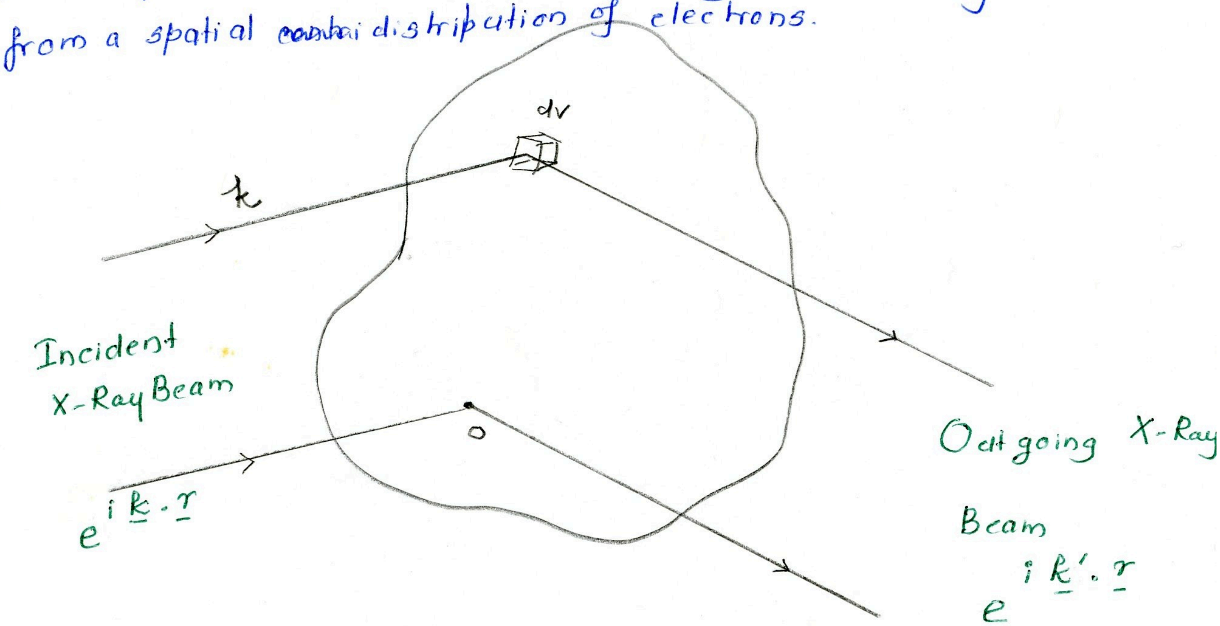
X-Ray Diffraction Conditions.

: Simple Bragg condition considers point particles at the Lattice points. Here we are considering the intensity of scattering from a spatial ~~[illegible]~~ distribution of electrons.



The amplitude of the wave scattered from a volume element is proportional to the electron concentration.

So the amplitude of the scattered wave in the direction k' is proportional to the integral over the crystal of $n(r)\,dV$ times $e^{i(k-k')r}$

The scattering amplitude

$$A = \int dV\, n(r)\, e^{-i\Delta k\cdot\bar{r}}$$

$k + \Delta k = k'$

Now inorder to write the Fourier Components:

$$A = \sum_G \int dV\, n_G\, e^{iG\cdot r}\, e^{-i\Delta k\cdot r}$$

$$n(r) = \sum_G n_G\, e^{iG\cdot r}$$

Recall for 1-D we wrote

$$n(x) = \sum_p n_p e^{i\frac{2\pi p}{a}x}$$

The Direct generalization to 3-D

$$n_G = \sum_G n_G e^{iG \cdot r}$$

$G \rightarrow$ Reciprocal Vectors.

Let's consider the Diffraction Condition

$$A = \sum_G \int dV\, n_G e^{iG \cdot r} e^{-i\Delta k \cdot r}$$

When the scattering vector ~~is~~ $\Delta \bar{k}$ is equal to the Reciprocal vector G, the argument of the exponent vanishes.

$k + \Delta k = k'$ becomes

$$\boxed{k + G = k'} \longrightarrow \text{Diffraction Condition.}$$

This condition must be equivalent to Bragg Diffraction Condition

Let's further simpify this.

$$k + G = k'$$

$$k^2 + 2k \cdot G + G^2 = k'^2$$

Here we are considering elastic waves ; $k^2 = k'^2$

$$2k\cdot G + 1G^2 = 0$$

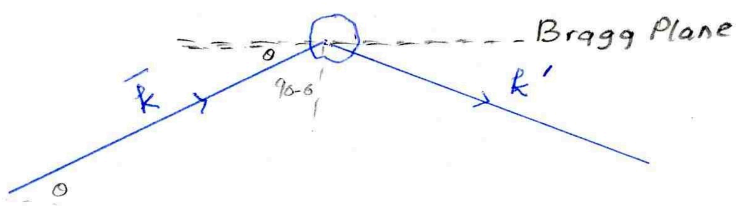
$$2k\cdot G = |-G|^2$$

Let's look at the geometric representation of these vector

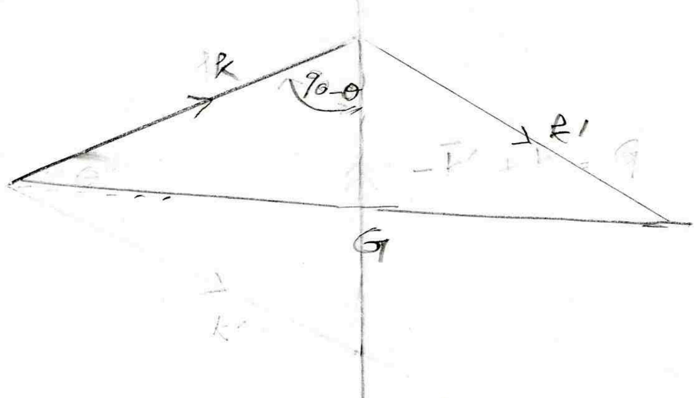
$$\bar{k} - \bar{k}' = \bar{G}$$

$$\bar{G} = h\bar{A} + k\bar{B} + l\bar{C}$$

(Here I choose $\bar{A}, \bar{B}, \bar{C}$ as the Reciprocal Lattice Vect



I want to do $\bar{k} - \bar{k}'$



By Geometry

$$G = 2k\sin\theta$$

$$|k| = |k'|$$

$$k = \frac{2\pi}{\lambda}$$ (Wave Num

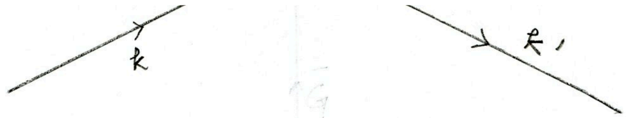
$$2\bar{k}\cdot\bar{G} = 2|k||G|$$

$$= 2|k||G|\sin\theta$$

$$2k\cdot G = |G|^2$$

$$2|k||G|\sin\theta = |G|^2$$

$$2\frac{2\pi}{\lambda}\sin\theta = |G|$$



Now we are looking at the planes perpendicular to $\bar{G}$. In the next home work, you will prove that the lattice planes normal to the Direction

$$G \quad h\bar{A} + k\bar{B} + lC = d_{hkl}$$

$$d_{hkl} = \frac{2\pi}{|G|}$$

With that

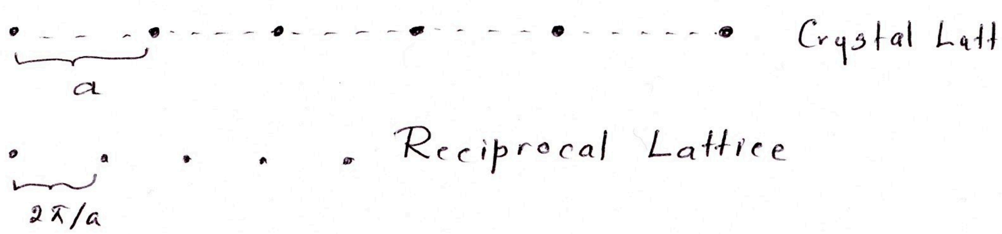
So now our Diffraction condition becomes

$$d_{hkl} \qquad 2\left(\frac{2\pi}{\lambda}\right)\sin\theta = \cancel{2\pi}\,|G|$$

$$2\left(\frac{2\pi}{\lambda}\right)\sin\theta = \frac{2\pi}{d_{hkl}}$$

$$\boxed{2d\sin\theta = \lambda}$$ Bragg Condit

$\boxed{\text{Note}}$ Laue Condition introduces a set of Reciprocal Lattice Vectors. We know in 1-D, for a lattice with periodicity a, the periodicity $\frac{2\pi}{a}$.



What are the Reciprocal Lattice in 3-D

Reciprocal Lattice Vectors in 3-D

What are the reciprocal vectors. Where does it come from?

$$n(x) = n(x+T)$$

$$= \sum_p n_p e^{i\frac{2\pi p}{a} \cdot x}$$

$$n(r) = n(r+T)$$

$$= \sum_G n_G e^{i\bar{G}\cdot\bar{r}}$$

We find a set of vectors $\bar{G}$ such that $n(r)$ is invariant under all lattice translations.

$$\sum_G n_G e^{iG\cdot r} = \sum_G n_G e^{i\bar{G}\cdot(\bar{r}+\bar{T})}$$

$$\Rightarrow e^{i\bar{G}\cdot\bar{T}} = 1$$

$\bar{T}$ = Translational vector.

$$\bar{T} = v_1\bar{a} + v_2\bar{b} + v_3\bar{c}$$

$\bar{a}, \bar{b}, \bar{c} \rightarrow$ Lattice Vectors

$$\bar{G} = u_1\bar{A} + u_2\bar{B} + u_3\bar{C}$$

$\bar{A}, \bar{B}, \bar{C} \rightarrow$ Reciprocal Lattice Vector

$$\cancel{e^{i\bar{G}\cdot\bar{T}} = e^{i(u_1\bar{a}+v_1}}$$

$$e^{i\bar{G}\cdot\bar{T}} = e^{i(u_1\bar{A}+u_2\bar{B}+u_3\bar{C})\cdot(v_1\bar{a}+v_2\bar{b}+v_3\bar{c})}$$

$$= e^{i(2\pi n)}$$

$\longrightarrow$ Then this becomes 1

In order for that condition to be satisfied :

We choose

$$\bar{A} \perp \underline{b} , \underline{c}$$

$$\bar{B} \perp \underline{a} , \underline{c}$$

$$\bar{C} \perp \underline{a} , \underline{b}$$

Now

$$e^{i \bar{G} \cdot \bar{T}} = e^{i (u_1 \bar{A}_1 + u_2 \bar{A}_2 + u_3 \bar{C}) \cdot (v_1 \underline{a} + v_2 \underline{b} + v_3 \underline{c})}$$

$$= e^{i (u_1 v_1 \bar{A} \cdot \bar{a} + u_2 v_2 \bar{B} \cdot \bar{b} + u_3 v_3 \bar{C} \cdot \bar{c})}$$

$$u_1 v_1 \bar{A} \cdot \bar{a} = 2\pi n_1$$

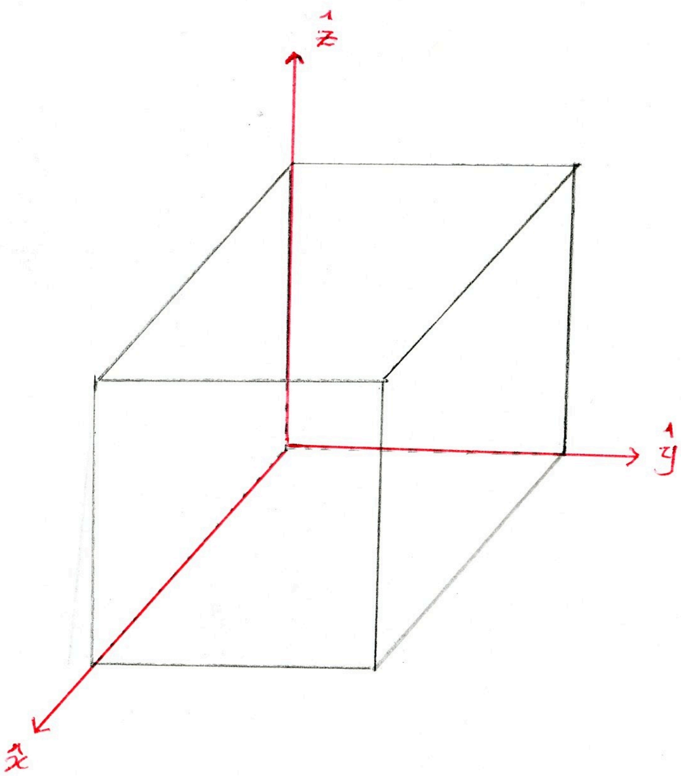
For that to be true, we choose

$$\bar{A} = \frac{2\pi \, \bar{b} \times \bar{c}}{\bar{a} \cdot \bar{b} \times \bar{c}}$$

$$\bar{B} = \frac{2\pi \, \bar{a} \times \bar{c}}{a \cdot \bar{b} \times \bar{c}}$$

$$\bar{C} = \frac{2\pi \, \bar{a} \times \bar{b}}{a \cdot (\bar{b} \times \bar{c})}$$

<u>Simple Cubic Lattice :</u>



$\bar{a} = a\,\hat{x} \qquad \bar{b} = a\,\hat{y} \qquad \bar{c} = a\,\hat{z} \qquad \bar{a}\cdot\bar{b}\times\bar{c} = a^3$

$$\bar{A} = \frac{2\pi\ \bar{b}\times\bar{c}}{\bar{a}\cdot\bar{b}\times\bar{c}} = \frac{2\pi\ a^2\ \hat{x}}{a^3} = \frac{2\pi}{a}\hat{x}$$

$$\bar{B} = \frac{2\pi\ \bar{c}\times\bar{a}}{\bar{a}\cdot\bar{b}\times\bar{c}} = \frac{2\pi}{a}\hat{y}$$

$$\bar{C} = \frac{2\pi\ a\times b}{\bar{a}\cdot\bar{b}\times\bar{c}} = \frac{2\pi}{a}\hat{z}$$

Body Centered Cubic Lattice.

The primitive Lattice vectors :

The First nearest neighbors are located at :

$$\left(\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\right)\left(-\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\right)\left(\tfrac{1}{2}\ -\tfrac{1}{2}\ \tfrac{1}{2}\right)\left(\tfrac{1}{2}\ \tfrac{1}{2}\ -\tfrac{1}{2}\right)\left(-\tfrac{1}{2}\ -\tfrac{1}{2}\ \tfrac{1}{2}\right),$$

$$\left(-\tfrac{1}{2}\ -\tfrac{1}{2}\ -\tfrac{1}{2}\right)\left(-\tfrac{1}{2}\ +\tfrac{1}{2}\ -\tfrac{1}{2}\right)\left(\tfrac{1}{2}\ -\tfrac{1}{2}\right.$$

We cam make a symmetric primitive cell by choosing

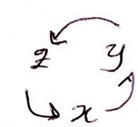
$$a' = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$b' = \frac{a}{2}(-\hat{x} + y + \hat{z})$$

$$c' = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

$\bar{a}' . \bar{b}' \times \bar{c}' \longrightarrow$ We cam of course make a guess.

$$\bar{b}' \times \bar{c}' = \frac{a^2}{4}[-\hat{x} + \hat{y} + \hat{z}] \times [\hat{x} - \hat{y} + \hat{z}]$$



$$= \frac{a^2}{4}[\hat{z} + \hat{y} - \hat{z} + \hat{x} + \hat{y} + \hat{x}]$$

$$= \frac{a^2}{2}[\hat{y} + \hat{x}]$$

$$a' . b' \times \hat{c} = \frac{a}{2}(\hat{x} + \hat{y} - z) \cdot (\hat{y} + \hat{x}] \frac{a^2}{2}$$

$$= \frac{a^3}{4}[1 + 1] = \frac{a^3}{2}$$

$$A = \frac{2\pi\ b' \times c'}{\bar{a} . b' \times c'} = \frac{2\pi}{a^3/2}\ \frac{a^2}{2}(\hat{y} + \hat{x}) = \frac{2\pi}{a}(\hat{y} + \hat{x})$$

Simillar way we can calculate the $\bar{B}$ & $\bar{C}$ vectors

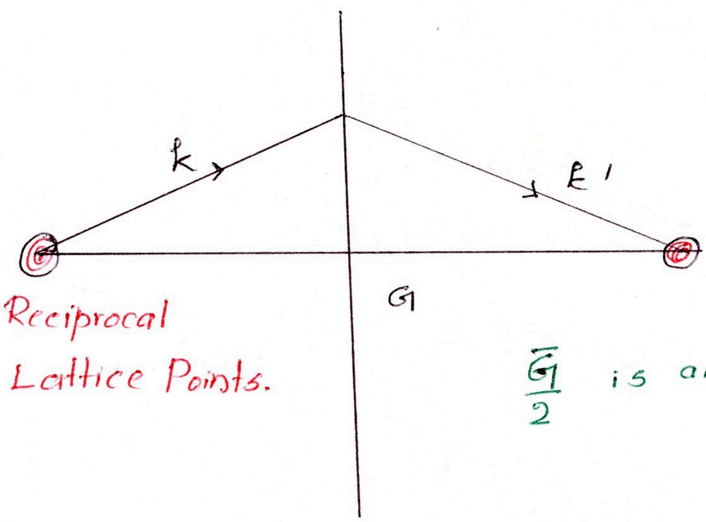
Similarly we can calculate the Reciprocal Vectors for any Lattice.

Let's look at Some important properties of Reciprocal vectors.

The Diffraction condition reads:

$$2 \bar{k} \cdot \bar{G} = G^2$$

$$k \cdot \frac{G}{2} = \left(\frac{G}{2} \right)^2$$



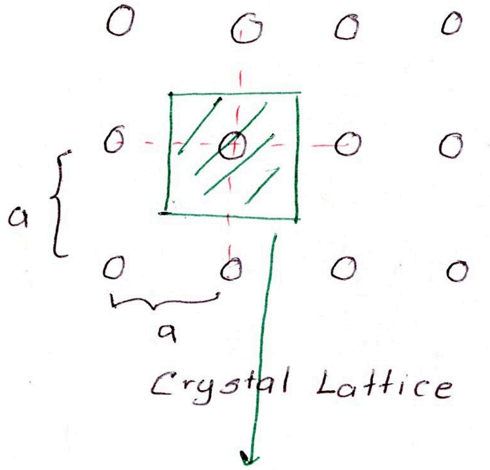
$\frac{\bar{G}}{2}$ is an important quantity

A wave whose wave vector drawn from the origin terminates an any of these planes will satisfy the Bragg diffraction condition.

These planes divides the fourier space into pieces.

Let's think about the square lattice.

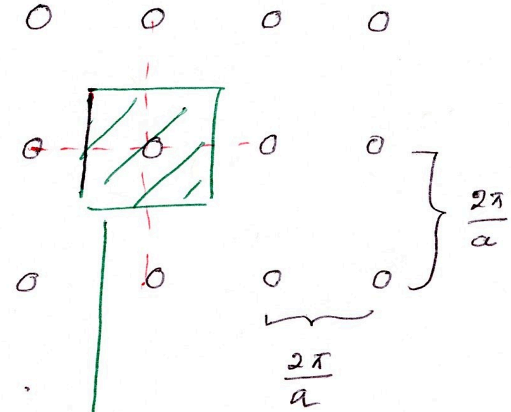
Reciprocal Lattice will also be square.



Crystal Lattice

Wigne Seitz Cell for the Real Crystal

$\Rightarrow$

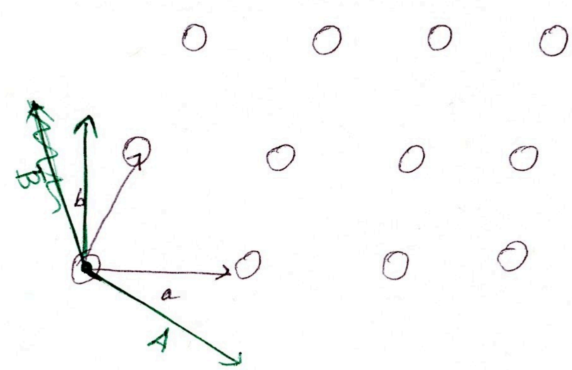


Reciprocal Lattice

Brillouin Zone of the Reciprocal Lattice

Brillouin Zone is equivalen to the Wigner Seitz cell in the Reciproc space.

Hexagonal Lattice



$$\bar{A} = 2\pi \frac{b \times c}{a \cdot \bar{b} \times \bar{c}}$$

$$\bar{B} = 2\pi \frac{a \times c}{a \cdot \bar{b} \times \bar{c}}$$

Reciprocal Lattice of a Hexagonal Lattice

Do it for Home Work.