X-ray diffraction :-

X-rays are electromagnetic waves like oridinary light, they should exhibit interference and diffraction. The wavelength of X-rays is of the order of 1Å, So that ordinary devices such as ruled diffraction gratings do not produce observable effects with X-rays. In 1912, German Physicist Laue Suggested that a crystal which consisted of a three-dimensional array of regularly spaced atoms could Serve the purpose of grating. The crystal differs from the ordinary grating in the sense that the diffracting centres in the crystal are not in one plane. Hence the crystal acts as a space grating rather than a plane grating.

On the suggestion of Laue, his associates, Friedrich and Knipping succeeded in diffractiong X-rays by passing them through a thin Crystal of Zinc blende. The diffraction pattern obtained consists of a central spot and a series of spots arranged in a definite pattern about the central spot. This symmetrical pattern of spots is Known as Laue pattern and proves the X-rays are electromagnetic radiation. A simple interpretation of the diffraction pattern was given by W.L. Bragg. According to him, the spots are produced due to the reflection of some of incident X-rays from the various sets of parallel crystal planes which contain a large number of atoms.

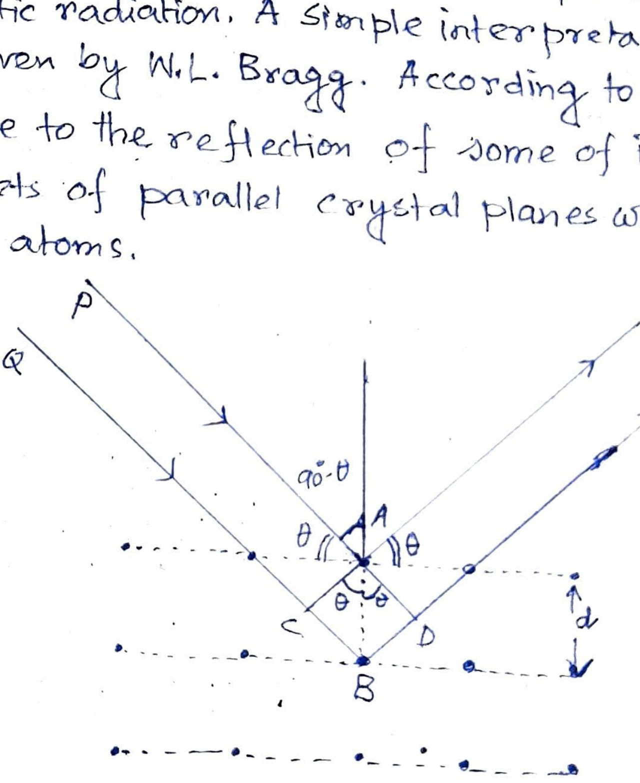


Fig.(19)

Bragg's Law:-

Consider a ray PA reflected at atom A in the direction AR from plane 1 and another ray QB reflected at another atom B in the direction BS. Now from the atom A, draw two normals AC and AD on QB and BS respectively. The two reflected rays will be in phase or out of phase depending on the path difference. When the path difference (CB+BD) is a whole wavelength λ or multiple of whole wavelength (nλ), then the two rays will reinforce each other and produce an intense spot. Thus condition of reinforcement is

$$CB + BD = n\lambda$$

From fig (19)

$$CB = BD = d\sin\theta$$

Where θ = glancing angle, the angle between incident ray and planes of reflection

Therefore,

$$\boxed{2d\sin\theta = n\lambda} \quad \ldots \quad (1)$$

Where d is the interplanar spacing and $n = 1, 2, 3 \ldots$ stands for first, second, … order maxima respectively. Eqn (1) is known as Bragg's law. Different directions in which intense maxima will be produced different values of θ, i.e.

$$\sin\theta_1 = \frac{\lambda}{2d} \quad \text{for 1st max}^{m}$$

$$\sin\theta_2 = \frac{2\lambda}{2d} \quad \text{for 2nd max}^{m}$$

and So on.

The intensity of reflected x-rays decrasing gradually as the order of spectrum increases.

Thus we see that when a beam of monochromatic x-rays falls on a crystal, each atom becomes a source of scattering radiations. The combined Scattering of x-rays from these planes can be looked upon as reflections from these planes. Generally, the Bragg Scattering is regarded as Bragg reflection.

Reciprocal Lattice:-

The diffraction of x-rays occurs from various sets of parallel planes having different orientations and interplanar spacings. In certain situations involving the presence of different sets of parallel with different orientations, it becomes difficult to visualize all such planes because of their two dimensional nature. The problem was simplified by P.P. Ewald by devloping a new type of lattice known as reciprocal lattice. The idea underlying the devlopment was that each set of parallel planes could be represented by a normal to these planes having ~~the~~ length equal to the reciprocal of interplanar spacing. Thus direction of each normal represents the orientation of the set of parallel planes and length is proporti~~ond~~onal to the reciprocal of interplanar spacing.

The normals are drawn with reference to any arbitray origin and points are marked at their ends. These points form a regular arrangement which is called a reciprocal lattice.

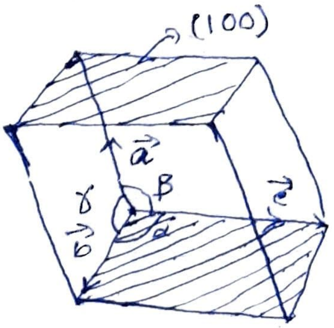
A reciprocal lattice vectors, $\vec{\sigma}_{hkl}$ is defined as a vector having magnitude equal to the reciprocal of the interplanar spacing d_{hkl} and direction coinciding with normal to the (hkl) planes. Thus, we have

$$\vec{\sigma}_{hkl} = \frac{1}{d_{hkl}}\hat{n}$$

where $\hat{n}$ is the unit vector normal to the (hkl) planes. In fact, a vector drawn from the origin to any point in the reciprocal lattice vector.

Like a direct lattice, a reciprocal lattice also has a unit cell which is of the form of a parallelopiped. The unit cell is formed by the shortest normals along the three directions, i.e. along the normals to the planes (100), (010) and (001). These normals produce reciprocal lattice vectors designated as $\vec{\sigma}_{100}$, $\vec{\sigma}_{010}$ and $\vec{\sigma}_{001}$ which represent the fundamental reciprocal lattice vectors.

Let $\vec{a}$, $\vec{b}$ and $\vec{c}$ be the primitive translational vectors of the direct lattice as shown in fig. (20). The base of the unit cell is formed by vectors $\vec{b}$ and $\vec{c}$ and its height is equal to d_{100}. The volume of the cell is



unit cell of monoclinic crystal.

Fig. (20)

$$V = \text{area} \times d_{100}$$

$$\text{or, } \frac{1}{d_{100}} = \frac{\text{area}}{V} = \frac{|\vec{b}\times\vec{c}|}{V}$$

In vector form $$\frac{\hat{n}}{d_{100}} = \frac{\vec{b}\times\vec{c}}{V} = \vec{\sigma}_{100} = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \quad \cdots (1)$$

Denoting the fundamental reciprocal vectors $\vec{\sigma}_{100}$, $\vec{\sigma}_{010}$ and $\vec{\sigma}_{001}$ by $\vec{a}^*$, $\vec{b}^*$ and $\vec{c}^*$ respectively, eqn (1) is.

$$\left.\begin{aligned} \vec{a}^* &= \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \\ \text{Similarly, } \quad \vec{b}^* &= \frac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \\ \vec{c}^* &= \frac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \end{aligned}\right\} \quad \cdots (2)$$

From eqn (2), we have, $\vec{a}^*$ is normal to $\vec{b}$ and $\vec{c}$
$\vec{b}^*$ is normal to $\vec{c}$ and $\vec{a}$
$\vec{c}^*$ is normal $\vec{a}$ and $\vec{b}$

In vector notations, it means

$$\left.\begin{array}{ll} \vec{a}^{*}\cdot\vec{b}=0 & \vec{a}^{*}\cdot\vec{c}=0 \\ \vec{b}^{*}\cdot\vec{c}=0 & \vec{b}^{*}\cdot\vec{a}=0 \\ \vec{c}^{*}\cdot\vec{a}=0 & \vec{c}^{*}\cdot\vec{b}=0 \end{array}\right\} \text{———} ③$$

Similarly, $\vec{a}^{*}\cdot\vec{a}=\vec{b}^{*}\cdot\vec{b}=\vec{c}^{*}\cdot\vec{c}=1$ . . . . (4)

A crystal lattice is a lattice in real or ordinary space i.e., the space defined by the co-ordinates, whereas a reciprocal lattice is a lattice in the reciprocal space, associated $\vec{K}$-space or Fourier Space. The translation lattice vector $\vec{T}$ is given by

$$\vec{T}=n_1\vec{a}+n_2\vec{b}+n_3\vec{c} \quad . . . (5)$$

where n_1, n_2, n_3 are integers. Similarly, reciprocal lattice vectors defined as

$$\vec{G}=h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*} \quad . . . (6)$$

where h, k, l are integers.

In some other books, eqn (2) and ④ write as

$$\vec{a}^{*}\cdot\vec{a}=\vec{b}^{*}\cdot\vec{b}=\vec{c}^{*}\cdot\vec{c}=2\pi \quad . . . (7)$$

and

$$\left.\begin{array}{l} \vec{a}^{*}=2\pi\dfrac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \\ \vec{b}^{*}=2\pi\dfrac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \\ \vec{c}^{*}=2\pi\dfrac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \end{array}\right\} \quad . . . (8)$$

<u>Reciprocal lattice to SC lattice:-</u>

The primitive translation vectors of a simple cubic lattice may be written as

$$\vec{a}=a\hat{i}, \quad \vec{b}=a\hat{j}, \quad \vec{c}=a\hat{k}$$

Volume of the simple cubic unit cell $=\vec{a}\cdot(\vec{b}\times\vec{c})$

$$=a^3[\hat{i}\cdot(\hat{j}\times\hat{k})]$$

$$=a^3$$

Using eqn(8), the reciprocal lattice vectors to the Sc lattice are obtained as

$$\left.\begin{array}{l} \vec{a}^{*}=2\pi\dfrac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}=2\pi\dfrac{a\hat{j}\times a\hat{k}}{a^3}=\dfrac{2\pi}{a}\hat{i} \\ \text{Similarly, } \vec{b}^{*}=\dfrac{2\pi}{a}\hat{j} \\ \text{and } \vec{c}^{*}=\dfrac{2\pi}{a}\hat{k} \end{array}\right\} \quad . . . (9)$$

Eqn (9) indicate that all the three reciprocal lattice vectors are equal in magnitude which means that the reciprocal lattice to SC lattice is also simple cubic but with lattice constant is $\frac{2\pi}{a}$.

Reciprocal lattice to BCC lattice:-

The primitive translation vectors of a body-centred cubic lattice as shown in fig. (21), are

$$\left.\begin{aligned}\vec{a}' &= \frac{a}{2}(\hat{i}+\hat{j}-\hat{k})\\ \vec{b}' &= \frac{a}{2}(-\hat{i}+\hat{j}+\hat{k})\\ \vec{c}' &= \frac{a}{2}(\hat{i}-\hat{j}+\hat{k})\end{aligned}\right\} \cdots (10)$$

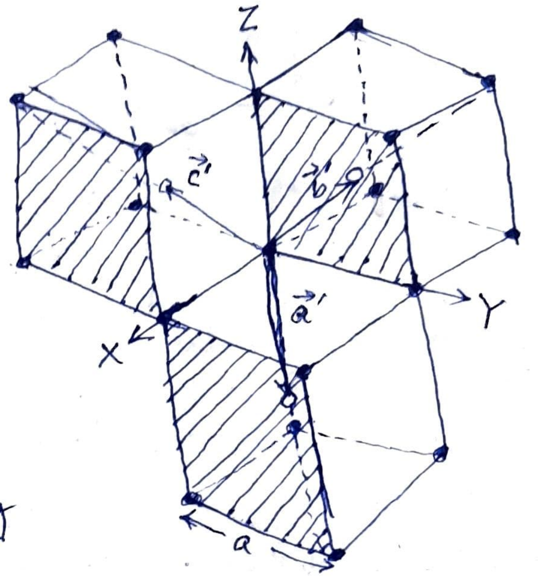


Fig. (21)

where 'a' is the length of the cube edge and $\hat{i}$, $\hat{j}$ and $\hat{k}$ are the orthogonal unit vectors along cube edges. The volume of the primitive cell is given by

$$V = \vec{a}'\cdot(\vec{b}'\times\vec{c}')$$

$$= \frac{a^3}{8}\left[(\hat{i}+\hat{j}-\hat{k})\cdot\{(-\hat{i}+\hat{j}+\hat{k})\times(\hat{i}-\hat{j}+\hat{k})\}\right]$$

$$= \frac{a^3}{2}$$

Using eqn(8), the reciprocal lattice vectors as obtained as

$$\left.\begin{aligned}\vec{a}^* &= 2\pi\frac{\vec{b}'\times\vec{c}'}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = 2\pi\times\frac{a^2/2\,(\hat{i}+\hat{j})}{a^3/2} = \frac{2\pi}{a}(\hat{i}+\hat{j})\\ \text{Similarly, } \vec{b}^* &= 2\pi\frac{\vec{c}'\times\vec{a}'}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = \frac{2\pi}{a}(\hat{j}+\hat{k})\\ \vec{c}^* &= 2\pi\frac{\vec{a}'\times\vec{b}'}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = \frac{2\pi}{a}(\hat{k}+\hat{i})\end{aligned}\right\} \cdots (11)$$

As will be seen later, these are the primitive translation vectors of an fcc lattice. Thus the reciprocal lattice to a bcc lattice is fcc lattice.

Reciprocal lattice to FCC lattice:-

The primitive translation vectors of an fcc lattice, as shown in fig. (22)

$$\left.\begin{aligned}\vec{a}' &= \frac{a}{2}(\hat{i}+\hat{j})\\ \vec{b}' &= \frac{a}{2}(\hat{j}+\hat{k})\\ \vec{c}' &= \frac{a}{2}(\hat{k}+\hat{i})\end{aligned}\right\} \cdots (12)$$

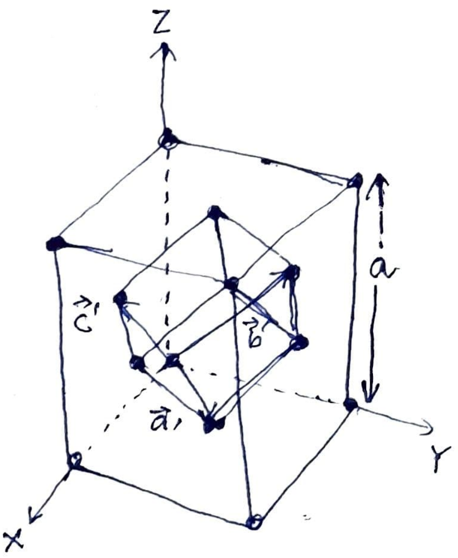


Fig. (22)

Volume of the primitive cell

$$\vec{a}'\cdot(\vec{b}'\times\vec{c}') = \frac{a}{2}(\hat{i}+\hat{j})\cdot\left[\frac{a}{2}(\hat{j}+\hat{k})\times\frac{a}{2}(\hat{k}+\hat{i})\right]$$

$$= \frac{a^3}{8}(\hat{i}+\hat{j})\cdot(\hat{i}+\hat{j}-\hat{k})$$

$$= \frac{a^3}{4}$$

From eqn (8), the primitive translation vectors of the reciprocal lattice are obtained as

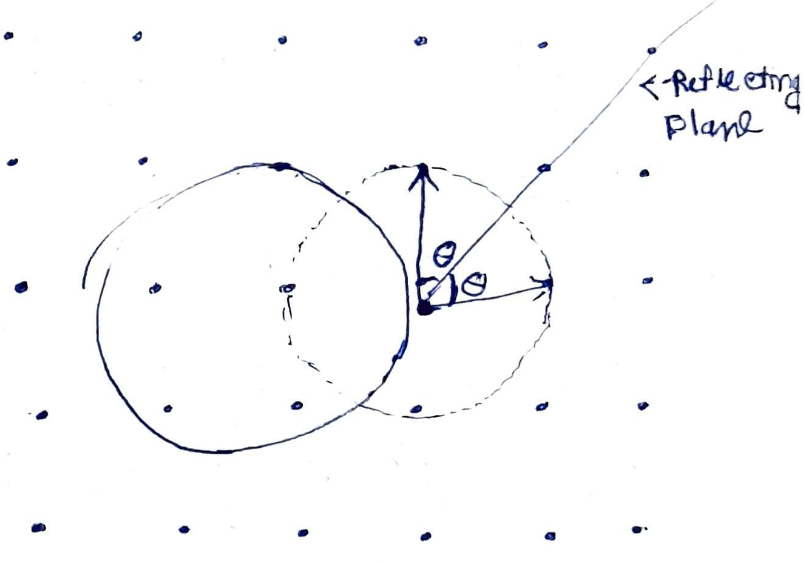
$$\left.\begin{aligned}\vec{a}^* &= 2\pi\,\frac{\vec{b}'\times\vec{c}'}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = 2\pi\,\frac{\frac{a^2}{4}(\hat{i}+\hat{j}-\hat{k})}{\frac{a^3}{4}} = \frac{2\pi}{a}(\hat{i}+\hat{j}-\hat{k})\\ \text{Similarly, } \vec{b}^* &= \frac{2\pi\,(\vec{c}'\times\vec{a}')}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = \frac{2\pi}{a}(-\hat{i}+\hat{j}+\hat{k})\\ \text{and } \vec{c}^* &= \frac{2\pi\,(\vec{a}'\times\vec{b}')}{\vec{a}'\cdot(\vec{b}'\times\vec{c}')} = \frac{2\pi}{a}(\hat{i}-\hat{j}+\hat{k})\end{aligned}\right\}\cdots(13)$$

Comparing eqn (13) and eqn (10), we find that these are the primitive translation vectors of a bcc lattice having length of the cube edge as $\frac{2\pi}{a}$.

Thus the reciprocal lattice to an fcc lattice is a bcc lattice.

Bragg's law in Reciprocal lattice :-

The Bragg's diffraction condition.



Bragg's Law in Reciprocal lattice:-

Bragg's law of x-ray diffraction can be expressed as a relation between vectors in the reciprocal lattice.

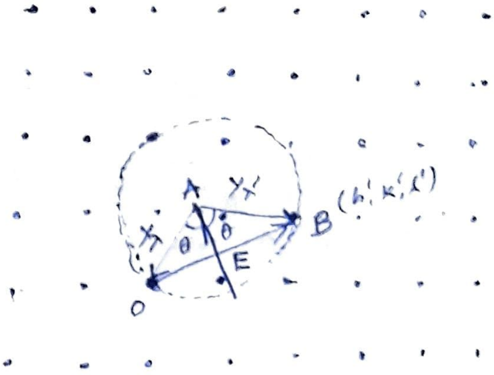


Fig (23)

In fig. (23) $\vec{AO}$ is a vector length $\frac{1}{\lambda}$ in the direction of incident x-ray beam and terminates at the origin O of the reciprocal lattice. With A as the centre we draw sphere of radius $|\vec{AO}| = \frac{1}{\lambda}$, which intersects some point B in reciprocal lattice.

The co-ordinates of B is (h', k', l') which may have a highest common factor n i.e., $h' = nh$, $k' = nk$, $l' = nl$, where h, k, l have common factor unity. $\vec{OB}$ then represents a vector joining the origin O of the reciprocal lattice and $B(h', k', l')$, OB therefore, must be normal to the plane $(h'k'l')$ and is of length

$$|\vec{OB}| = \frac{n}{d_{hkl}} \quad \cdots \quad (1)$$

From the fig (23), ΔAOB,

$$OB = 2 \times OE = 2\, OA \sin\theta = 2\frac{\sin\theta}{\lambda} \quad \cdots \quad (2)$$

From eqn (1) and (2)

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

$$\text{or,} \quad \boxed{2d_{hkl} \sin\theta = n\lambda}$$

~~Vectors form~~

Vector form of Bragg's law:-

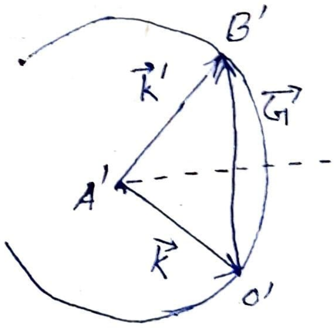


Fig. 24

Let the vectors $\vec{A'O'}$, $\vec{O'B'}$ and $\vec{A'B'}$ be the magnified form by a constant factor 2π such that $A'O' = 2\pi(OA)$, $O'B' = 2\pi(OB)$ and $A'B' = 2\pi(AB)$

Since $OA = \frac{1}{\lambda}$

$\therefore$ $A'O' = \frac{2\pi}{\lambda}$ can represent the wave vector $\vec{k}$ by the vector $\vec{A'O'}$, Then $\vec{O'B'}$ is a reciprocal vector $\vec{G}$.

Now from the triangle law of vectors, $\vec{A'B'} = \vec{A'O'} + \vec{O'B'}$

$$\vec{k}' = \vec{k} + \vec{G}$$

$$\text{or.} \quad \vec{k}' \cdot \vec{k}' = (\vec{k} + \vec{G}) \cdot (\vec{k} + \vec{G})$$

$$\text{or.} \quad k'^2 = k^2 + 2\vec{k} \cdot \vec{G} + G^2$$

Since $k^2 = k'^2$, so

$$\boxed{2\vec{k}\cdot\vec{G} + G^2 = 0} \quad \cdots \quad (3)$$

This is the vectorform of Bragg's law and used in the construction of the Brillouin Zones.

Now from the fig (24) $|\vec{A'O}| = |\vec{A'B}|$

$$\left.\begin{aligned} & k^2 = k'^2 \\ \text{and} \quad & \vec{k'} - \vec{k} = \Delta\vec{k} = \vec{G} \end{aligned}\right\} \quad \cdots \quad (4)$$

This shows that

(i) Scattering changes the direction of $\vec{k}$ not change the magnitude of wave vector.

(ii) The Scattered wave differs from the incident wave by a reciprocals lattice vector $\vec{G}$.

Brillouin Zones:-

A Brillouin zone is the locus of all those k- values in the reciprocal lattice which are Bragg reflected.

We construct the Brillouin zone for a simple square lattice of sides 'a'. The primitive translation vectors of this lattice are $\vec{a} = a\hat{i}$, $\vec{b} = a\hat{j}$

The corresponding translation vector in reciprocal lattice are $\vec{a}^* = \frac{2\pi}{a}\hat{i}$, $\vec{b}^* = \frac{2\pi}{a}\hat{j}$

Therefore, the reciprocal lattiee vector is written as

$\vec{G} = \frac{2\pi}{a}(h\hat{i} + k\hat{j})$ where h, k are integers.

The wave vector $\vec{k} = k_x\hat{i} + k_y\hat{j}$

Now from Bragg's Condition

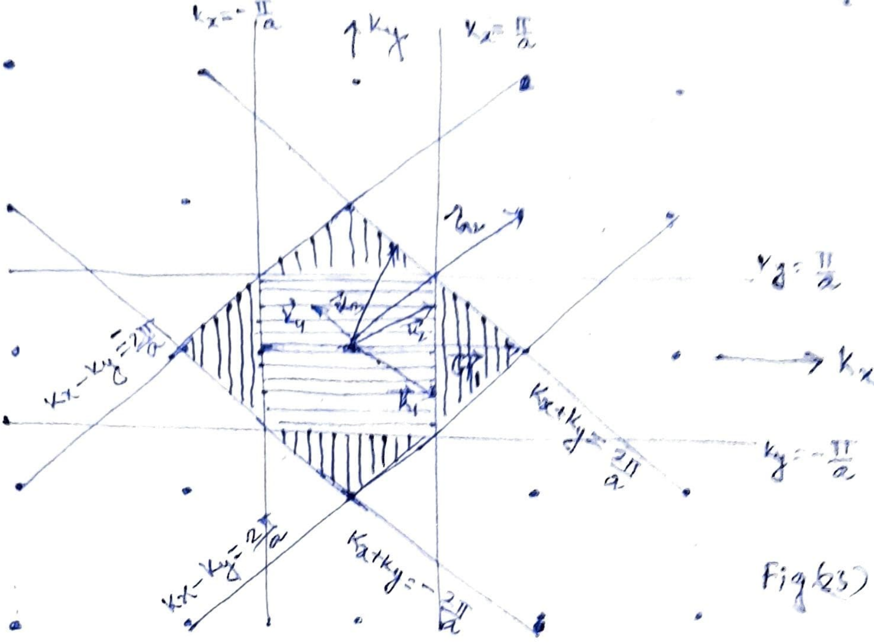
$$2\vec{k}\cdot\vec{G} + G^2 = 0$$

$$\text{or,} \quad \frac{4\pi}{a}\left[(k_x\hat{i} + k_y\hat{j})\cdot(h\hat{i} + k\hat{j})\right] + \frac{4\pi^2}{a^2}(h^2+k^2) = 0$$

$$\text{or,} \quad \boxed{hk_x + kk_y = -\frac{\pi}{a}(h^2+k^2)} \quad \cdots \quad (5)$$

The $\vec{k}$ values which are Bragg reflected are obtained by considering all possible Combinations of h and k.

For $h = \pm 1$ and $K = 0$, $k_x = \pm \frac{\pi}{a}$ and k_y is arbitrary.
Also, for $h = 0$ and $K = \pm 1$, $k_y = \pm \frac{\pi}{a}$ and k_x is arbitrary.



Fig(25)

$k_x = \pm\frac{\pi}{a}$ and $k_y = \pm\frac{\pi}{a}$ are plotted in fig. (25). The square bounded by these lines are 1st Brillouin Zone.
In addition to this set of lines, some other sets of lines are also possible which satisfy the eqn (5). For example, $h = \pm 1$ and $K = \pm 1$, the eqn (5) gives the following set of four lines

$$\pm k_x \pm k_y = \frac{2\pi}{a} \quad \ldots \quad (6)$$

Additional area included by $\pm k_x \pm k_y = \frac{2\pi}{a}$ is the Second Brillouin Zone and so on.
The boundaries of the Brillouin Zones represent the loci ~~the~~ of $\vec{k}$-values which are Bragg reflected and may be considered as reflecting planes. Boundaries of the 1st Zone represent the reflecting planes for the 1st order, those of the second Zone represent the reflecting planes for the 2nd order, and so on. A $\vec{k}$-vector that doesnot terminate at a zone boundary cannot produce Bragg reflection. Thus the Brillouin Zone pattern can be employed to determine the X-ray diffraction pattern of a crystal and vice versa.

The Brillouin zones for a three-dimensional cubical lattice are constructed using the generalised equation

$$hk_x + Kk_y + lk_z = -\frac{\pi}{a}(h^2 + K^2 + l^2) \quad \ldots \quad (7)$$

where 'a' is the length of cube edge.

Atomic Scattering factor or form factor :-

So far we discussed the diffraction conditions which are scattering of x-rays from a lattice point in a space lattice. Since an electron is the smallest Scattering centre, the diffraction Conditions would ideally be applicable to a lattice in which every lattice point is occupied by an electron. This is not actual situation. Lattice points are occupied by atoms which may certain number of electrons. Also, x-rays Scattered from different portions of an atom are not in phase. Thus the amplitude of radiation scattered by a single atom is not necessarily equal to the product of the amplitude of radiation scattered by a single electron and the number of electrons present in the atom. The atomic Scattering factor or form factor, f, describes the scattering power by a single atom to the scattering power of a single electron and is given by

$$f = \frac{\text{amplitude of radiation scattered from an atom}}{\text{amplitude of radiation Scattered from an electron}}$$

To calculate f, we consider an atom containing electrons arranged in a spherically symmetric configuration around its centre which is taken as origin. Let r be the radius of the atom and ρ (r) the charge density at a point r.

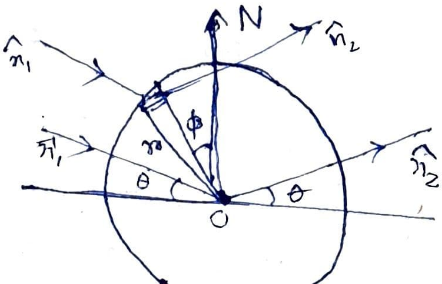


Fig.(26)

Considering a small volume element dv at r, the charge located at r is ρ(r) dv. We first consider the scattering from the charge ρ(r) dv and an electron located at the origin. If $\hat{n}_1$ and $\hat{n}_2$ represent the directions of the incident and Scattered beam respectively as shown in fig.(26). The phase difference between the wave scattered from the charge ρ(r) dv is

$$\phi = \frac{2\pi}{\lambda} \vec{r} \cdot \vec{N} \qquad \dots (1)$$

Where $\vec{N}$ is the Scattering normal. Let the scattering amplitude from the ~~charge~~ point electron in direction

$\hat{n}_2$ be written as $A e^{i(kx-\omega t)}$ where x is the distance covered along $\hat{n}_2$ and k is the wave number. Then the scattering amplitude from the charge $\rho(r)\,dv$ is

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

where $e^{i\phi_r}$ is a phase factor.

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

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

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

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

$$f = \int_V \rho(r) e^{i\phi_r} dv \quad \cdots \quad (2)$$

Since charge distribution is spherically symmetric,

$$dV = 2\pi r^2 \sin\phi\, d\phi\, dr \quad \cdots \quad (3)$$

and $|\vec{N}| = 2\sin\theta$

Therefore, from eqn (1), $\phi_r = \frac{2\pi}{\lambda} r N \cos\phi$

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

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

$$= \mu r \cos\phi \quad \cdots (4) \quad \text{where } \mu = \frac{4\pi}{\lambda}\sin\theta$$

From eqns (2), (3) and (4) we have

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

$$= \int_0^{\infty} 4\pi r^2 \rho(r) \frac{\sin \mu r}{\mu r} dr \quad \cdots (5) \quad \left[\int_0^{\pi} e^{i\mu r\cos\phi} \sin\phi\, d\phi = \frac{2\sin(\mu r)}{\mu r} \right]$$

This is the general expression for scattering factor.

The results obtained by the application of these models are fairly accurate and match with the experimental values of X-rays intensities. The variation of 'f' with $\frac{\sin\theta}{\lambda}$ for magnesium $(Z=12)$ is shown in fig (27). It is clear that $f \to Z$ at $\theta \to 0$, so from eq (5) gives

$$f = \int_0^{\infty} 4\pi r^2 \rho(r)\, dr.$$

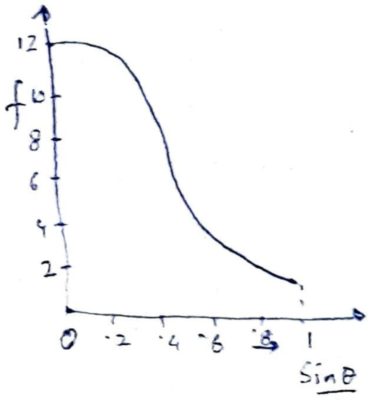


Fig (27)

Geometrical Structure Factor :-

The intensity of the x-ray beam diffracted from a crystal depends upon the contents of the unit cell, i.e., on the number, type and distribution of atoms involved within the cell. The phase of the scattered x-rays from different atoms may also differ. To find out an expression for the geometrical structure factor(S). let the nucleus of j^{th} atom by at $\vec{r}_j$ given by

$$\vec{r}_j = u_j \vec{a} + v_j \vec{b} + w_j \vec{c} \quad \ldots (1)$$

Where u_j, v_j and w_j represent the co-ordinates of jth atom.

The total scattering amplitude $F(h^{\circ}kl)$ is given by

$$F(hkl) = \sum_j f_j e^{i\phi_j}$$

$$= \sum_j f_j e^{i\frac{2\pi}{\lambda}(\vec{r}_j \cdot \vec{N})} \quad \ldots (2)$$

where f_j is the atomic scattering factor for the jth atom, ϕ_j is the phase difference between the scattered radiation from atom and electron respectively.

Therefore $$F(hkl) = \sum_j f_j e^{i2\pi(u_j h + v_j k + w_j l)} \quad \ldots (3)$$

For identical atoms, all the f_j's have the same value f. Therefore, eqn (3) gives as

$$F(hkl) = fS$$

Where $$S = \sum e^{2\pi i(u_j h + v_j k + w_j l)} \quad \ldots (4)$$

is called the geometrical structure factor

Now, the intensity of radiation is given by

$$I = |F|^2 = F \times F^*$$

$$= \left[\sum_j f_j \cos 2\pi(u_j h + v_j k + w_j l)\right]^2 + \left[\sum_j f_j \sin 2\pi(u_j h + v_j k + w_j l)\right]^2 \quad \ldots (5)$$

Geometrical Structure factor for Some Simple Crystals:-

(i) Simple cubic (SC) crystal:-

In SC crystal the effective number of atoms in unit cell is one which lies at the origin, then the structure factor from eqn(4) we have is unity. Then the total diffraction amplitude from eqn (3) is $F(hkl) = f$. Hence all the diffraction lines predicted by Bragg's law will appear in the diffraction pattern.

(ii) Body Centred Cubic (BCC) Crystal:-

A body-centred cubic contains two atoms per unit cell. The contributions from eight corner-atoms give rise to one atom and other is situated at the centre of the unit cell. If the ~~co-ordination~~ co-ordinates of the corner atom is (0,0,0), then the co-ordinates of the central atom is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Since both the atoms are identical, from eqn ④ we have

$$F(hkl) = f \sum_j e^{2\pi i (u_j h + v_j k + w_j l)}$$

$$= f\left[1 + e^{\pi i (h+k+l)}\right] \quad \cdots \quad (6)$$

It is evident from eqn (6), that the geometrical structure factor becomes zero for odd values of $(h+k+l)$, Since $e^{n\pi i} = -1$, if n is odd. If $(h+k+l)$ is even, then $F(hkl) = 2f$ and intensity from eqn ⑤ is $4f^2$. Thus, the reflection from (100), (111), (210)- planes etc. are missing and those from (110), (200), etc are present in BCC lattice. It is to be noted that the presence or absence of a reflection is considered only in terms of first order reflection.

(iii) Face Centred Cubic (FCC) Crystal.

A face centred cubic crystal has four atoms per unit cell. If the co-ordinates of a corner atom be (000), then the remaining three atoms of the unit cell have the co-ordinates $(\frac{1}{2}0\frac{1}{2})$, $(\frac{1}{2}\frac{1}{2}0)$, $(0\frac{1}{2}\frac{1}{2})$. Then the diffraction amplitude becomes

$$F(hkl) = f\left[1 + e^{\pi i (h+l)} + e^{\pi i (h+k)} + e^{\pi i (k+l)}\right] \cdots ⑦$$

Thus, we note from eqn (7) that $F(hkl)$ is non zero, when h, k, l are all even or all odd. Therefore reflections from (111), (200), (220) are present but those from (100), (110) (211) are absent.