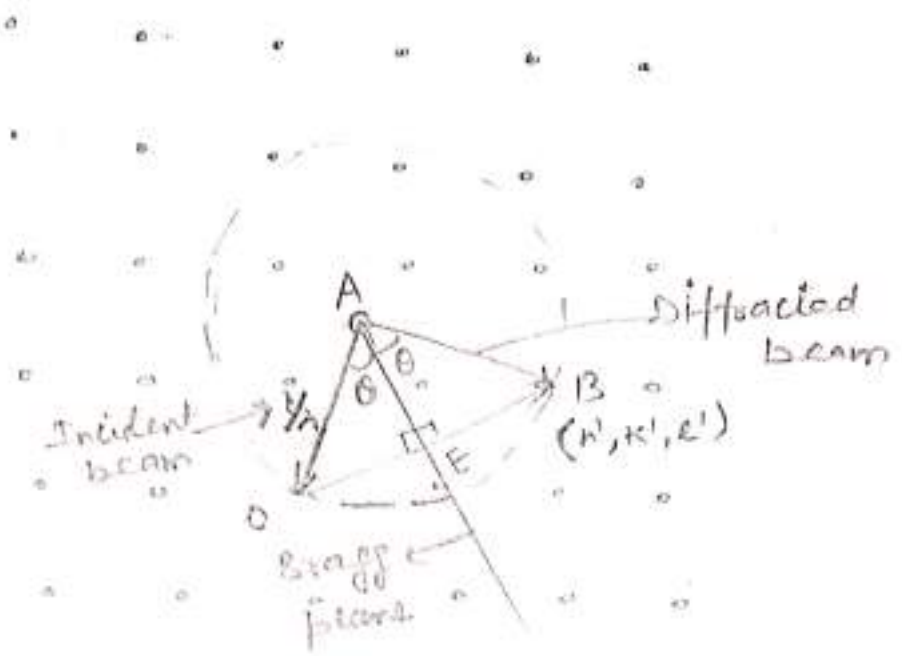
Bragg's law in Reciprocal lattice
(Ewald's construction)



Consider a reciprocal lattice as shown above in fig. From any arbitrary point A (not neccessarily a reciprocal lattice pt.), draw a vector $\vec{AO}$ of length $1/\lambda$ such that it point to any reciprocal lattice point, Let it be O. Now Taking A as center, draw a sphere of radius AO which must intersect at any other lattice point B of the reciprocal lattice.

Let the coordinates of point B be (h', k', l'). Join $\vec{AB}$ & $\vec{OB}$.

(2)

$\vec{OB}$ = Reciprocal lattice vector

Since $B = (h'k'l')$

$= (nh, nk, nl)$

from A, draw a ⊥ to OB, let it intersect OB at point E. AE is a bragg plane.

(Bragg Plane:— In Reciprocal space, if from origin, we draw a vector from one point to another lattice point & then draw a ⊥ bisector of that vector. This line in 2D (or plane in 3D) that we will get is known as Bragg plane)

$OB = 2OE$

$\therefore |\vec{OB}| = \frac{2\sin\theta}{\lambda}$ — (1)

In Δ AOE

$\sin\theta = \frac{OE}{1/\lambda}$

$OE = \frac{1}{\lambda}\sin\theta$

also, $|\vec{OB}| = \frac{1}{d_{h'k'l'}}$ [Distance from plane at origin & plane at pt B $= \frac{1}{d_{h'k'l'}}$]

$= \frac{1}{d_{nh\,nk\,nl}} = \frac{n}{d_{hkl}}$ — (2)

equating (1) & (2)

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

$$\boxed{2d_{hkl}\sin\theta = n\lambda}$$ → Bragg's law in Reciprocal lattice

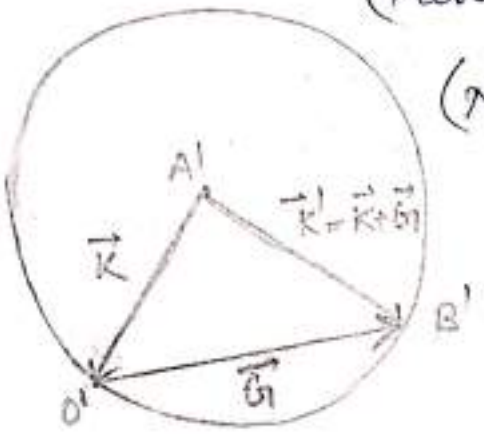
n = order of reflection

Note that, if the coordinates of a reciprocal lattice point (nh, nk, nl) contain a common factor n, then its represents n^{th} order reflection from the planes (hkl).

Such a construction is called Ewald's Construction.

Bragg's law in vector form:

(Modified form of Bragg's law)
or
(Magnified Ewald's Construction)



multiply all the dimensions by 2π

$$OA \times 2\pi = \frac{1}{\lambda} \times 2\pi = \frac{2\pi}{\lambda} = K = O'A' \text{ (new vector)}$$

$\vec{K}$ = Incident wave vector

$\vec{K'}$ = Scattered wave vector, $\vec{G}$ = Reciprocal lattice vector

$$|A'O'| = |A'B'| \quad \text{[Both are radius]}$$

$$K^2 = (K+G)^2$$

(4) $K'^2 = K^2 + G^2 + 2\bar{K}\cdot\bar{G}$

$$\boxed{G^2 + 2\bar{K}\cdot\bar{G} = 0}$$

vector form of Bragg's law.

Note!- K & K' have same magnitude ie Incident & diffracted beam has same magnitude, only directions are different

⇒ Scattering does not changes the magnitude of wave vector K, only its direction is changed. Also scattered wave differs from the incident wave by reciprocal lattice vector(G_1).

This vector form of Bragg's law will be helpful in the construction of Brillouin zone.

Atomic scattering factor or Atomic form factor (f)

Atomic scattering factor (f) describes the scattering power of a single atom relative to the scattering power of single electron.

$$\therefore f = \frac{\text{Amplitude of radiation's scattered from an atom}}{\text{Amplitude of radiation's scattered from an e}^{\ominus}.}$$

If Z is the number of electrons present in the atom.

$$f = \frac{Z \times \text{amplitude of radiation's scattered from an e}^{\ominus}}{\text{Amplitude of radiation's scattered from an e}^{\ominus}}$$

$f = Z$, but this is not true because X rays scattered from different positions (due to different e⊖) of an atom are, in general, not in phase always.

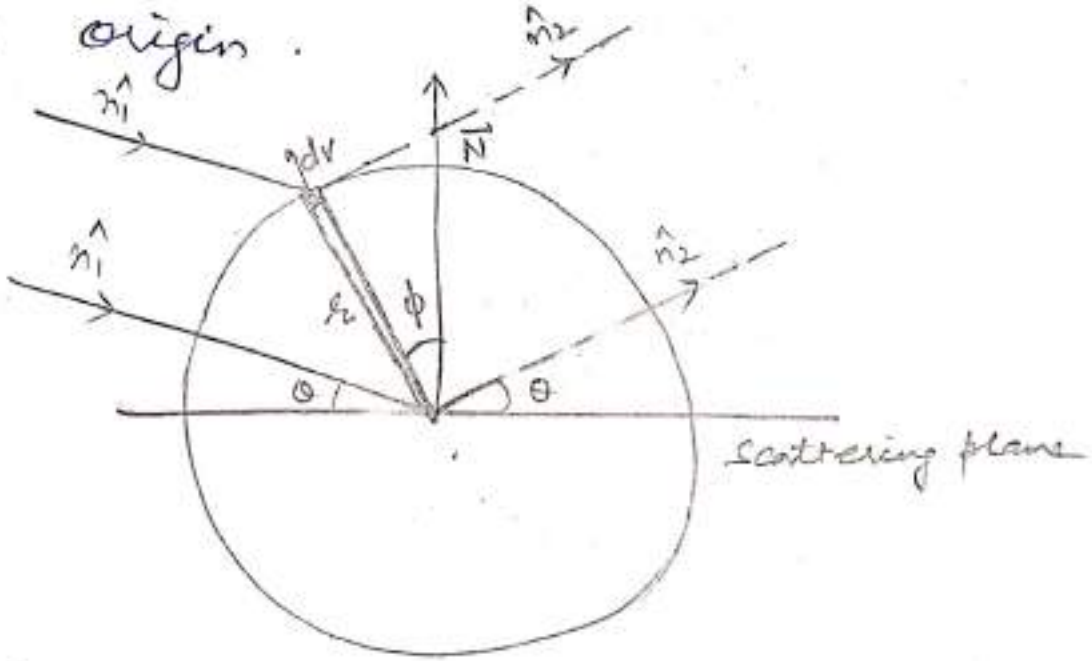
$$\therefore \boxed{f < Z}$$

⑥

Derivation of form factor (f) :

(for spherically symmetric charge distribution of electrons)

Consider an atom containing e⊖'s arranged in a sph. sym configuration around its center which is taken as origin.



Consider a small volume element dV at $\vec{r}$, the charge located at r is $\underline{f(r)\,dv}$.

$\hat{n}_1$, $\hat{n}_2$ be the direction of incident and scattered beam respectively.

The phase difference between the wave scattered from the charge $f(r)dv$ & that scattered from the electron is given by

$$\phi_r = \frac{2\pi}{\lambda}\,\vec{r}.\vec{N}$$

N = scattering normal

Let the scattering amplitude from the point electron in the direction $\hat{n}_2$ be $= A e^{i(Kx - \omega t)}$

x = distance covered along $\hat{n}_2$.

K = wave vector

Now, the scattering amplitude from the charge $\rho(r)dv$ in the same direction will be proportional to the magnitude of charge & will contain the phase factor $e^{i\phi_r}$ ie

$$A e^{i(Kx - \omega t) + i\phi_r} \cdot \rho(r) dv$$

∴ ratio of amplitude of radiation scattered by the charge element to that scattered by the point electron at the origin is

$$df = \frac{A e^{i(Kx - \omega t) + i\phi_r} \rho(r) dv}{A e^{i(Kx - \omega t)}}$$

$$df = e^{i\phi_r} \rho(r) dv$$

Thus, the ratio of amplitude from the whole atom to that from an electron is

$$f = \int_V \rho(r)\, e^{i\phi_r}\, dv$$

V = volume of the atom.

Since, the electron in the atom have spherically symetric charge distibuted

$\therefore dv = 2\pi r^2 \sin\phi\, d\phi\, dr$ (using sph. polar coordinates)

$|N| = 2\sin\theta \longrightarrow$ (Von-Laue treatment derivation)

$$\phi_r = \frac{2\pi}{\lambda} r \cdot N \cos\phi$$

$$= \frac{2\pi}{\lambda} r \cdot 2\sin\theta \cos\phi = \frac{4\pi}{\lambda} r \sin\theta \cos\phi$$

$$= \mu r \cos\phi \qquad \text{where } \mu = \frac{4\pi}{\lambda}\sin\theta$$

$$f = \int_{r=0}^{\infty} \int_{\phi=0}^{\pi} \rho(r)\, e^{i\mu r\cos\phi}\, 2\pi r^2 \sin\phi\, d\phi\, dr$$

Taking together ϕ term

Now, $\int_0^{\pi} e^{i\mu r\cos\phi} \sin\phi\, d\phi = 2\,\frac{\sin\mu r}{\mu r}$

$$\boxed{f = \int_0^{\infty} 4\pi r^2 \rho(r)\, \frac{\sin\mu r}{\mu r}\, dr}$$

as $\theta \to 0$ $\quad \mu \to 0$

for $\mu \to 0$ $\quad \frac{\sin \mu r}{\mu r} = 1$

$$\therefore \quad f = \int_0^\infty 4\pi r^2 \rho(r)\, dr$$

This integral represents the charge inside the spherical shell of radius r and thickness dr which is equal to the total electronic charge stored inside the atom $= Z$

Total scattering amplitude : $F(h'k'l')$

Total scattering amplitude for the $(h'k'l')$ reflection is defined as ratio of ---

$$F(h'k'l') = \frac{\text{Amplitude of radiation scattered by the entire unit cell}}{\text{Amplitude of radiation scattered by a single point electron}}$$

$$F(h'k'l') = \sum_j f_j e^{i\phi_j}$$

$$= \sum_j f_j e^{i(2\pi/\lambda)(r_j \cdot N)}$$

f_j → Atomic scattering factor for the j^{th} atom.

(10) ϕ_j = phase difference between the radiation scattered from the j^{th} atom of the unit cell & scattered from the $e^{\ominus}$ placed at the origin.

r_j = position of j^{th} atom

N = Scattering normal

$r_j = u_j a + v_j b + w_j c$

$$r_j \cdot N = \lambda(u_j h' + v_j k' + w_j l') \qquad \{a.N = h'\lambda\}$$

$$F(h'k'l') = \sum_j f_j \underbrace{e^{i2\pi(u_j h' + v_j k' + w_j l')}}_{= (S)}$$

$$F(h'k'l') = f \cdot S$$

where, $\boxed{S = \sum_j e^{2\pi i(u_j h' + v_j k' + w_j l')}}$ is

known as Geometrical structure factor.

ie it depends upon the geometrical arrangement of atoms with in a unit cell.

$$S = \frac{F(h'k'l')}{f}$$

$$S = \frac{\text{Total scattering amplitude}}{\text{Atomic scattering factor}}$$

Now, we know that

Intensity of radiation is proportional to square of amplitude.

∴ Intensity of diffracted beam (I) is also proportional to square of scattering amplitude (F).

$$\boxed{I = F^2}.$$

×

(12) Geometric structure factor for

1) Simple cubic : we know that,

$$S = e^{2\pi i \sum_j (u_j h' + v_j k' + w_j l')} \quad -(1)$$

$u_j v_j w_j$ = Coordinates representing the position of atoms in a unit cell

$(h' k' l')$ = Miller Indices

for simple cubic, $z = 1$ [$\because$ no of atoms / u.c = 1]

$(u_j v_j w_j) = (0, 0, 0)$

$$S = e^{2\pi i (0+0+0)} \quad \text{[Putting in eq (1)]}$$

$$S = e^{0} = 1$$

$$S = 1$$

Reflections are allowed for all possible values of $(h' k' l')$.

[Note:- Reflections will be forbidden if $S = 0$ & Allowed if $S = 1$]

2) Body centered cubic :

Total Number of atoms / U.C = 2

$Z = 2$

Positions of two atoms are given by the coordinates $(u_j v_j w_j)$

1) $(u_1 v_1 w_1) = (0\ 0\ 0)$

2) $(u_2 v_2 w_2) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

$$S = e^{0} + e^{2\pi i\left(\frac{1}{2}h' + \frac{1}{2}k' + \frac{1}{2}l'\right)}$$

$$\boxed{S = 1 + e^{\pi i (h'+k'+l')}}$$

Case I If $h'+k'+l' =$ odd

$$e^{i\pi\,(\text{odd no})} = (-1)$$

$\therefore$ $S = 1 - 1 = 0$ $\Rightarrow$ forbidden Reflection

Case II If $h'+k'+l' =$ even

$$e^{i\pi\,(\text{even No.})} = +1$$

$\therefore$ $S = 1 + 1 = 2$

$\Rightarrow$ Allowed Reflections

3) Face centered Cubic

Total number of atoms / unit cell

$= 4$

$\therefore Z = 4$. The positions of four atoms are given by the coordinates $(u_j v_j w_j)$.

$(u_1 v_1 w_1) = (0,0,0)$; $(u_2 u_2 w_2) = (\frac{1}{2}, \frac{1}{2}, 0)$

$(u_3 u_3 w_3) = (\frac{1}{2}, 0, \frac{1}{2})$; $(u_4 v_4 w_4) = (0, \frac{1}{2}, \frac{1}{2})$

$$S = e^{0} + e^{i\pi(h'+k')} + e^{i\pi(h'+l')} + e^{i\pi(k'+l')}$$

$$\boxed{S = 1 + e^{i\pi(h'+k')} + e^{i\pi(h'+l')} + e^{i\pi(k'+l')}}$$

Case I When all indices are even, such as

$(h'k'l') = (000), (2,0,0), (222), (220)$ & so on ...

i) Let us consider (0,0,0)

$S = 1 + e^{0} + e^{0} + e^{0}$

$S = 4 \Rightarrow$ allowed reflection

ii) for (200)

$S = 1 + e^{i\pi(2)} + e^{i\pi(2+0)} + e^{i\pi(0)}$

$S = 1 + 1 + 1 + 0 = 3$

$S = 3 \Rightarrow$ allowed reflection

iii) for (222)

$$S = 1 + e^{i\pi(4)} + e^{i\pi(4)} + e^{i\pi(4)}$$

$$S = 1 + 1 + 1 + 1 = 4$$

$S = 4 \Rightarrow$ Allowed Reflections

Therefore, for all the even miller indices, the S remain finite ($S \neq 0$), giving the conditions of allowed reflections.

Case II when all the miller indices are odd eg. (111), (3,3,3) (3,1,1) ---- so on.

i) For (111)

$$S = 1 + e^{2\pi i} + e^{2\pi i} + e^{2\pi i}$$

$S = 4 \Rightarrow$ allowed reflections.

ii) For (333)

$$S = 1 + e^{6\pi i} + e^{6\pi i} + e^{6\pi i}$$

$$S = 1 + 1 + 1 + 1 = 4$$

$S = 4 \Rightarrow$ allowed reflections

iii) For (3,1,1)

$$S = 1 + e^{4\pi i} + e^{4\pi i} + e^{2\pi i}$$

$$S = 1 + 1 + 1 + 1$$

$S = 4 \Rightarrow$ Allowed Reflections

Therefore, again for all the odd miller indices also, S remains finite ($S \neq 0$), hence the reflections are allowed from such planes.

Case III — When the miller indices are mixed (odd & even) both such as

(101), (211), (201) --- & soon

i) For (101)

$$S = 1 + e^{\pi i} + e^{2\pi i} + e^{\pi i}$$

$$S = 1 - 1 + 1 - 1$$

$S = 0 \Rightarrow$ forbidden reflections

ii) For (211)

$$S = 1 + e^{3\pi i} + e^{3\pi i} + e^{2\pi i}$$

$$S = 1 - 1 - 1 + 1$$

$S = 0 \Rightarrow$ forbidden reflections

iii) For (201)

$$S = 1 + e^{2\pi i} + e^{3\pi i} + e^{\pi i}$$

$$S = 1 + 1 - 1 - 1$$

$S = 0 \Rightarrow$ forbidden reflections

Hence, for mixed miller indices - the S becomes zero, thereby indicating forbidden reflections.

Selection Rules for Allowed Reflections:-

SCC : All possible values of (h,k,l)

BCC : (h+k+l) should be even.

FCC : All (h,k,l) should be even or odd. (Not mixed)

Practice ques: Check for the allowed (✓) and forbidden(✗) Reflections.

(h,k,l)	SCC	BCC	FCC
i) (100)	✓	✗	✗
ii) (110)	✓	✓	✗
iii) (111)	✓	✗	✓
iv) (211)	✓	✓	✗
v) (131)	✓	✗	✓
vi) (201)	✓	✗	✗
vii) (131)	✓	✗	✓
viii) (300)	✓	✗	✗