

Course Name: Solid State Physics (PHY503)
Unit 2:Crystal Diffraction and reciprocal lattice

Dr Kamal Devlal

Department of Physics

Uttarakhand Open University, Haldwani

kdeolal@uou.ac.in

Mob. 8791477949

UNIT 2: CRYSTAL DIFFRACTION AND RECIPROCAL LATTICE

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1. INTRODUCTION

- Wavelengths of X-rays are of the order of 10^{-8} to 10^{-9} cm and spacing between the layers of these atoms in a crystal is in order of 10^{-8} cm, which are of the same order.
- Therefore, in 1912, German physicist Max Vor Laue suggested that the ordered arrangement of atoms in a crystal must make it to act as a three-dimensional grating.
- Thus the three dimensional crystal would be suitable for the diffraction of X-rays and diffraction pattern so obtained can give the information about the crystal structure.
- Later on, WL Bragg presented a suitable explanation of X-ray diffraction by crystal. Now x ray diffraction techniques have become a n important tool study the crystal structure.

2. X RAY DIFFRACTION AND BRAG'S LAW

- The diffraction occurs when the incident rays are reflected by atoms on the different parallel planes and these reflected rays interfere constructively and make diffraction pattern.
- By analyzing the diffraction patterns we can find out the lattice parameters, size, shape, orientation of crystal, inter planner distance etc.
- In 1913, Bragg presented a method to explain the diffraction of x ray beam.

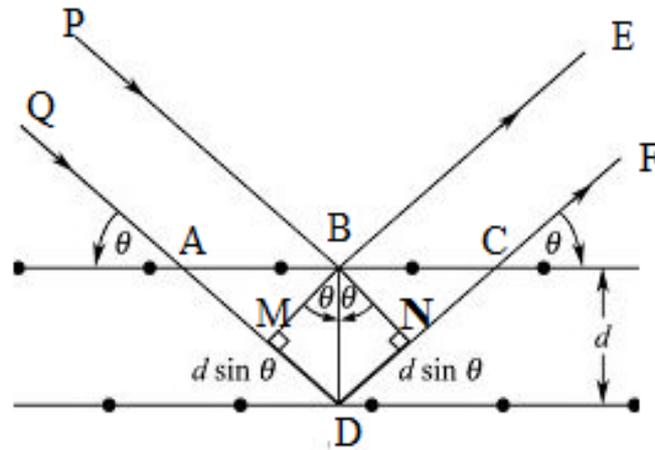


Figure 2.1: Bragg's diffraction by crystal planes

- In figure the path difference between rays PBE and QDF can be given as

$$\Delta = MD + DN = 2MD = 2d \sin \theta$$
- For constructive interference the path difference should be integral multiplication of therefore $2d \sin \theta = n\lambda$
- This is Bragg's law. The condition occurs only at certain values of λ and θ
- Thus by observing the parameters by experiment we can determine the crystal lattice spacing, size, shape, orientation and we can study the crystal structure.

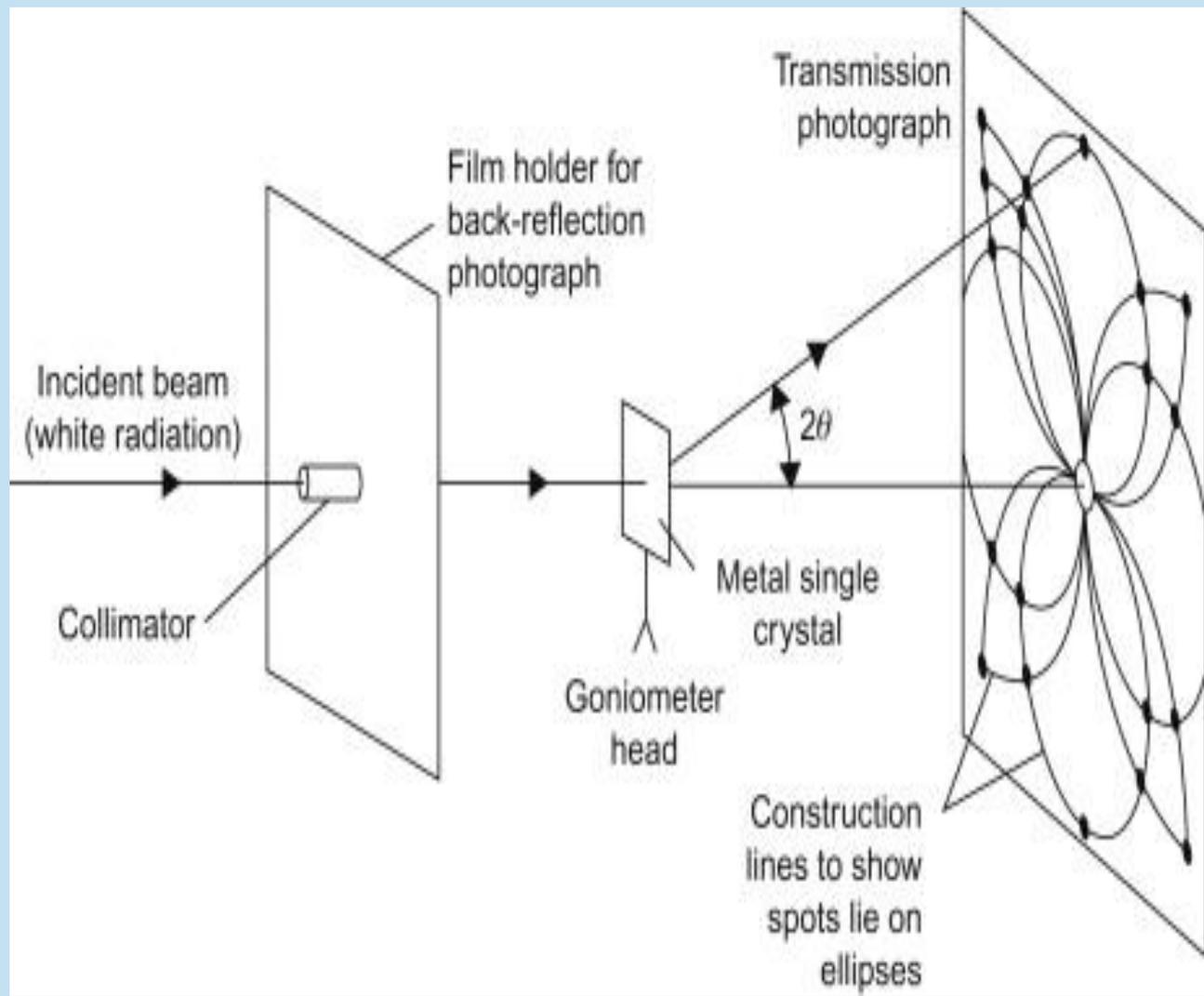
3. Diffraction methods

- The diffraction occurs whenever the Bragg's condition is satisfied.
- In general when monochromatic x ray beam falls on a single crystal, for arbitrary setting x rays will not produce any diffraction pattern.
- But some way if we continuously vary wavelength (λ) or diffraction angle (θ) then at a particular setting of single crystal, the Bragg's condition satisfies, and diffraction occurs.
- The ways, in which these quantities vary, there are three diffraction method as given below:

Method	Wavelength	Angle	Specimen type
Laue Method	Variable	Fixed	Single crystal
Rotating crystal method	Fixed	Varying	Single crystal
Powder method	Fixed	Variable	powder

4. Laue Diffraction method:

- The first diffraction methods, ever used till today and it reproduces Von Laue's original experiment
- Mainly used to determine the orientations of large single crystals.
- While radiations is reflected or transmitted through a fixed single crystal, the Bragg's angle that is fixed in this particular case, for every set of planes, in the crystal and each set picks out and diffracts that particular wavelength which satisfies the Bragg's law for the particular values of d and θ
- In this particular region on to the particular film we are getting some kinds of white spots over there, which are the different diffraction picks, or maybe the spots.



- Now we know that the Elastic Scattering

$$|\mathbf{K}| = |\mathbf{K}'|$$

where $\mathbf{K} = \frac{\mathbf{S}_0}{\lambda} =$ incident wave vector

$$\mathbf{K}' = \frac{\mathbf{S}}{\lambda} = \text{diffracted wave vector}$$

$\mathbf{S}_0 =$ incoming X ray beam

$\mathbf{S} =$ Scattered X ray beam

The Laue's theory states that for diffractions the differences in the two wave vectors must be equal to a reciprocal lattices vector.

$$\mathbf{K}' - \mathbf{K} = \boldsymbol{\sigma}^*$$

Now from this particular case, we are going to discuss about the Ewald sphere. The Ewald sphere is a pictorial way to show the diffraction condition. We construct a sphere which is known as the Ewald constructions as shown in figure 2.3.

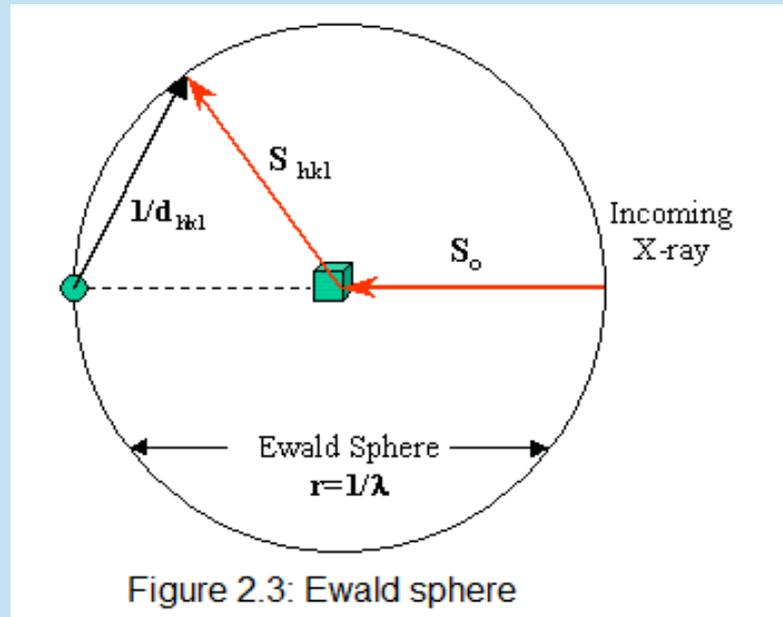


Figure 2.3: Ewald sphere

- Ewald sphere is a virtual or imaginary sphere, that sphere whose radius is $1/\lambda$.
- The geometrical construction of Ewald sphere provides the relationship between the orientations of a crystal and the directions of the beams diffracted by it.
- If the origin of reciprocal space is placed at the tip of incident beam then diffractions will occur only for those reciprocal lattice points that lie on the surface of the Ewald sphere

5. Rotating Crystal method

- In rotating crystal method, a single crystal is mounted at a point on the axis of a cylindrical shape in such a way that the monochromatic x-rays strike perpendicular on the crystal.
- A cylindrical photographic film is placed around the crystal and crystal is rotated about the axis in a chosen direction.
- The axis of the photographic film is same as the axis of rotation of the Crystal.
- As crystal rotates, sets of lattice points come at the positions that are suitable for Bragg's diffraction. At some particular positions, lattice points correctly at Bragg angle for reflection of X-Ray beam, and at this instant diffraction beam will be formed.
- The diffracted beam are located on the surface of imaginary cone when the film is laid out from the cylinder, flat it, the diffraction spots lies on the film in horizontal lines.
- By recording the diffraction pattern, both angle and intensities for various crystal orientations can be obtained.

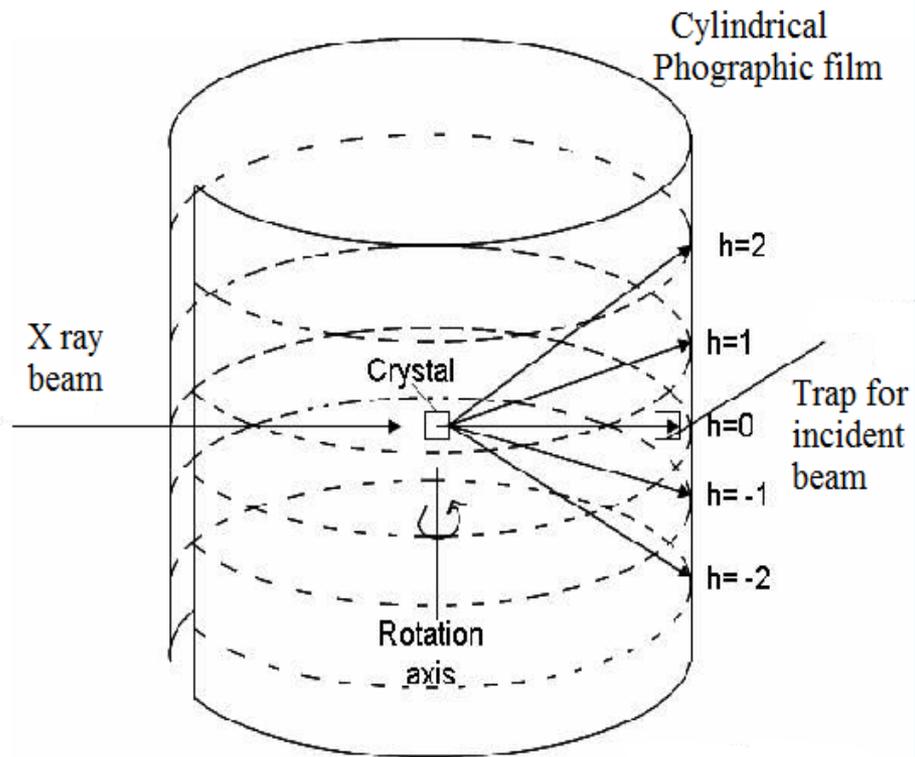


Figure 2.4: Rotating crystal method

▪ Crystal structure determination by the rotating crystal method

- By recording the diffraction pattern, both angle and intensities for various crystal orientations can be obtained and the shape and size of unit cell of the crystal and arrangement of atoms inside the crystal can be determined.
- If the wavelength of X-Rays is λ and angle of diffraction is θ at which a reflection occurs, the inter-planar spacing d can be determined by using Bragg's law as given below:

$$2d \sin \theta = n\lambda$$

$$d = \frac{a}{\sqrt{(h)^2 + (k)^2 + (l)^2}}$$

6. Powder method:

- Wavelength of X-ray, λ is fixed but angle of incident x ray with crystal plan Θ variable.
- The sample consists of powder and it consists of large number of crystallites with various orientations. The crystal to be examined is reduced to a very fine powder and placed in a beam of monochromatic X-rays.
- When the X-rays falls on the sample, tiny crystal are oriented in random directions with respect to the incident X rays and some of the crystals will be correctly oriented with the X-ray beam and give diffraction pattern.
- For example, in particular planes, say, (100) planes can reflect the incident beam and other crystals will be correctly oriented for the other planes say (110) and so on.
- Thus in Powder method every set of lattice planes will be capable of reflection as all the orientations of crystal are available on the sample.
- if the sample consists of many randomly oriented single crystals, the diffraction beams are seen to lie on the surface of several cones. The cones may merge in all directions, in forward and backwards as shown in figure

In powder method, a sample has hundreds of tiny crystals show that the diffraction beam form continuous cones.

A circle of film is used to record the diffraction pattern. Each cone intersects this film gives diffraction line. The lines are seen as arc on the as shown in figure.

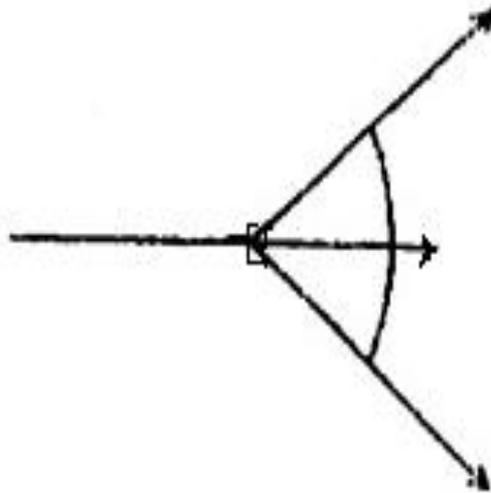


Figure 2.5: Diffraction by a single crystal

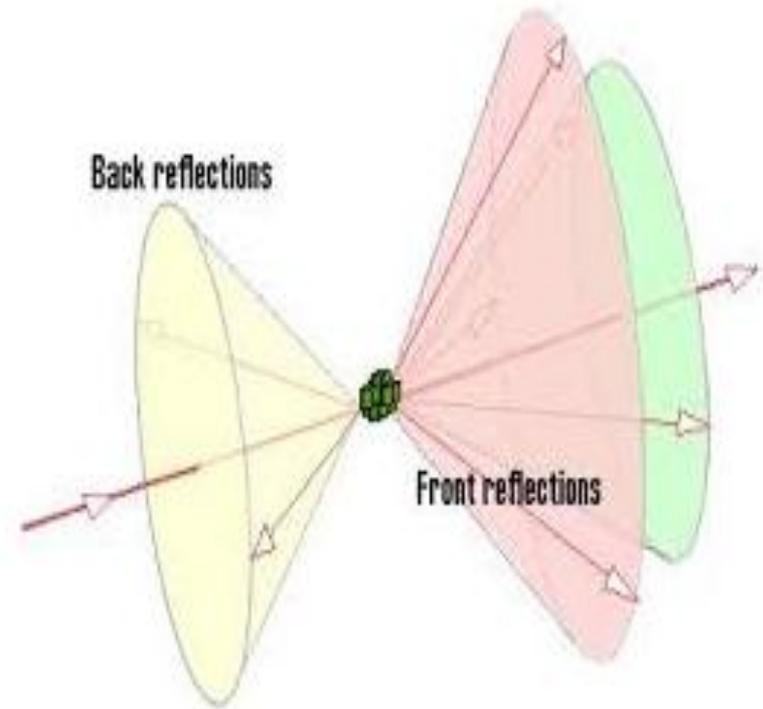


Figure 2.6: Diffraction by a powdered crystal

■ Powder diffraction film:

- The cones of diffracted radiation intersect the cylindrical strips of film inline or arc and when the strips is unrolled and make it flat, the strip shows diffraction lines as shown in figure 2.8.
- Each diffraction line is made up of a large number of small spots. Each line is formed by a separate crystal particle. The spots lying so closer together and they appear as a continuous line.
- The lines are generally curved as cone of diffracted rays cut the strip a curved line but at $2\theta = 90^\circ$, the line will be straight.
- From the measured position of a given diffraction line on the film, angle θ can be determined.
- If we know the wavelength λ of X-Rays, we can calculate the inter planar spacing (d) of reflecting lattice planes.
- Figure 2.8 shows the different positions of lines corresponding to different lattice planes.

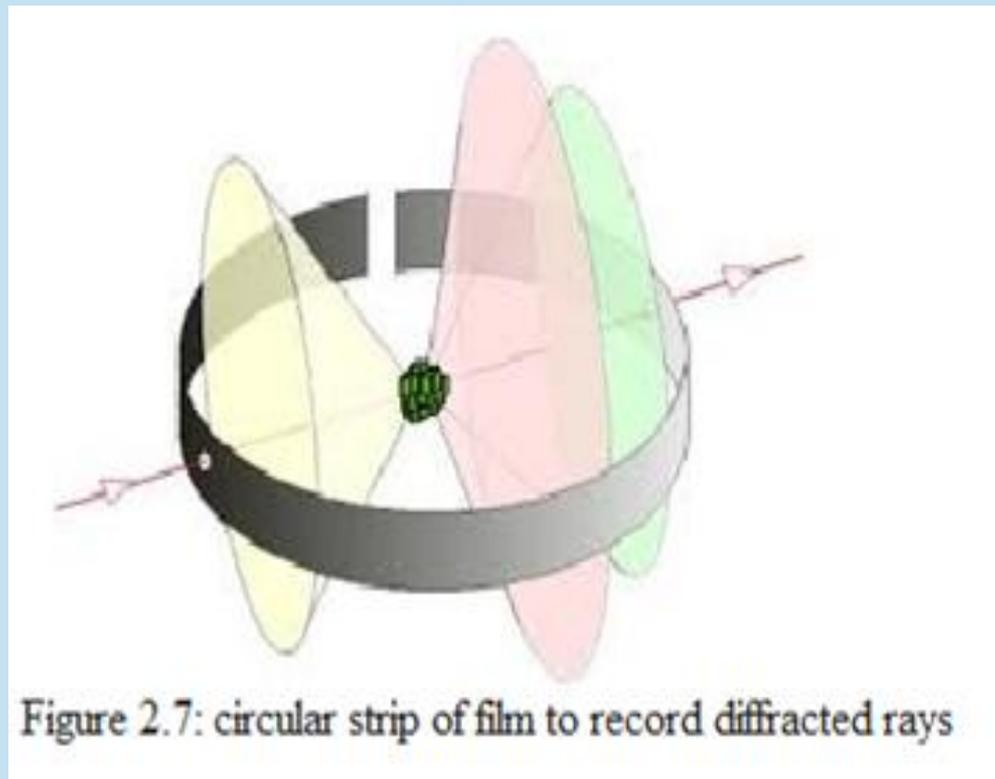


Figure 2.7: circular strip of film to record diffracted rays

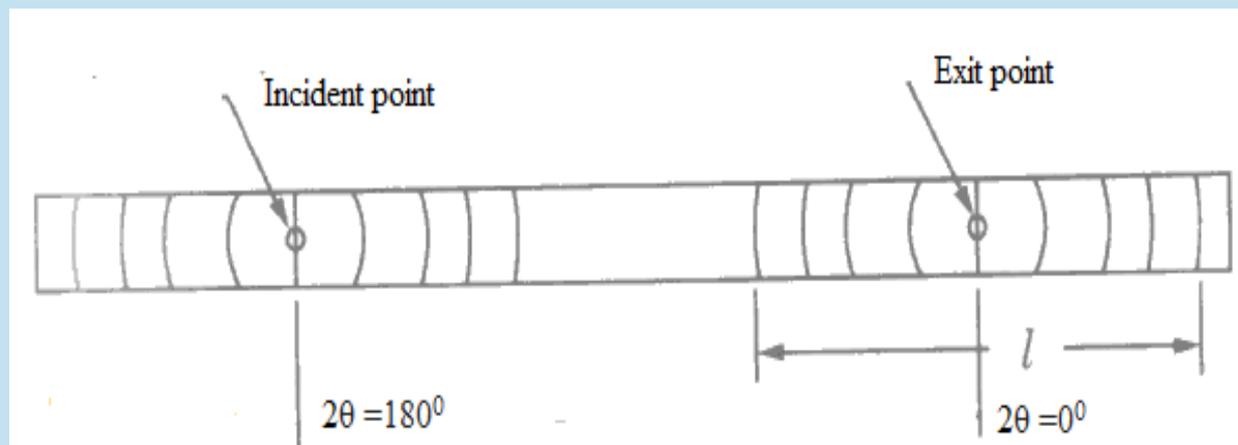


Figure 2.8: appearance of strip of photographic film

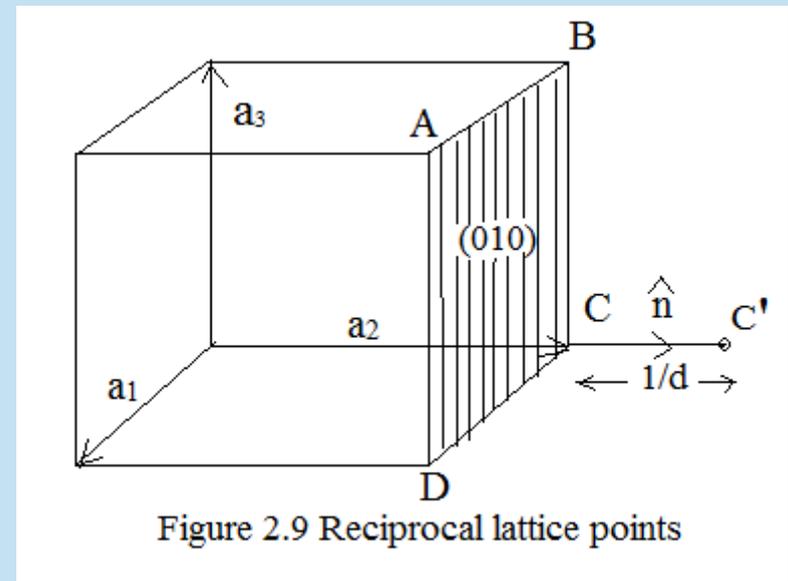
7. Reciprocal lattice System

- When we observe diffraction patterns, the diffraction spots form a picture of crystal lattice. This periodic structure like lattice is not a direct picture of crystal but an image of actual crystal. This is called reciprocal lattice.
- Reciprocal lattice points are inverse of actual lattice points. Thus the distance in reciprocal lattice system is $1/d$, where d is the distance corresponding to actual distance d in actual crystal lattice.
- All the periodic points of reciprocal lattice form a reciprocal lattice system. Such space is called reciprocal space or Fourier space.
- In direct lattice system, the lattice vectors are denoted by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (or $\mathbf{a}, \mathbf{b}, \mathbf{c}$). Similarly, in reciprocal lattice system, the reciprocal lattice vectors are denoted by $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ (or $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$).
- Any vector in reciprocal space called a reciprocal vector \mathbf{G} can also be given as

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 \quad \text{where } v_1, v_2, v_3 \text{ are integer numbers.}$$

Construction of Reciprocal lattice:

- 1. Consider a crystal lattice in real space as shown in figure. We know that a plane (hkl) shows a set of parallel equidistance planes with interspacing d_{hkl} .
- 2. Now consider a normal on any arbitrary lattice point, on the plane (hkl) and find out a point at distance $1/d_{hkl}$. This point is reciprocal lattice point.
- 3. The array of all such point are called reciprocal lattice. In figure ABCD is plane (101) then C' is reciprocal point.



$$a_1, a_2, a_3$$

■ Reciprocal lattice of a monoclinic crystal

- monoclinic crystal have lattice constants as shown in figure 2.10. We construct a unit cell in which vectors a and b are along the plane of paper and vector c is perpendicular to this plane. Consider a plane $(h0k)$ which makes intercepts at a/h at point A and b/k at point C, and this plane is parallel to axis c . The normal to this plane is along the direction of plane containing vectors a and b i.e. plane of paper as shown by vector OO' as shown in figure 2.11. If we go $1/d_{hkl}$ distance from the arbitrary plane $(h0k)$ perpendicular to line AC, along the direction perpendicular to plane $(h0l)$ i.e. OO' , we get the reciprocal lattice point corresponding to point O.
- We can extend the same manner to get other reciprocal lattice points as shown in figure 2.12. In this figure OA and OC represent two faces (sides) of monoclinic crystal. Line AC represents a plane $(h0k)$ which is perpendicular along line AC. Now for reciprocal point, normal is drawn on planes $(h0l)$ at a distance $1/d_{h0l}$. Similarly, we draw normal to all (hkl) planes and arranged the points at distance $1/d_{hkl}$ in the direction of normals, the three dimensional reciprocal lattice is obtained. It can be seen that plane (200) have half the interplaner spacing with respect to plane (100) but reciprocal point (200) is twice far from the origin.

Construction of reciprocal lattice of monoclinic crystal

- monoclinic crystal have lattice constants as

$$a_1 \neq a_2 \neq a_3 \text{ and } \alpha = \gamma = 90^\circ; \beta \neq 90^\circ$$

- We construct a unit cell in which 2 vectors a_1, a_3 are along the plane of paper and 1 vector a_2 is perpendicular to this plane. Consider a plane (h0k) which makes intercepts at points A and C.
- Line AC represents a plane (h0k) which is perpendicular along line AC. The normal to this plane is along the direction of vector OO'
- If we go $1/d_{hkl}$ distance from the arbitrary plane (h0k) along OO', we get the reciprocal lattice point corresponding to point O.
- Similarly, extend the same manner.
- draw normal to all (hkl) planes and arranged the points at distance $1/d_{hkl}$ in the direction of normals, the three dimensional reciprocal lattice is obtained.
- It can be seen that plane (200) have half the interplaner spacing with respect to plane (100) but reciprocal point (200) is twice far from the origin.

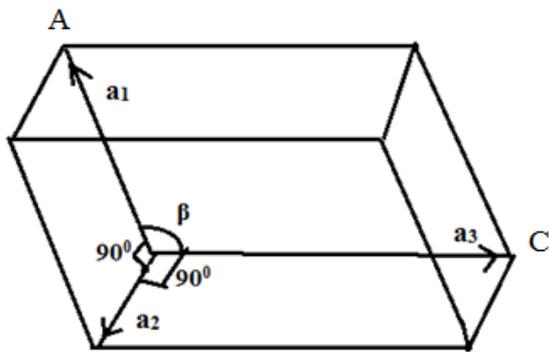


Figure 2.10: Monoclinic lattice point in real space

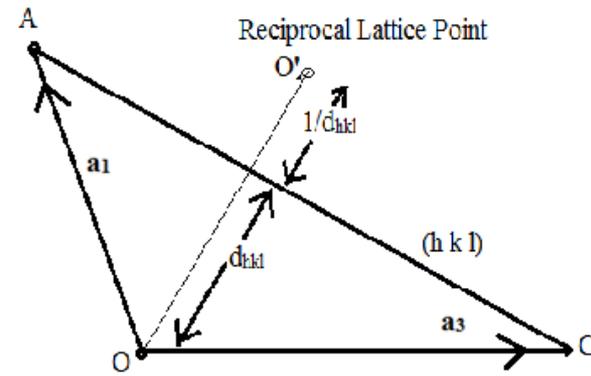


Figure 2.11: Reciprocal lattice point in real space for monoclinic crystal

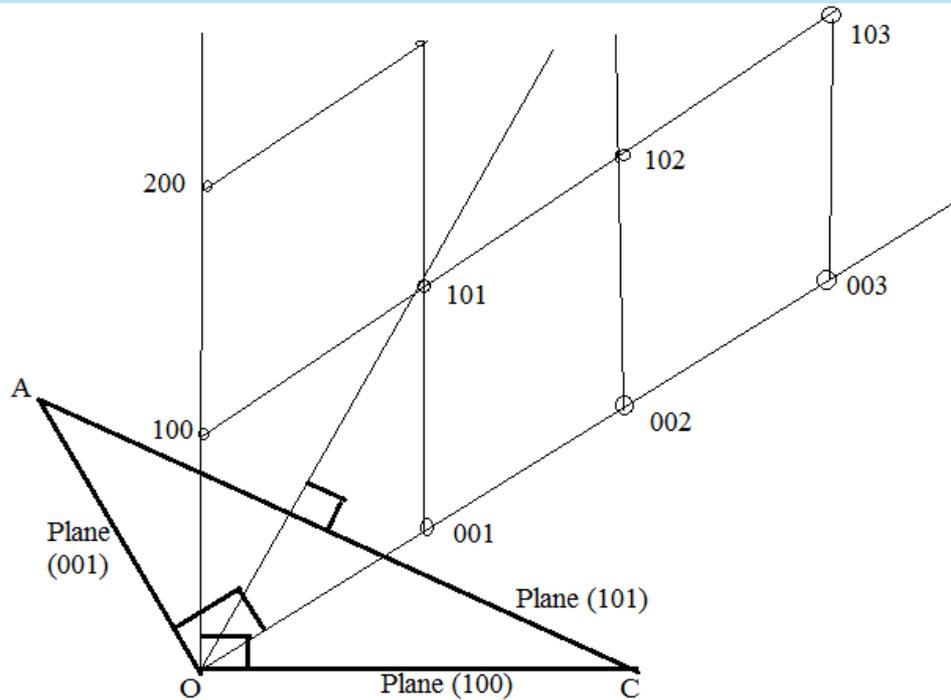


Figure 2.12: Reciprocal lattice points for monoclinic lattice in 2D

7. Reciprocal lattice vectors:

- Reciprocal lattice vector is defined as the vector has magnitude $1/d_{hkl}$ and direction perpendicular to the plane (hkl). Generally reciprocal lattice vector is denoted by

$$\sigma_{hkl} = \frac{1}{d_{hkl}} \hat{n} \quad \text{where } \hat{n} \text{ unit vector along the normal to } (hkl) \text{ plane}$$

- If lattice vectors of a crystal are denoted by a_1, a_2, a_3 in direct lattice system and in reciprocal lattice system, the reciprocal lattice vectors are denoted by b_1, b_2, b_3 then the volume of crystal unit cell in direct lattice system can be given by

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

- For simplest case if we choose plane (100) then

$$V = \text{area} \times \text{height} = \text{area} \times d_{hkl}$$

$$\frac{1}{d_{100}} = \frac{\text{area}}{V} = \frac{a_2 \times a_3}{[a_1 \cdot a_2 \times a_3]}$$

$$\sigma_{100} = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]}$$

The fundamental reciprocal lattice vectors are defined as

$$\mathbf{b}_1 = \sigma_{100} = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]}$$

Similarly

$$\mathbf{b}_2 = \sigma_{010} = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]}$$

$$\mathbf{b}_3 = \sigma_{001} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]}$$

Since each reciprocal vector is orthogonal to two axis vectors of direct lattice

$$\mathbf{b}_1 \cdot \mathbf{a}_2 = \mathbf{b}_1 \cdot \mathbf{a}_3 = \mathbf{b}_2 \cdot \mathbf{a}_1 = \mathbf{b}_2 \cdot \mathbf{a}_3 = \mathbf{b}_3 \cdot \mathbf{a}_1 = \mathbf{b}_3 \cdot \mathbf{a}_2 = 0$$

Above relations are equally valid if we introduce a term 2π , since wave vector is $k = 2\pi/\lambda$ thus the reciprocal lattice vectors are

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]} \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]} \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]}$$

9.1 Reciprocal lattice of simple cubic crystal:

- Consider unit cell in a simple cubic crystal which have primitive lattice vectors indirect lattice system is given by

$$\mathbf{a}_1 = a\hat{i} ; \mathbf{a}_2 = a\hat{j} ; \mathbf{a}_3 = a\hat{k}$$

Where $\hat{i}, \hat{j}, \hat{k}$ are unit vector along x y z Axis respectively. Now the reciprocal lattice vectors are given as

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3]} = 2\pi \frac{a^2 \hat{j} \times \hat{k}}{a^3 \hat{i} \cdot \hat{j} \times \hat{k}} = \frac{2\pi}{a} \hat{i} \quad \text{where } [\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3] \text{ is volume (V) of unit cell.}$$

$$\text{or } \mathbf{b}_1 = \frac{2\pi}{a} \hat{i} \quad \text{Similarly } \mathbf{b}_2 = \frac{2\pi}{a} \hat{j} \quad \text{And} \quad \mathbf{b}_3 = \frac{2\pi}{a} \hat{k}$$

Thus a simple cubic lattice of lattice parameter \mathbf{a} , transformers to a simple cubic lattice of lattice parameter $\frac{2\pi}{a}$ in reciprocal lattice system. Figure 2.13 and 2.14 show the simple cubic lattice in direct and reciprocal lattice system.

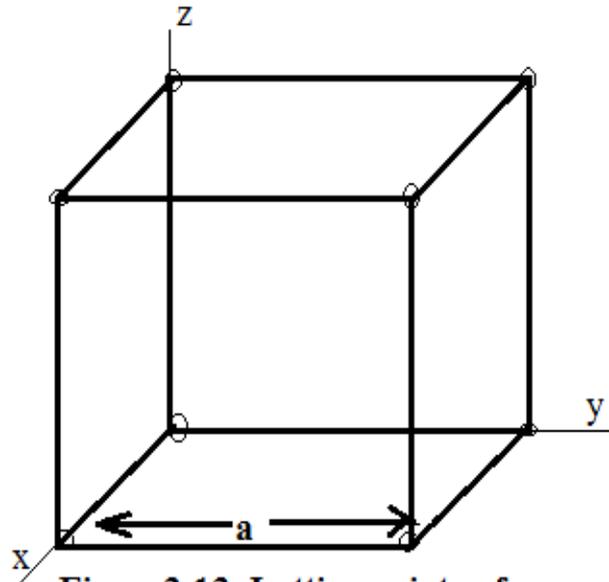


Figure 2.13: Lattice points of sc crystal in direct lattice

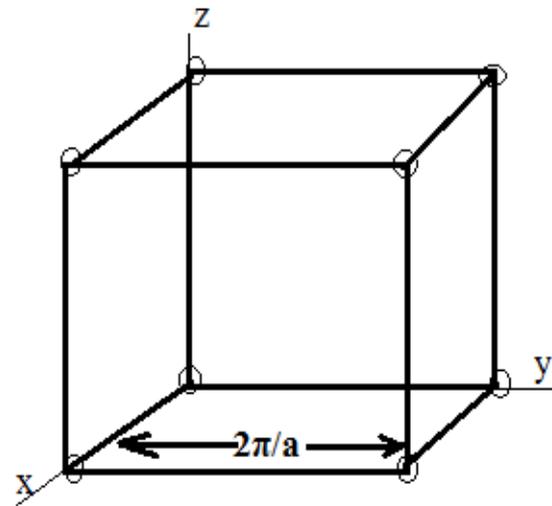


Figure 1.14 : lattice points of sc crystal in reciprocal lattice

9.2 Reciprocal lattice of body centered cubic crystal:

- The primitive lattice vectors bcc crystal in direct lattice system is given as

$$a_1 = \frac{a}{2}(\hat{i} + \hat{j} - \hat{k}); a_2 = \frac{a}{2}(-\hat{i} + \hat{j} + \hat{k}); a_3 = \frac{a}{2}(\hat{i} - \hat{j} + \hat{k})$$

- These vectors are shown in figure 2.15. Now the reciprocal lattice vectors are given as

$$b_1 = 2\pi \frac{a_2 \times a_3}{[a_1 \cdot a_2 \times a_3]} = 2\pi \frac{(a^2/4)(-\hat{i} + \hat{j} + \hat{k}) \times (\hat{i} - \hat{j} + \hat{k})}{(a^3/2)} = \frac{2\pi}{a}(\hat{j} + \hat{k})$$

$$b_1 = 2\pi \frac{(a^2/4)2(\hat{i} + \hat{j})}{(a^3/2)} = \frac{2\pi}{a}(\hat{j} + \hat{k})$$

or $b_1 = \frac{2\pi}{a}(\hat{j} + \hat{k})$ Similarly $b_2 = \frac{2\pi}{a}(\hat{k} + \hat{i})$ And $b_3 = \frac{2\pi}{a}(\hat{i} + \hat{j})$

If we recall fcc crystal lattice the primitive vectors can be given

$$a_1 = \frac{a}{2}(\hat{i} + \hat{j}); a_2 = \frac{a}{2}(\hat{j} + \hat{k}); a_3 = \frac{a}{2}(\hat{k} + \hat{i})$$

Thus we can say that the unit cell of body centered cubic lattice in reciprocal lattice space is a face centered with lattice.

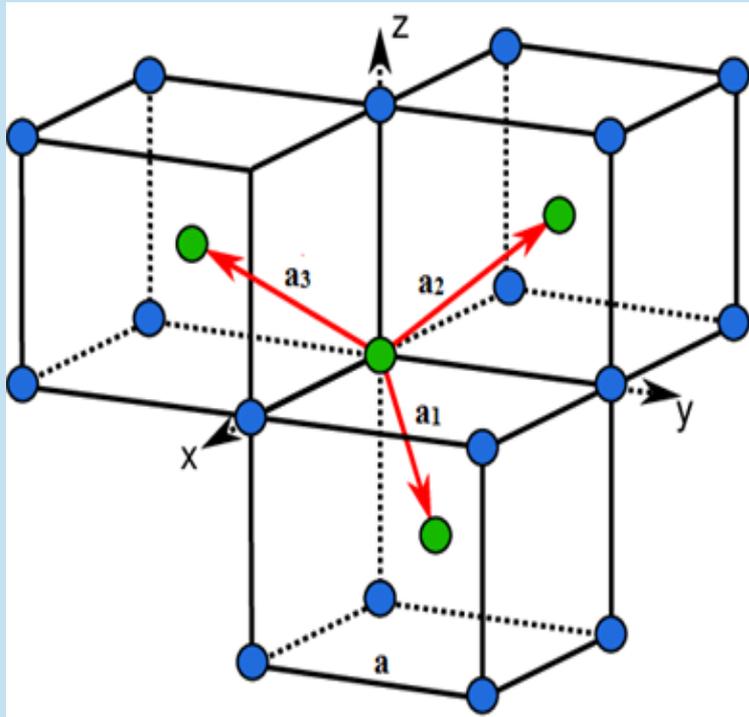


Figure 2.15 : Primitive lattice vectors of bcc crystal

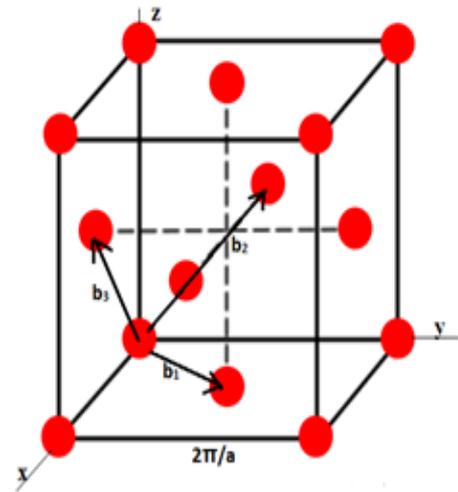


Figure 2.16 Reciprocal lattice to bcc crystal (i.e. fcc).

9.3. Reciprocal lattice to fcc crystal:

- Consider a unit cell of fcc crystal with lattice parameter a . The primitive lattice vectors for fcc crystal are given as

$$\mathbf{a}_1 = \frac{a}{2}(\hat{i} + \hat{j}); \quad \mathbf{a}_2 = \frac{a}{2}(\hat{j} + \hat{k}); \quad \mathbf{a}_3 = \frac{a}{2}(\hat{k} + \hat{i})$$

- Figure 2.16 represents a fcc lattice. Reciprocal lattice vectors of this unit cell is given

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)]} = 2\pi \frac{(a^2/4)(\hat{j} + \hat{k}) \times (\hat{i} + \hat{k})}{\frac{a^3}{8} [(\hat{i} + \hat{j}) \cdot ((\hat{j} + \hat{k}) \times (\hat{i} + \hat{k}))]} = 2\pi \frac{(a^2/4)(\hat{i} + \hat{j} - \hat{k})}{\frac{a^3}{4}}$$

or $\mathbf{b}_1 = \frac{2\pi}{a}(\hat{i} + \hat{j} - \hat{k})$ Similarly $\mathbf{b}_2 = \frac{2\pi}{a}(-\hat{i} + \hat{j} + \hat{k})$ And $\mathbf{b}_3 = \frac{2\pi}{a}(\hat{i} - \hat{j} + \hat{k})$

- Thus the reciprocal lattice to fcc in the form of bcc lattice with lattice parameter to $\frac{2\pi}{a}$. Figure 2.15 can be considered as reciprocal lattice to fcc.

10. Diffraction condition in Reciprocal lattice system:

- In direct lattice system, diffraction takes place when the condition $2d \sin \theta = n\lambda$ is satisfied. This condition can also be obtained from reciprocal lattice system.
- We know the reciprocal points are the points $1/d_{hkl}$ distant along a normal to crystal plane (h k l). Now consider a reciprocal lattice space which has a large number of such reciprocal lattice points as shown in figure 2.17.
- Take a Reciprocal lattice point O as a centre, we draw a circle of radius $1/\lambda$ which is called Ewald circle in two dimensional space, and in three dimension it is called Ewald sphere.
- Ewald stated that whenever a beam of x rays coming in the direction OA and strikes at point O, the centre of circle, and if the beam diffracted in the direction OB and passes through any another lattice point B on the circle, then the Bragg diffraction takes place.

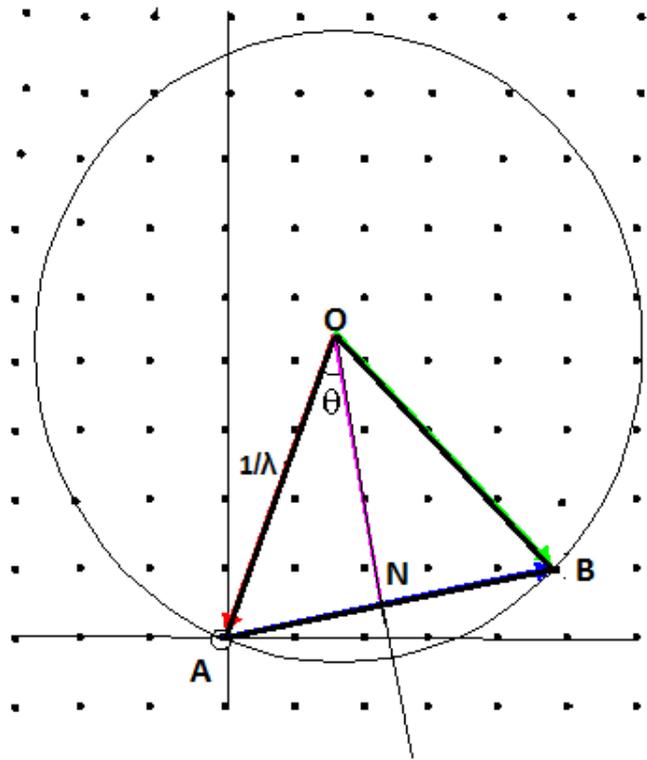


Figure 2.17: Ewald circle in reciprocal lattice system

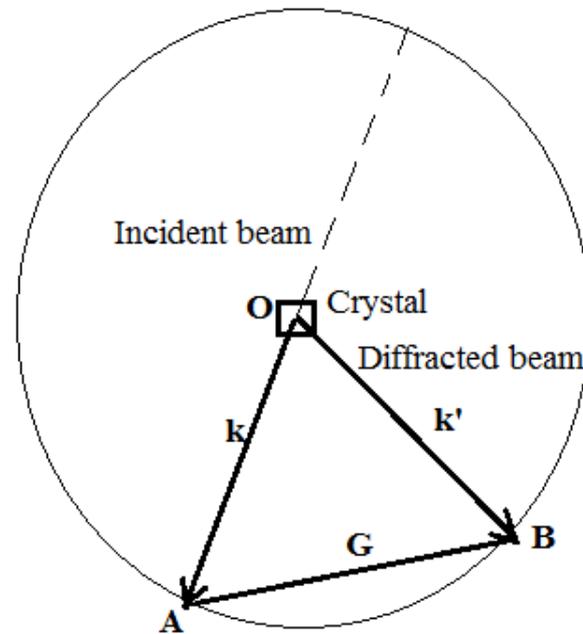


Figure 2.18: Diffraction in reciprocal lattice system

- Support an x-ray beam is coming in the direction of OA, strike at a lattice point O where a crystal is placed then OA represents the incident wave vector \mathbf{k}
- The incident wave strikes at point O, the diffracted x ray \mathbf{k}' passes through another lattice point B on the circle then Bragg diffraction occurs.
- Thus the reciprocal vector $AB = \mathbf{G}$ can be given as

$$AB = \mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 \quad \text{where } v_1, v_2, v_3 \text{ are integer numbers.}$$
- If we draw a perpendicular bisector of a vector AB, then it passes through point N where ON is nothing but plane of diffraction (h k l) which is perpendicular to plane of paper.
- We know that the separation between two reciprocal planes is d_{hkl} then distance between points A and B in reciprocal space can be given as:

$$AB = \frac{n}{d_{hkl}}$$

- Similarly by geometry

$$AB = 2AN = 2 OA \cdot \sin \theta = \frac{2 \sin \theta}{\lambda}$$

using above two expressions for a AB

$$\frac{n}{d_{hkl}} = \frac{2 \sin \theta}{\lambda} \quad \text{or} \quad 2d \sin \theta = n\lambda$$

This is nothing but diffraction condition in direct lattice system.

- Now we find out the diffraction condition in reciprocal lattice system. We know that in reciprocal space (Fourier space) the lattice parameter is denoted by wave vector k' . Figure 2.18 is the simplified representation of diffraction in reciprocal lattice system shown. Now $OA + AB = BO$

$$K + G = K' \quad \text{or} \quad K - K' = G \quad \text{or} \quad \Delta K = G$$

- Since OA and OB are radius of the Eward circle and magnitude of both vectors are same only direction are different thus

$$|OA|^2 = |OB|^2 \quad |K|^2 = |K + G|^2 \quad G^2 + 2KG = 0$$

- This is diffraction condition in reciprocal lattice system

11. Brillouin Zones:

- The concept of a Brillouin zone was developed by Leon Brillouin (1889–1969), a French physicist.
- In direct lattice system we defined Wigner Seitz cell which is nothing but a type of unit cell constructed by the area enclosed by perpendicular bisectors of nearest neighbours.
- If we construct a unit cell by area enclosed by perpendicular bisectors of nearest neighbours reciprocal lattice points that is called Brillouin zone.
- The first Brillouin zone: Now we draw perpendicular bisectors AB, BC, CD, DA of first nearest neighbor points, then the area enclosed by these perpendicular bisectors, i.e. ABCD is called first Brillouin zone.
- Similarly, the areas enclosed by the perpendicular bisectors of second nearest neighbours, EFGH, give the second Brillouin zone.
- There are also third, *etc.*, Brillouin zones, corresponding to a sequence of disjoint regions (all with the same volume) at increasing distances from the origin, but these are used less frequently.
- the *first* Brillouin zone is often called simply the *Brillouin zone*.
- In general, the n -th Brillouin zone consists of the set of points that can be reached from the origin by crossing exactly $n - 1$ distinct Bragg planes.

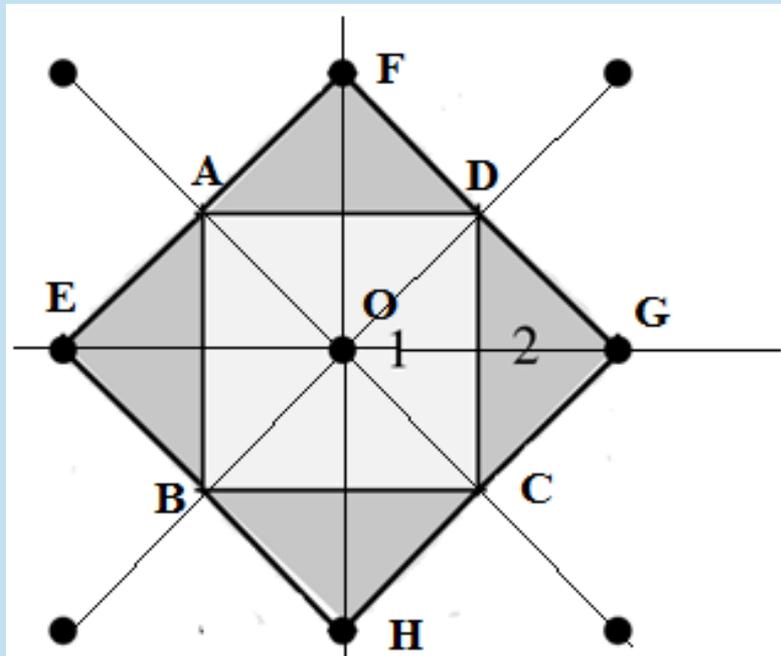


Figure 2.19: First and second Brillouin zone in 2D space.

- Brillouin zone In three dimensional space
- In three dimensional space, Brillouin zone is the minimum volume under perpendicular bisectors of Bragg planes in reciprocal lattice space.
- Brillouin zone can also be understood by Ewald construction. According to Ewald construction, Bragg diffraction occurs for all possible value of wave vector \mathbf{K} for which condition satisfies.
- A Brillouin zone is the locus of all such values of \mathbf{K} in reciprocal lattice system for which Bragg diffraction occurs.
- The importance of the Brillouin zone stems from the Bloch wave description of waves in a periodic medium, in which it is found that the solutions can be completely characterized by their behavior in a single Brillouin zone.

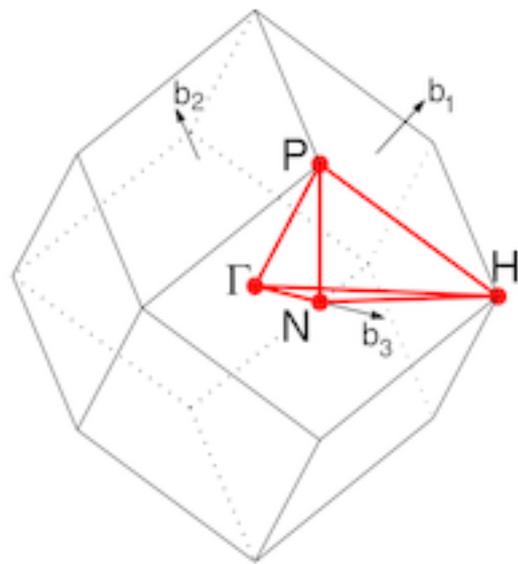


Figure 2.20: Brillouin zone of bcc crystal.

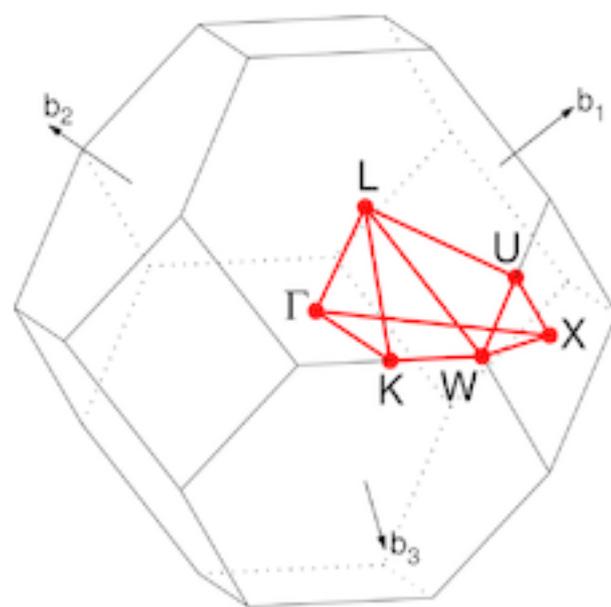


Figure 2.21: Brillouin zone of fcc crystal.

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