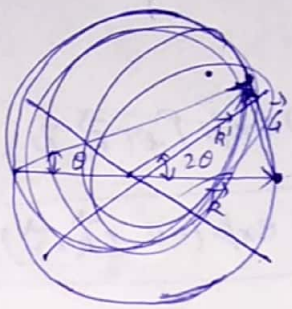
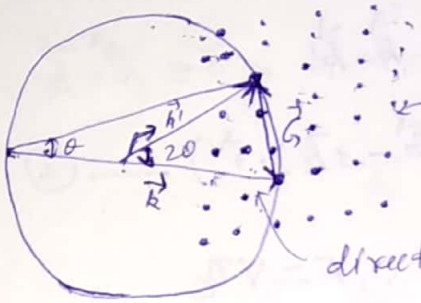
Ewald construction :-

Visualize diffraction condition in 3-D





R.L Points (Reciprocal Lattice Point)

direction of X-ray beam, $\vec{k}$ is chosen to show that $\vec{k}$ terminates at any R.L Point.

We draw a sphere of radius $|\vec{k}| = \frac{2\pi}{\lambda}$ about origin of $\vec{k}$.

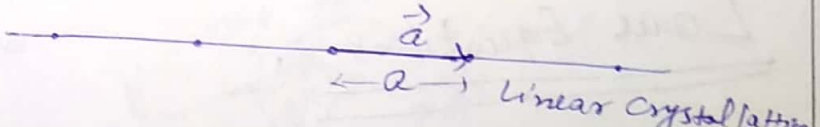
A Diffraction beam ~~too~~ will be formed if this sphere intersects any othe point in the R.L.

The sphere as drawn intercepts a point connected with the end of $\vec{k}$ by a R.L vector $\vec{G}$. Diffraction is in direction

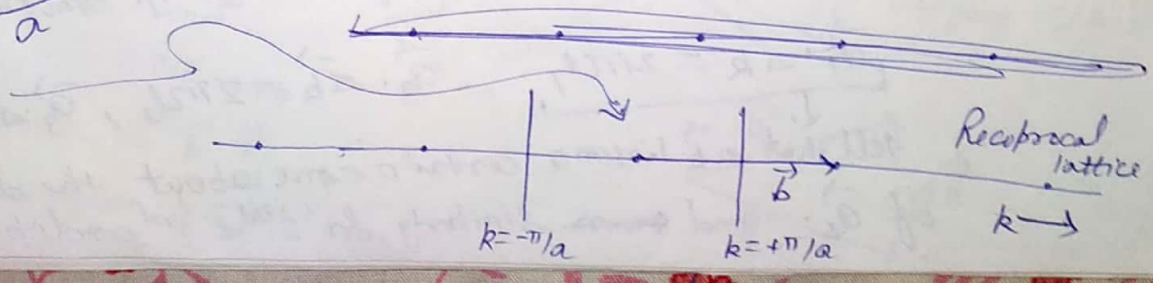
$$\vec{k'} = \vec{k} + \vec{G}, \quad \theta = \text{Bragg angle}$$

Brillouin Zone → Wigner-Seitz primitive cell in R.L.

In 1-D



$|\vec{b}| = \frac{2\pi}{a}$



Fourier Analysis of the basis

Structure factor · related to scattering amplitude

$$S_G = \int_{cell} dV\, n(\vec{r}) \exp(-i\vec{G}\cdot\vec{r})$$

↓ single cell with $r=0$ at one corner

$$n(\vec{r}) = \sum_{j=1}^{S} n_j(\vec{r}-\vec{r}_j)$$

↑ total e^- concentration at $\vec{r}$

$n_j(\vec{r}-\vec{r}_j)$ ↑ e^- conc. of atom j at $\vec{r}$.

, j = total # of atoms

r_j = vector to the centre of atom j

$$S_G = \sum_j \int dV\, n_j(\vec{r}-\vec{r}_j) \exp(-i\vec{G}\cdot\vec{r}) = \sum_j \exp(-i\vec{G}\cdot\vec{r}_j) \int dV\, n_j(\vec{\rho}) \exp(-i\vec{G}\cdot\vec{\rho})$$

Here $\vec{\rho} = \vec{r} - \vec{r}_j$

Define $\boxed{f_j = \int dV\, n_j(\vec{\rho}) \exp(-i\vec{G}\cdot\vec{\rho})}$

↑ atomic property; ↑ Integrated over all space

$$\boxed{S_G = \sum_j f_j \exp(-i\vec{G}\cdot\vec{r}_j)}$$

$\vec{G} = u_1\vec{b}_1 + u_2\vec{b}_2 + u_3\vec{b}_3$

Here $r_j = x_j\vec{a}_1 + y_j\vec{a}_2 + z_j\vec{a}_3$, $0 \le x_j, y_j, z_j \le 1$

↑ Position of the center of atom j relative to associated lattice Point.

$$\boxed{S_G(u_1u_2u_3) = \sum_j f_j \exp\left[-i2\pi(u_1x_j + u_2y_j + u_3z_j)\right]}$$

Remi

↑ differ from different atoms for one kind of atom in crystal it is same

$S \rightarrow$ need not to be real , ~~beca~~ because scattered Intensity involve ~~S*S~~ S^*S, S^* = complex conjugate of S.

$\Rightarrow S^*S \rightarrow$ real

$S_G = 0$, $I = 0$

If we choose ~~for~~ a conventional cell instead of Primitive cell The bassis is changed, but Physical scattering unchanged Thus for two choices 1 & 2.

$$N_1(\text{cell}) \times S_1(\text{basis}) = N_2(\text{cell}) \times S_2(\text{basis})$$

S for fcc Cubic cell has identical atoms at

$(x_j, y_j, z_j) \rightarrow (000), (0\tfrac{1}{2}\tfrac{1}{2}), (\tfrac{1}{2}0\tfrac{1}{2}), (\tfrac{1}{2}\tfrac{1}{2}0)$

$$S(u_1 u_2 u_3) = f\left[1 + \exp[-i\pi(u_2+u_3)] + \exp[-i\pi(u_1+u_3)] + \exp[-i\pi(u_1+u_2)]\right]$$

for all indices ~~odd~~ even/odd integers, $S = 4f$ and so on.

~~If all odd.~~

~~If one.~~

Atomic form factor → f_j → measures scattering power of j^{th} atom in the unit cell.

f involves number and distribution of atomic electrons and wavelength and angle of scattering of the radiation.

$$f_j = \int dV\, n_j(\vec{r}) \exp(-i\vec{G}\cdot\vec{r})$$

for spherical symmetric e^- distribution

$$f_j = 4\pi \int dr\, n_j(r)\, r^2 \frac{\sin Gr}{Gr}$$

If n_j's concentrated at $r=0$, $\lim_{r\to 0} \frac{\sin Gr}{Gr} = 1 \Rightarrow f_j = 4\pi \int n_j(r) r^2$

$$f_j = Z$$

↑ # of atomic electrons

Quasicrystals → - Not Bravais lattice
- Have symmetries intermediate between a crystal and a liquid.

Known quasicrystals are intermetallic alloys and are very poor electrical conductors

Note → only waves whose wavevector $\vec{k}$ drawn from the origin terminates on a surface of the B.Z. can be diffracted by the crystal.

Crystal lattice	First B.Z.
SC	Cube
fcc	Rhombic dodecahedron
bcc	Truncated octahedron