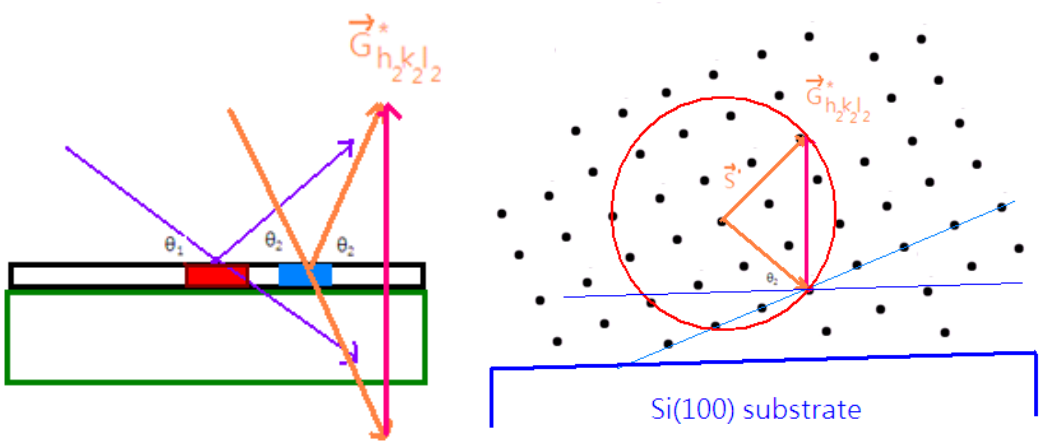
(a) Ewald sphere construction



Rotate the incident beam at until $\vec{G}_{h_1k_1l_1}{}^*$ meets the diffraction condition at $2\theta = 2\theta_1$

This is equivalent to at least one crystal with $(h_1k_1l_1)$ plane normal in parallel with the Si(100) surface normal.

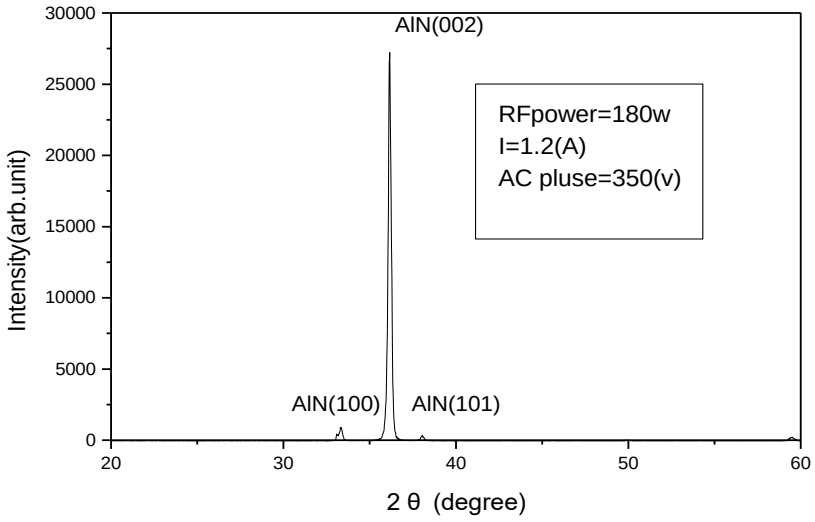
When the incident beam is rotated (rotating the Ewald sphere), different $\vec{G}_{h_2k_2l_2}{}^*$ will meet the diffraction condition at $2\theta = 2\theta_2$



This is equivalent to at least one crystal with $(h_2k_2l_2)$ plane normal also in parallel with the Si(100) surface normal.

If only one plane of the film is observed in the diffractometer measurement, the film is epitaxial or textured on Si(100).

(b)XRD spectrum of AlN deposited on Si(100)



A large number of grains with AlN(002) surface normal in parallel to Si(100) surface normal, but small amount of grains of

AlN(100) and AlN(101) are also in parallel to Si(100) surface normal.

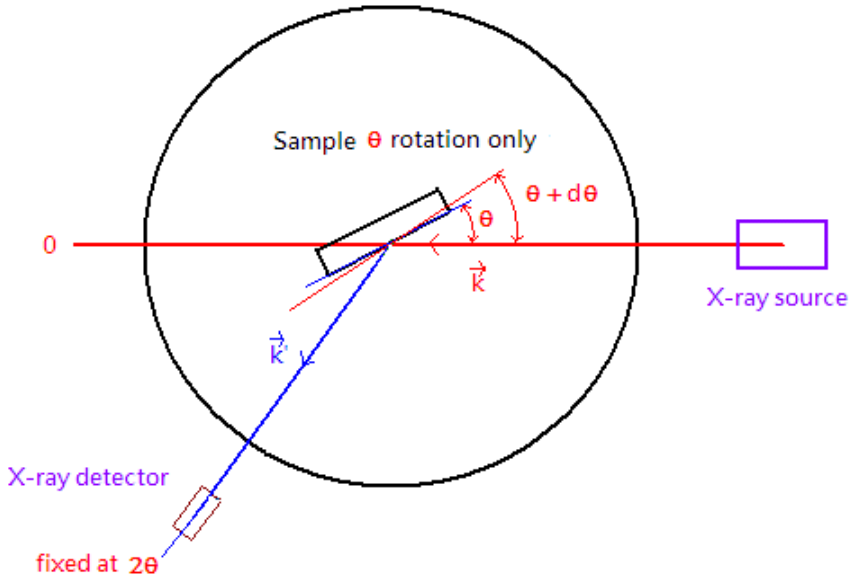
9-2-2-2 X-ray rocking curve

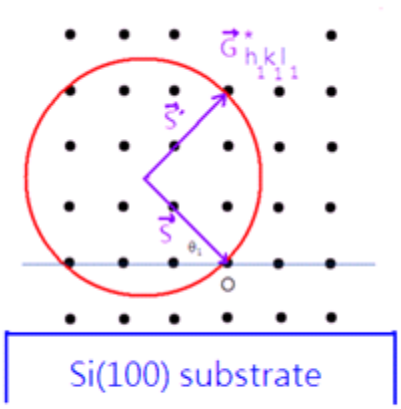
X-ray rocking is usually used to characterize the crystal quality of an epitaxial or textured film.
At a certain diffraction condition

$$\vec{\kappa}' - \vec{\kappa} = 2\pi\vec{G}^*_{h_1k_1l_1}$$

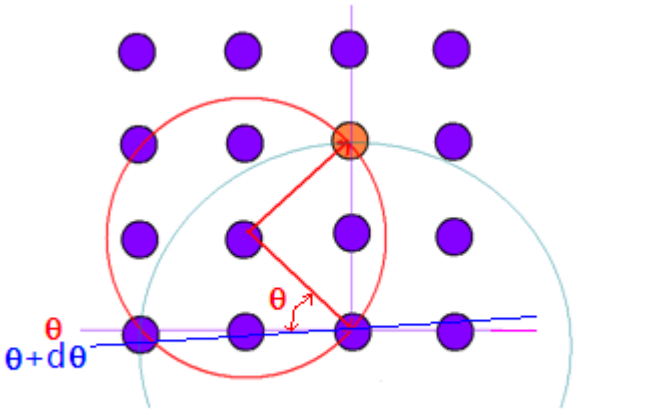
, the incident and outgoing directions of X-ray are fixed and the sample is rotated by θ scan.

When the crystal is rotated by dθ, this is equivalent to the detector being moved by the same dθ. The FWHM of the diffracted peak truly reflects the width of each reciprocal lattice point, i. e. the shape effect of a crystal.



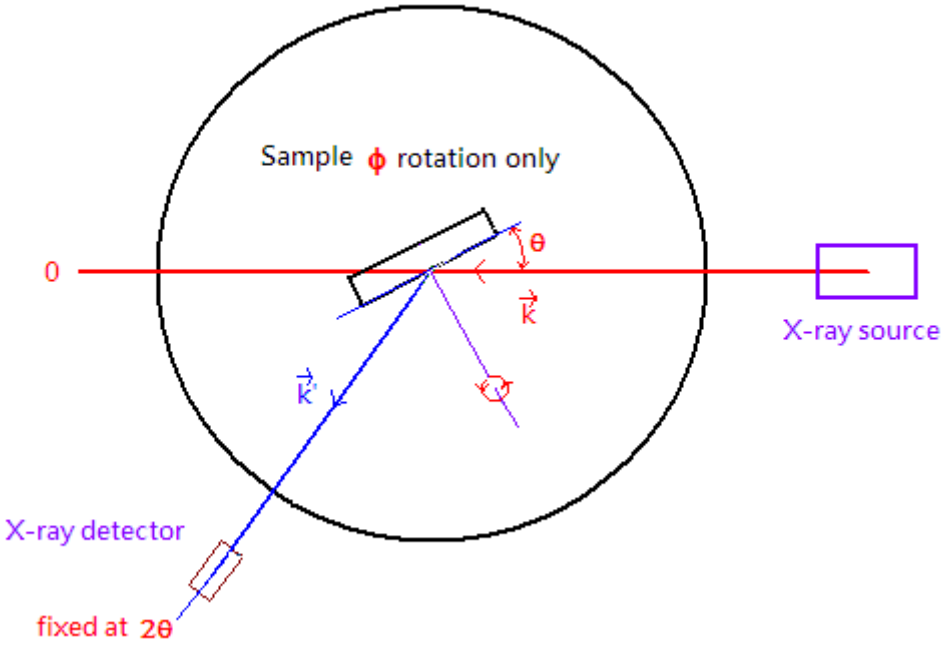


Find the diffracted peak at θ and then scan the sample

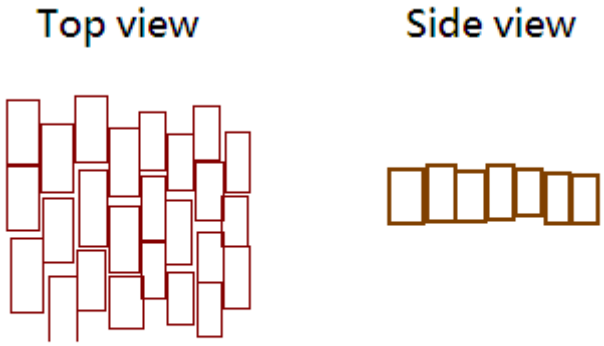


9-2-2-3 ϕ scan

The ϕ scan is used to characterize the quality of the epitaxial film around its plane normal by rotating ϕ $(0 - 2\pi)$

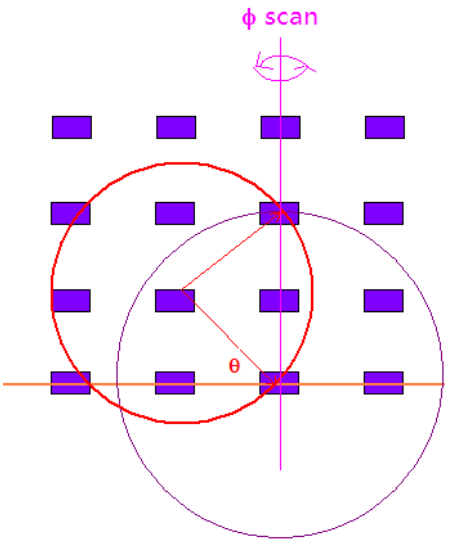


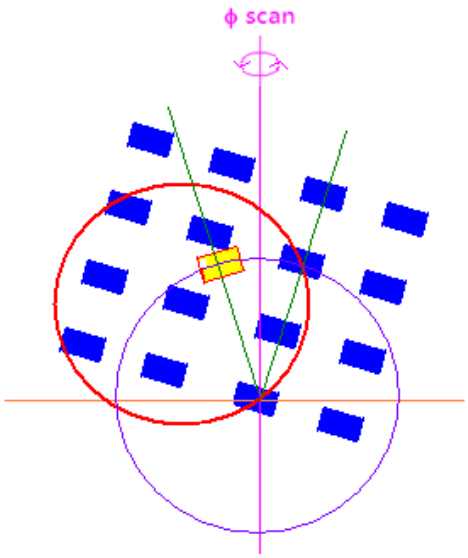
Example: the crystal quality of highly oriented grains each of which is a columnar structure shown below.



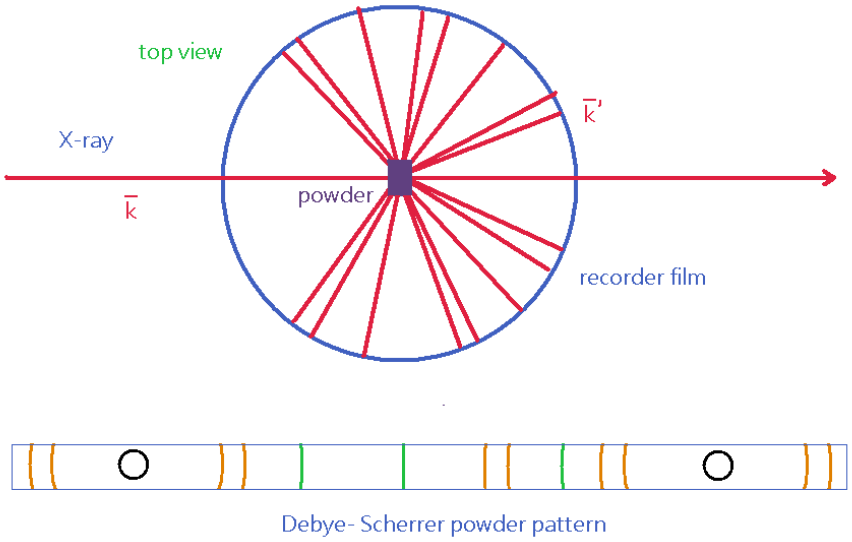
Mosaic columnar structure

Each lattice point in the reciprocal lattice will be expanded into an orthorhombic volume according to the shape effect. The ϕ scan can be used to confirm the orientation of the columnar structure relative to the substrate.

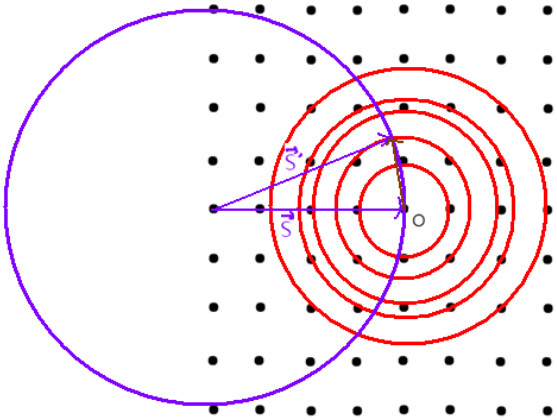

ϕ scan
θ
rotating reciprocal lattice by scanning ϕ


ϕ scan

9-2-4 Powder method (Debye-Scherrer Camera)



(a) Ewald sphere construction



$\vec{S}'$ forms a cone resulting from the intersection between Ewald sphere and the spherical reciprocal lattice.

Powder can be treated as a very larger number of polycrystals with grain orientation in a random distribution

$\Rightarrow$ Reciprocal lattice become a series of concentric spherical shells of $\left|\vec{G}_{hkl}^{\,*}\right|$ as their radius.

The intersection between the concentric spherical shells of $\left|\vec{G}_{hkl}{}^{*}\right|$ in radius and the Ewald sphere of radius $\frac{\kappa}{2\pi}$ are a series of circles.

$\Rightarrow$ The circles are recorded as lines in the film.

9-3. Intensities of diffracted beams

For powder pattern lines Debye-scherrer method

$$I = |F|^2 P \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta} A(\theta) e^{-2M}$$

where I = relative integrated intensity (arbitrary unit)

P = multiplicity factor

F = structure factor

θ= Bragg angle

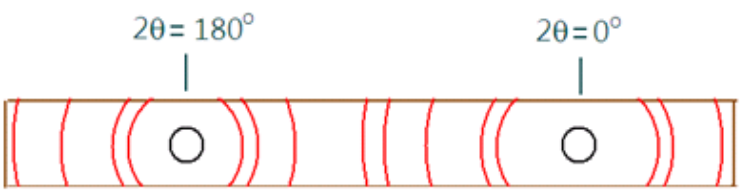
$\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$ = Lorentz-polarization factor

$A(\theta)$ = absorption

e^{-2M} = temperature factor

Example

Debye-Scherrer powder pattern of Cu made with Cu K_α radiation



1	2	3	4	5	6	7	8
line	hkl	$h^2+k^2+l^2$	$\sin^2\theta$	$\sin\theta$	$\theta(°)$	$\frac{\sin\theta}{\lambda}(Å^{-1})$	f_{Cu}
1	111	3	0.1365	0.369	21.7	0.24	22.1
2	200	4	0.1820	0.427	25.3	0.27	20.9
3	220	8	0.364	0.603	37.1	0.39	16.8
4	311	11	0.500	0.707	45.0	0.46	14.8
5	222	12	0.546	0.739	47.6	0.48	14.2
6	400	16	0.728	0.853	58.5	0.55	12.5
7	331	19	0.865	0.930	68.4	0.60	11.5
8	420	20	0.910	0.954	72.6	0.62	11.1

1	9	10	11	12	13	14
line	$\lvert F\rvert^2$	P	$\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$	Relative integrated intensity		
				Calc.	Calc.	Obs.
1	7810	8	12.03	7.52×10^5	10.0	Vs
2	6990	6	8.50	3.56	4.7	S
3	4520	12	3.70	2.01	2.7	s
4	3500	24	2.83	2.38	3.2	s
5	3230	8	2.74	0.71	0.9	m
6	2500	6	3.18	0.48	0.6	w
7	2120	24	4.81	2.45	3.3	s
8	1970	24	6.15	2.91	3.9	s

(a)

$$F = NS_{\vec{G}}$$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i \vec{G}\cdot\vec{r}_j} f_j$$

For f.c.c lattice

four atoms at [000], $\left[\frac{1}{2}\frac{1}{2}0\right]$, $\left[\frac{1}{2}0\frac{1}{2}\right]$, $\left[0\frac{1}{2}\frac{1}{2}\right]$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}\right)\cdot\left(u_j\vec{a}+v_j\vec{b}+w_j\vec{c}\right)} f_j$$

$$S_{\vec{G}} = \sum_{j}^{s} e^{-2\pi i\left(hu_j+kv_j+lw_j\right)} f_j$$

$$S_{\vec{G}} = f\left[e^{0} + e^{-2\pi i\left(\frac{h}{2}+\frac{k}{2}\right)} + e^{-2\pi i\left(\frac{h}{2}+\frac{l}{2}\right)} + e^{-2\pi i\left(\frac{k}{2}+\frac{l}{2}\right)}\right]$$

$$= f\left[1 + e^{-\pi i(h+k)} + e^{-\pi i(h+l)} + e^{-\pi i(k+l)}\right]$$

Hence,

$S_{\vec{G}} = 4f$ if h, k and l are unmixed.

$S_{\vec{G}} = 0$ if h, k and l are mixed.

$$\mathrm{F} = \mathrm{N}S_{\vec{G}}$$

$|\mathrm{F}|^2 = \mathrm{FF}^* = \mathrm{N}^2 \cdot 16\mathrm{f}^2$ for unmixed indices

(b)

$$2\mathrm{d}_{\mathrm{hkl}}\sin\theta = \lambda$$

$$\sin\theta = \frac{\lambda}{2\mathrm{d}_{\mathrm{hkl}}} = \frac{\lambda}{2\frac{\mathrm{a}}{\sqrt{\mathrm{h}^2+\mathrm{k}^2+\mathrm{l}^2}}}$$

$$\sin^2\theta = \frac{\lambda^2}{4\mathrm{a}^2}\left(\mathrm{h}^2+\mathrm{k}^2+\mathrm{l}^2\right)$$

Then,

Small θ is associated with small $(\mathrm{h}^2+\mathrm{k}^2+\mathrm{l}^2)$.

Total 8 lines can be derived through the reflection (selection) rule for fcc in the Debye-Scherrer powder pattern.

(c) Multiplicity P is the one counted in the point group stereogram.

In cubic,

$\{\mathrm{hkl}\}\ \mathrm{P} = 48;$

$\{\mathrm{hhl}\}\ \mathrm{P} = 24;$

$\{0\mathrm{kl}\}\ \mathrm{P} = 24;$

$\{0\mathrm{kk}\}\ \mathrm{P} = 12;$

$\{hhh\}$ P = 8;

$\{00l\}$ P = 6 , as counted in the point group m3m.

(d) Lorentz-polarization factor $\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$

(i) polarization factor

The scattered beam depends on the angle of scattering

Thomson equation

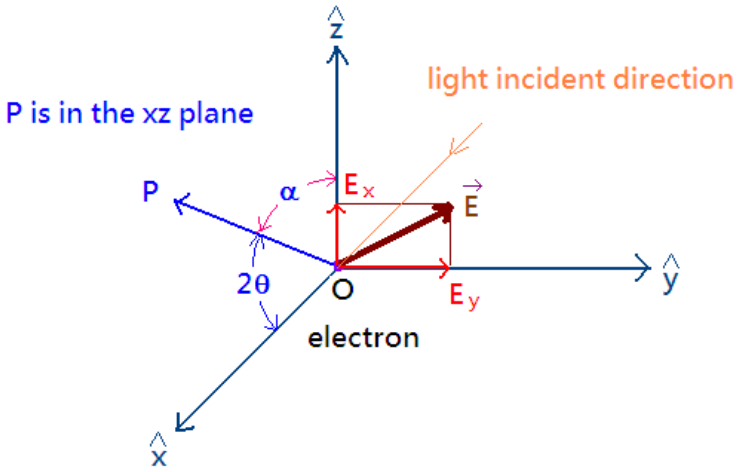
$$I = I_o \left(\frac{\mu_0}{4\pi}\right)^2 \left(\frac{e^4}{m^2 r^2}\right) \sin^2\alpha = I_o \left(\frac{k}{r^2}\right) \sin^2\alpha$$

I_o = intensity of the incident beam

$$\mu_0 = 4\pi \cdot 10^{-7} \frac{mKg}{C^2}$$

k = constant

α = angle between the scattering direction and the direction of acceleration of the electron



Assuming the incident beam is traveling in $\hat{x}$ direction

An unpolarized beam from X-ray tube has its electric field $\vec{E}$ in a random direction. The y and z components of the incident beam accelerate electrons in $\hat{y}$ and $\hat{z}$ directions, respectively.

$$E^2 = E_y^2 + E_z^2$$

Since

$$E_y^2 = E_z^2 = \frac{E^2}{2}$$

$$I_{oy} = I_{oz} = \frac{I_o}{2}$$

According to Thomson equation

$$I_{py} = I_{oy}\frac{k}{r^2}$$

$$I_{pz} = I_{oz}\frac{k}{r^2}\cos^2 2\theta$$

$$I_p = I_{py} + I_{pz} = I_{oy}\frac{k}{r^2} + I_{oz}\frac{k}{r^2}\cos^2 2\theta$$

$$I_p = I_{oz}\frac{k}{r^2}(1 + \cos^2 2\theta)$$

$$I_p = I_o\frac{k}{r^2}\left(\frac{1 + \cos^2 2\theta}{2}\right)$$

where I_p is the total scattered intensity at p

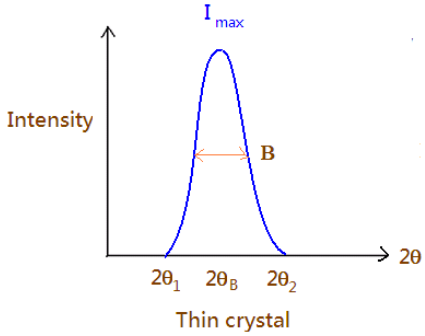
and the $\frac{1+\cos^2 2\theta}{2}$ is the polarization factor.

(ii)Lorentz factor $\frac{1}{\sin 2\theta} \cdot \cos\theta \cdot \frac{1}{\sin 2\theta}$

(ii-1) $\frac{1}{\sin 2\theta}$ factor due to grain orientation or crystal rotation

The factor is counted in powder method and in rotating crystal method.

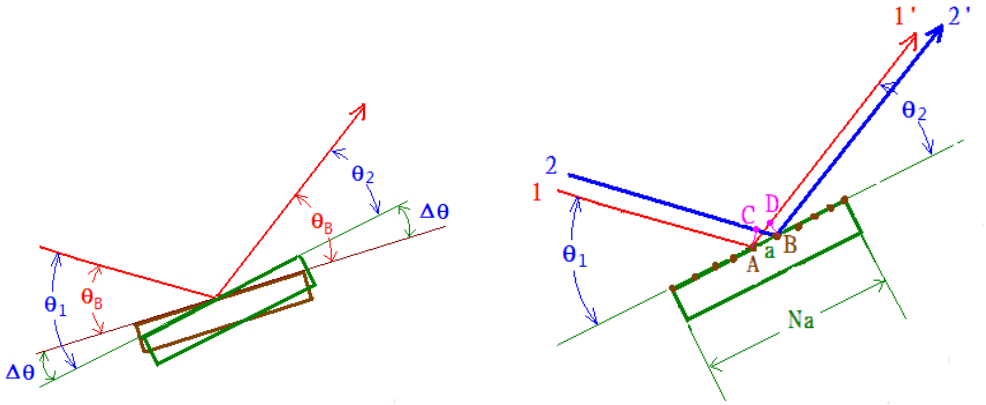
First, the integrated intensity $= \int I d(2\theta)$



integrated intensity = $I_{max} \cdot B$, where B is the width at $\frac{I_{max}}{2}$

$$I_{max} \propto \frac{1}{\sin\theta}$$
$$B \propto \frac{1}{\cos\theta}$$
$$I_{max} \cdot B \propto \frac{1}{\sin\theta\cos\theta} \propto \frac{1}{\sin 2\theta}$$

(a) $I_{max} \propto \frac{1}{\sin\theta}$



When the reflecting planes make an angle θ_B with the incident beam, the Bragg law is satisfied and the intensity diffracted in the direction $2\theta_B$ is maximum.

But, some are still diffracted in this direction when the angle of incident differs slightly from θ_B due to other crystals in the powder (or due to crystal rotation)

→ such that $\theta_1 = \theta_B + \Delta\theta$; $\theta_2 = \theta_B - \Delta\theta$ in the figure

The difference in path length for rays $1'$ and $2'$ is

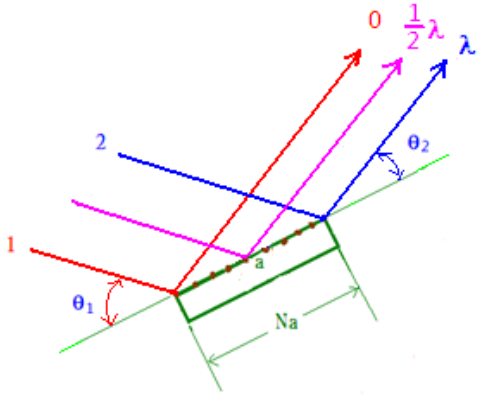
$$\delta_{1'2'} = AD - CB = a\cos\theta_2 - a\cos\theta_1$$
$$\delta_{1'2'} = a[\cos(\theta_B - \Delta\theta) - \cos(\theta_B + \Delta\theta)]$$
$$\delta_{1'2'} = 2a\sin(\Delta\theta)\sin\theta_B$$
$$\delta_{1'2'} = 2a\Delta\theta\sin\theta_B$$

where we have used $\sin(\Delta\theta) = \Delta\theta$

The path difference at either end of the plane is $N\delta_{1'2'}$ since the distance between twp ends is Na as shown in the figure.

Therefore, the maximum value of $\Delta\theta$, which allows the rays $1'$ and $2'$ detected at the angle of $2\theta_B$, occurs at

$$N\delta_{1'2'} = \lambda$$
$$2Na\Delta\theta\sin\theta_B = \lambda$$
$$\Delta\theta = \frac{\lambda}{2Na\sin\theta_B}$$



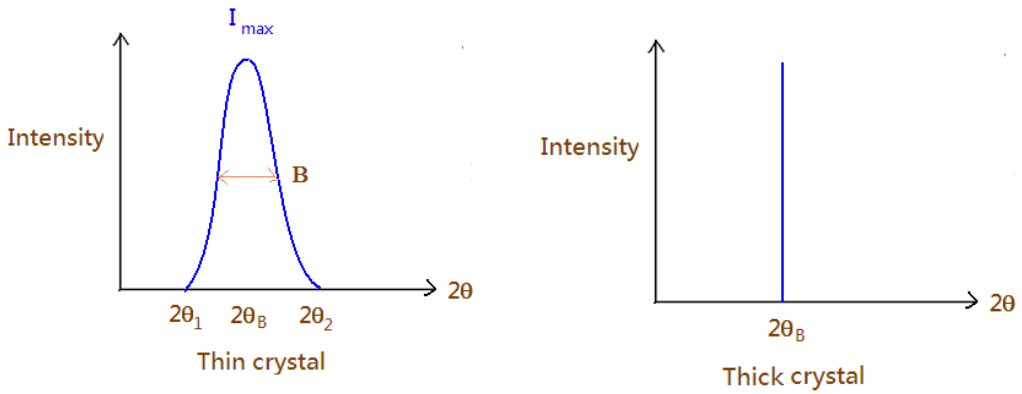
within the range of $\Delta\theta$,we still obtain I_{max} at θ_B

hence $I_{max} \propto \frac{1}{\sin\theta}$

Note that $\Delta\theta$=0 when N is infinite.

(b)why $B \propto \frac{1}{\cos\theta}$

the width B increases as the thickness of the crystal decreases , as shown in the figure in the next page



$$B = \frac{2\theta_2 - 2\theta_1}{2} = \theta_2 - \theta_1$$

write the path difference related to the total crystal thickness t.

t = md, where d is the planar spacing and m+1 is the number of atomic layers.

At $\theta = \theta_B$

$$2d\sin\theta_B = \lambda$$
$$2t\sin\theta_B = 2md\sin\theta_B = m\lambda$$

At $\theta = \theta_1$

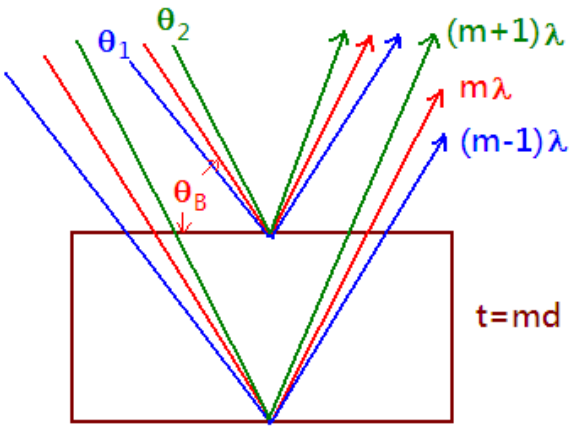
When the path difference in the atomic layers at top and bottom is λ, the path difference at top and at the center is $\frac{\lambda}{2}$.

The total phase difference in the crystal will be cancelled. In other words,

$$2t\sin\theta_1 = m\lambda - \lambda = (m-1)\lambda$$

`Similarly, at $\theta = \theta_2$

$$2t\sin\theta_2 = m\lambda + \lambda = (m+1)\lambda$$



Then

$$t(\sin\theta_2 - \sin\theta_1) = \lambda$$

$$2t\cos\left(\frac{\theta_1 + \theta_2}{2}\right)\sin\left(\frac{\theta_2 - \theta_1}{2}\right) = \lambda$$

$$2t\cos\theta_B \sin\left(\frac{\theta_2 - \theta_1}{2}\right) = \lambda$$

Since $\frac{\theta_2 - \theta_1}{2}$ is very small

$$2t\cos\theta_B\left(\frac{\theta_2 - \theta_1}{2}\right) = \lambda$$

$$B = \frac{\lambda}{t\cos\theta_B}$$

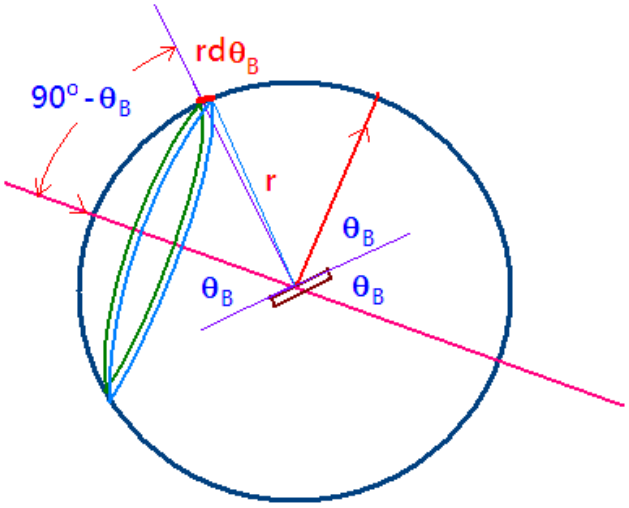
$$B = \frac{\lambda}{md\cos\theta_B}$$

Therefore

$$B \propto \frac{1}{\cos\theta}$$

Note that B=0 when m is infinite.

(iii-1) $\cos\theta$ factor due to the number of crystal counted in the powder method



The number of crystal is not constant for a particular θ_B even through the crystal are oriented completely at random.

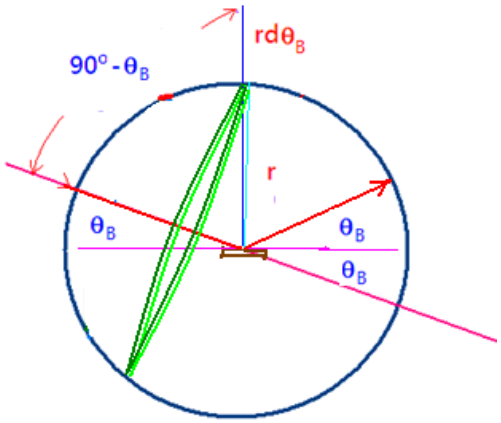
For the hkl reflection, the range of angle near the Bragg angle, over which reflection is appreciable, is $\Delta\theta$. Assuming that ΔN is the number of crystals located in the circular band of width $r\Delta\theta$

$$\frac{\Delta N}{N} = \frac{r\Delta\theta \cdot 2\pi r \sin\left(\frac{\pi}{2} - \theta_B\right)}{4\pi r^2}$$

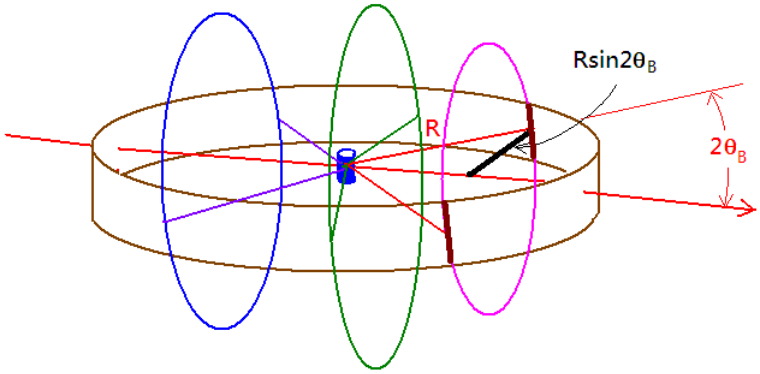
$$\frac{\Delta N}{N} = \frac{\Delta\theta \cdot \cos\theta_B}{2}$$

where N is the total number of crystal.

The number of grains satisfying the diffraction condition is proportional to $\cos\theta_B$. In other words, more grains satisfying the diffraction condition at higher θ_B as shown in the figure below.



(iii-2) $\frac{1}{\sin 2\theta_B}$ factor due to the segment factor in the Debye-scherrer film



The film receives a greater proportion of a diffraction cone when the reflection is in the forward or backward direction than it does near $2\theta = \frac{\pi}{2}$

The relative intensity per unit length is proportional to

$$\frac{1}{2\pi R \sin 2\theta_B}$$

i.e. proportional to

$$\frac{1}{\sin 2\theta}$$

Therefore, the Lorentz factor for the powder method is

$$\frac{1}{\sin 2\theta}\cos\theta\frac{1}{\sin 2\theta} = \frac{\cos\theta}{\sin^2 2\theta} = \frac{1}{4\sin^2\theta\cos\theta}$$

and for the rotating crystal method and the diffractometer method is

$$\frac{1}{\sin 2\theta}$$

(iv) Plot of polarization and Lorentz factors

$$\alpha := 0\pi, 0.001\pi .. 0.5\pi$$

$$f(\alpha) := \frac{(1 + \cos(2\alpha)\cos(2\alpha))}{\sin(\alpha)\sin(\alpha)\cos(\alpha)}$$