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**B.Sc. => Solid-State Physics
Chapter - 1
Crystal Structure**

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Crystal Structure

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Syllabus: Amorphous and Crystalline Materials. Lattice Translation Vectors. Lattice with a Basic – Central and Non – Central Elements. Unit cell. Miller Indices. Reciprocal Lattice. Types of Lattices. Brillouin Zones. Diffraction of X- rays by Crystals. Bragg's Law. Atomic and Geometrical Factor.

Q.1. What are crystalline and amorphous solids? Give examples.

Ans. (i) Crystalline Solids: For example, Quartz, sugar, mica, sodium chloride (NaCl), potassium iodide (*K, I*), carbon (*C*), cesium chloride (CsCl) etc., are all crystalline solids.

Characteristics of crystalline solids

1. The atoms or molecules are arranged in a regular three dimensional throughout the crystal, so these solids have definite geometrical shape.
2. Periodicity in the arrangement of atoms or molecules over many million atomic diameters i.e. there is long range order of the atoms in the structure of crystalline solids.
3. Crystalline substances are bounded by flat surfaces.
4. Crystalline material possess uniform chemical composition i.e., bond between all ions atoms or molecules are of equal strength.
5. Crystalline solids are anisotropic i.e. their physical properties like thermal conductivity, electrical conductivity, refractive index, mechanical strength etc, are different along different directions.

(ii) Glassy (or amorphous) Solids: The solids which do not possess a regular and periodic arrangement of atoms (or molecules/ions) and are in a more or less chaotic and random distribution throughout the solids are called glassy (or amorphous) solids. Thus amorphous solids can be regarded to be highly viscous supercooled liquids without any sharp melting points and non-periodic and regularity of the arrangement of atoms.

For example: Glass, rubber, sulphur etc. are all glassy solids.

Q. 2. What is the difference between crystalline and glassy solids?

Ans. Crystalline solids

1. In crystalline solids, the atoms arranged in regular way.
2. They possess long range order of atoms.
3. These solids have sharp melting points.

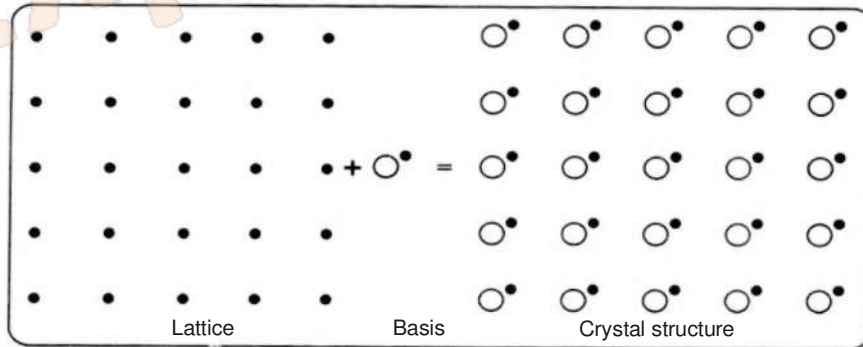
4. These are anisotropic in character i.e. the physical properties (like mechanical, optical and electrical) have different value in different directions.
5. These are treated as true solids. alllabexperiments.com
6. The examples are quartz, mica, diamond, NaCl, Co, Zn, lead etc.

Glassy solids:

1. In glassy solids, the atoms are arranged in irregular way.
2. They possess short range order of atoms.
3. These do not have sharp melting points.
4. These are isotropic in character i.e. they have same value of physical in all the directions.
5. These are not true solids.
6. The examples are glass, lamp block, rubber, plastic, sulphur etc.

Q.3. What is Basis, Unit cell and primitive cell in a crystal structure?

Ans. Lattice is simply the network of points in space, until we associate these lattice points with one or more atoms (i.e. unit assembly of atoms of same composition) we do not get crystal structure. This unit assembly which make the given lattice a crystal is known as basis. Thus, basis is the assembly of atoms, ions or molecules which when repeated in three dimensions generates a crystal structure. Thus a crystal lattice combined with a basis generates the crystal structure. $\text{crystal structure} = \text{space lattice} + \text{basis}$.

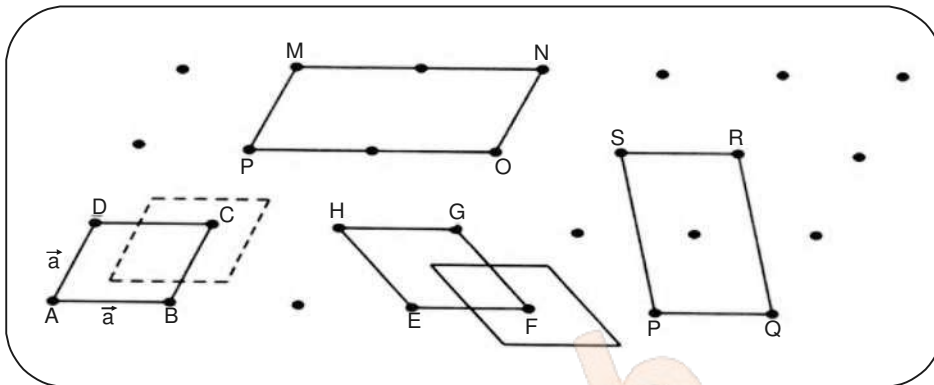


Crystal structure

Crystal lattice is purely a geometrical conception consisting of a periodic arrangement of points, such that by placing different atoms (or groups of atoms) on these points, we obtain the actual crystal.

Unit cell

The smallest geometrical figure which repeats itself in space to produce a crystal is called unit cell. Consider a two dimensional lattice array as shown in fig. We find that if the parallelogram $ABCD$ is



Two dimensional lattice and different unit cell.

Repeatedly translated by the vectors \vec{a} and \vec{b} along AB and AD we obtain the same lattice of which this parallelogram is a part. Thus, $ABCD$ is called a unit cell. The choice of unit cell is not unique, some other unit cell are also shown in the fig. In three dimensional case we have parallelepipeds as unit cells.

Therefore, we include that the entire lattice can be derived by repeating a unit cell by means of translation vectors as edges of the unit cell.

Lattice Parameters of a Unit Cell

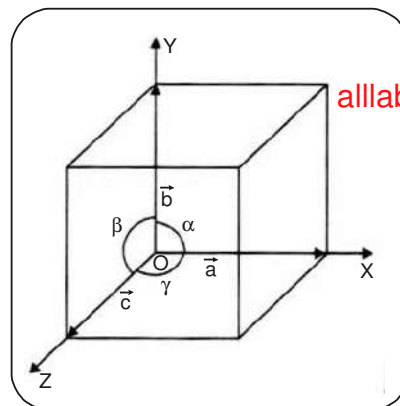
Crystallographic Axis

The lines drawn along the lines of intersection of any three faces of a unit cell, which do not lie in the same plane are called crystallographic axis.

In figure. OX , OY and OZ are crystallographic axis.

Interfacial angles

The angles between the three crystallographic axis are called interfacial angles.



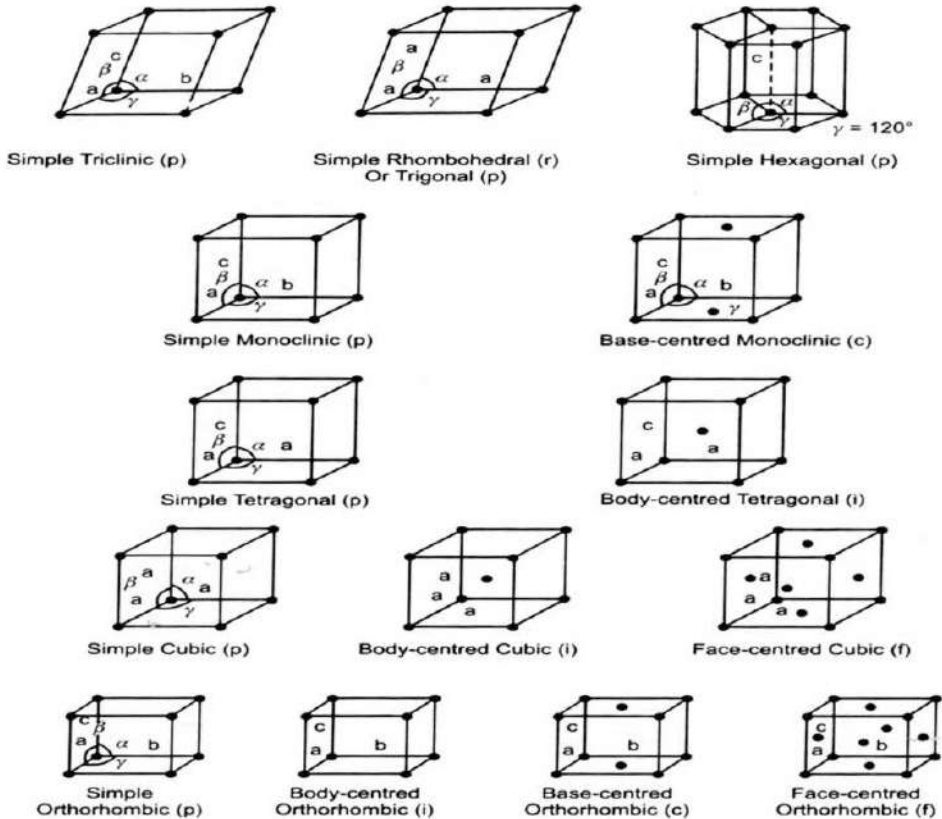
Unit cell

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Q. 4. What is Bravais lattice, give its types?

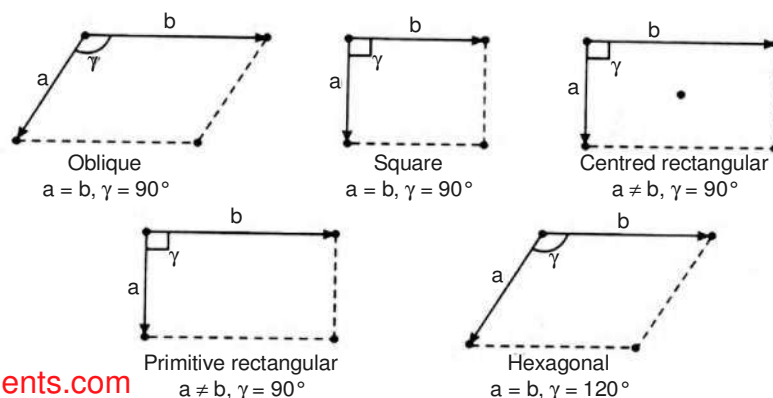
Ans.



Bravais Lattice in two and three Dimensions

Bravais introduced the concept of space lattice to describe the structure of crystals. According to him there are five lattice types or unit cells in two dimensions and fourteen in three dimensions.

(i) **Two dimensional lattices:** There are in all five Bravais lattice types in two dimensions, i.e. oblique, hexagonal, rectangular and centered rectangular. These are shown in fig.



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Fig. Bravais lattice types in two dimensions

(ii) **Three dimensions lattices:** There are seven crystal systems in three dimensions namely triclinic, monocline, cubic, Tetragonal, orthorhombic, trigonal and hexagonal. These seven types of crystal systems generate 14 types of Bravais lattices in which triclinic lattice is of general type and other 13 are of special type. These 14 space lattices are shown in fig. and table gives the seven systems and fourteen lattices.

Table: The crystal system

S. No.	System	Number of lattices in the system	Bravais lattices	Axis length and interfacial angles
1.	Triclinic	1	1. Simple	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90$
2.	Trigonal (or rhombohedral)	1	1. Simple	$a = b = c, \alpha = \beta = \gamma \neq 90$
3.	Hexagonal	1	1. Simple	$a = b \neq c, \alpha = \beta = 90, \gamma = 120$
4.	Monocline	2	1. Simple 2. Base centred	$a \neq b \neq c, \alpha = \beta = 90^\circ, \gamma \neq 90$
5.	Tetragonal	2	1. Simple 2. Body centred	$a = b \neq c, \alpha = \beta = \gamma = 90$

Q.5. Define Miller indices. Determine it for different planes of cubic crystal?

Ans. The miller indices of a plane are determined as follows. Consider the plane shown in fig.

(i) Take any atom or point as origin and construct co – ordinate axis. Find the intercepts of the plane along the a, b and c axis, in of the words determine the coordinates of the intercepts.

$$\begin{array}{ccc} x & y & z \\ 3a & 2b & 2c \end{array}$$

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(ii) Express the intercepts as multiples of a , b , and c

$$\frac{3}{3} \quad \frac{2}{2} \quad \frac{2}{2}$$

(iii) Take reciprocals of the intercepts

$$\frac{1}{3} \quad \frac{1}{2} \quad \frac{1}{2}$$

(iv) Reduce these reciprocals into the smallest set of integers in the same ratio by multiplying with their LCM.

$$\begin{array}{ccc} 6 \times \frac{1}{3} & 6 \times \frac{1}{2} & 6 \times \frac{1}{2} \\ 2 & 3 & 3 \end{array}$$

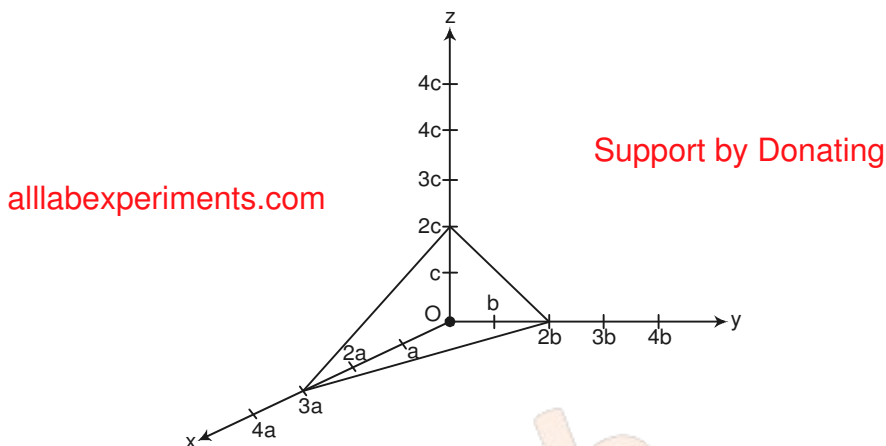


Fig. A crystal plane making intercepts 3, 2, and 2 on a , b and c axis respectively

(v) Enclose these integers (smallest set) into Parentheses and we get miller indices (233)

In general miller indices of a plane are denoted by (hkl) . If n_1 , n_2 , n_3 and I_1 , I_2 , I_3 are the coordinates of the intercepts made by the plane on the three crystallographic axes, the miller indices are given as

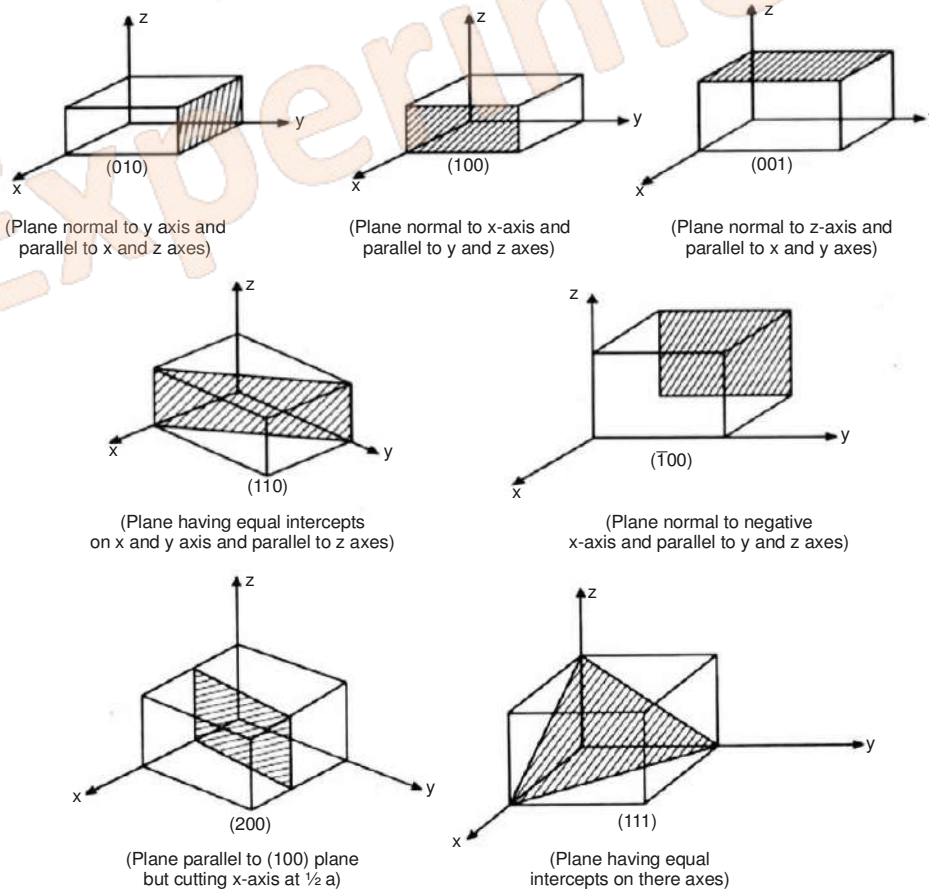
$$\frac{1}{n_1} : \frac{1}{n_2} : \frac{1}{n_3} = h : k : l$$

By taking reciprocals, we bring all the planes in a single unit cell, so that we can discuss or study all the crystal planes passing through a single unit cell. If an intercept is at infinity, the corresponding index is zero e.g., for intercepts of a plane at ∞ , $1b$, $2c$ the miller indices are (0, 2, 1). The indices (hkl) may denote a single plane or a set of parallel planes. If a plane cut an axis on the negative side of the origin, the corresponding index is negative and denoted by placing a minus sign on the index $(\bar{h}kl)$ as called as bar h , k , l .

Planes equivalent by symmetry may be denoted by curly brackets around indices e.g. the family of planes with numbers (100) , (010) , (001) , $(\bar{1}00)$, $(00\bar{1})$ is denoted by $\{100\}$. These family of planes need not be parallel to each other.

Similarly family of planes with members (233) , (323) , (332) , $(\bar{2}33)$, $(\bar{3}23)$ etc, is denoted as $\{233\}$, where curly bracket stands for family of planes.

The miller indices of some important planes in a cubic crystal are shown below:

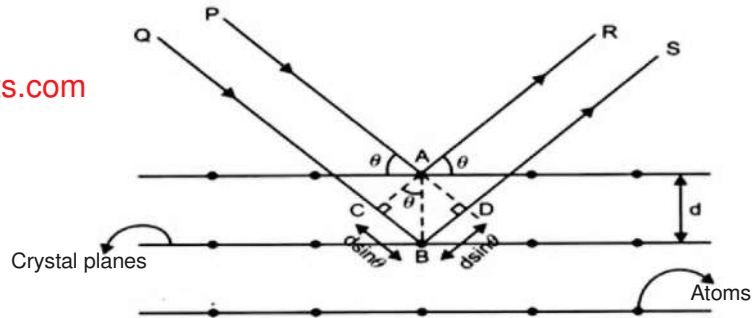


Q.6. What is Bragg's law of X-ray diffraction

Ans.

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The multiple reflected rays interfere constructively and the diffraction pattern is obtained. Consider parallel lattice planes as shown in fig. Let the planes be at a distance of 'd' from each other and having Miller indices (*hkl*). Let a parallel beam of X- rays of wavelength λ be incident on these parallel planes at a glancing angle θ s.t, the ray lies in the plane of paper. Let two rays PA and QB incident at A and B, are reflected in the direction AR and BS respectively as shown in fig. Draw AC and AD perpendiculars on QB respectively. The reflected rays AR and BS interfere constructively, if the path difference ($CB + BD$) is equal to the integral multiple of wavelength λ .

i.e. $CB + BD = n\lambda$.

From fig. It is clear that

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

Where θ is the angle of incidence as well as the angle of reflection and is also known as glancing angle. Hence the condition for reinforcement is

$$d \sin \theta + d \sin \theta = n\lambda.$$

$$2d \sin \theta = n\lambda \quad \dots(2.1)$$

Where $n = 1, 2, 3, 4, \dots$ stand for first order, second order... etc, maxima. Equation (2, 1) is known as Bragg's law. Eq. 2.1 is also called fundamental equation of solid state physics. As $\sin \theta$ lies between 0 and 1, hence it is obvious that λ must be $\leq 2d$, As $d \approx 1A$, $\therefore \lambda = 2A$. That is why visible light can not be used in crystal diffraction.

Characteristic Feature of Bragg's Law [Important]

1. Bragg's law is consequence of the periodicity of the space lattice.
2. The law does not tell about the arrangement or basis of atoms associated with its lattice point.
3. The composition of the basis determines the relative intensity of the various order of diffraction from a given set of parallel planes.
4. Bragg's reflection can occur only for wavelength $\lambda \leq 2d$. This is the reason why visible wavelength cannot be used in diffraction.
5. For the same order and spacing the angle θ decreases. Consequently for gamma rays, glancing angles must be used.

Q.7. X-rays of wavelength 1.75 Ang. undergoes first order Bragg reflection from [111] plane at 300. What is inter-atomic spacing of crystal?

Ans. $a = 1.75 \text{ \AA} = 1.75 \times 10^{-10} \text{ m.}$

$$\text{Angle} = 30^\circ$$

$$n = 1$$

Now
$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where a = interatomic spacing, $h, k, l \rightarrow$ Miller indices

d = inter planes distance

so
$$d_{111} = \frac{a}{\sqrt{1+1+1}} = \frac{a}{\sqrt{3}}$$

using Bragg's equation $2d \sin \theta = n\lambda$.

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$$2 \times \frac{a}{\sqrt{3}} \sin 30^\circ = 1 \times 1.75 \times 10^{-10}$$

$$\Rightarrow a = \frac{\sqrt{3}}{2} \times 1.75 \times 10^{-10} \times 2 = 3.03 \times 10^{-10} \text{ m.}$$

Q.8. What is Brillouin Zone? Draw and explain first and second Brillouin zones of a square lattice.

Ans. Brillouin zone is a primitive cell in reciprocal lattice. It is constructed by selecting every \vec{G} from origin and placing planes perpendicular to \vec{G} at the vector mid point. It gives all the wave vectors which can diffract.

Let us construct Brillouin zones for a simple square lattice of side a . The primitive translations vectors for this lattice are

$$\vec{a} = a\hat{i}; \vec{b} = b\hat{j} = a\hat{j} = [\because a = b]$$

The corresponding reciprocal lattice translations vectors are

$$\vec{a}^* = \frac{2\pi}{a}\hat{i}; \vec{b}^* = \frac{2\pi}{a}\hat{j}$$

$$\therefore \vec{G} = h\vec{a}^* + k\vec{b}^* = \frac{2\pi}{a}(h\hat{i} + k\hat{j})$$

Where h and k are integers.

Let the wave vector for an X- ray be given by

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

Where it is measured from the origin of the reciprocal lattice. From Bragg's condition, we have

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

or
$$2\vec{k} \cdot \vec{G}^2 = -\vec{G}^2$$

or
$$2(k_x\hat{i} + k_y\hat{j}) \cdot \frac{2\pi}{a}(h\hat{i} + k\hat{j}) = \frac{4\pi^2}{a^2}(h^2 + k^2)$$
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or
$$hk_x + kk_y = -\frac{\pi}{a}(h^2 + k^2)$$

This equation represents a family of straight lines in the k_x and k_y plane. Their k_x and k_y intercepts are

$$k_x = -\frac{\pi}{a} \left(\frac{h^2 + k^2}{h} \right) \text{ (for } k_y = 0 \text{)}$$

$$k_y = -\frac{\pi}{a} \left(\frac{h^2 + k^2}{k} \right) \text{ (for } k_x = 0 \text{)}$$

If we take

$$h = 0, k = \pm 1$$

and

$$k = 0, h = \pm 1.$$

we obtain four lines

$k_x = \pm \frac{\pi}{a}$ [This is a set of four lines and area enclosed by these lines is first Brillouin zone]

and

$$k_y = \pm \frac{\pi}{a}$$

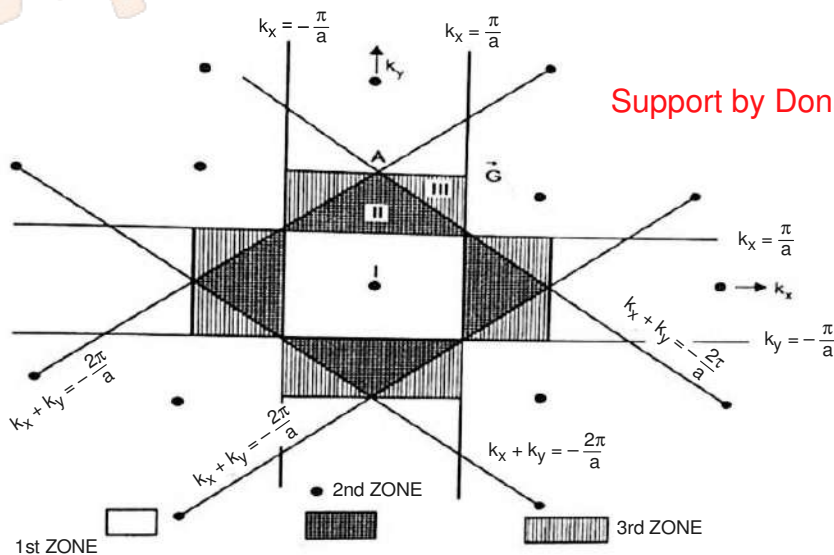


Fig. Construction of first three Brillouin zones for a square lattice.

The four lines are plotted in fig. All \vec{k} vectors originating at the origin and terminating on these lines will produce Bragg's reflection. Besides this set of lines, some other sets of lines, are also possible by taking $h = \pm 1$ in e.q. The four possible lines are

$$\pm k_x + k_y = \frac{-2\pi}{a}; \text{ which can separately be written as:}$$

$$\left. \begin{array}{l} k_x + k_y = \frac{-2\pi}{a} \\ k_x - k_y = \frac{-2\pi}{a} \\ -k_x + k_y = \frac{-2\pi}{a} \\ -k_x - k_y = \frac{-2\pi}{a} \end{array} \right\} \text{set of four lines'}$$

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The area enclosed by these four lines is 2nd Brillouin zone.

Q.9. Define Reciprocal lattice. Give its graphical construction?

Ans. Reciprocal Lattice: X-ray diffraction is equivalent to reflection by the sets of parallel lattice planes in the crystal. But the picture of X-ray diffraction as given by $n\lambda = 2d \sin \theta$ (Bragg's law) is very much over simplified. There exist many sets of planes, with varying slopes and spacings, which can diffract a given beam of X-ray. It is difficult to visualize several slopes of two dimensional surfaces, such as planes. We know that the slope of a plane is determined by its normal which is a line, so it has one dimension. Hence if we are concerned with a multitude of planes, we can think in terms of their normals. (A normals represents the slope of a set of parallel planes).

If the length assigned to each normal is proportional to the reciprocal of the inter planer spacing of that plane, then the points at the end of their normal drawn from a common origin is called reciprocal lattice.

Graphical Construction of Reciprocal lattice: The reciprocal lattice can be constructed by using the above rules. We shall have graphical representation for a monoclinic lattice, the formation of two dimensional reciprocal lattice is discussed as below. Fig. (a) represents a monoclinic unit cell. Here $a \neq b \neq c$ and $a = \beta = 90^\circ; \gamma > 90^\circ$. It is clear from the fig. that \vec{a} and \vec{b} lie in the plane of paper, but \vec{b} is perpendicular to the plane of the paper. In the two dimensional view, \vec{a} and \vec{c} are represented by sides OA and OB (fig (b)). Also the side \vec{b} is represented by a dot (\bullet) at O . It is important to note here that the planes

(hol) will be perpendicular to the plane of the paper and normals to these planes are represented by the lines. Therefore, the line OA actually represents the (001) planes, the line OB represents the (100) planes the line AB represents the (101) planes.

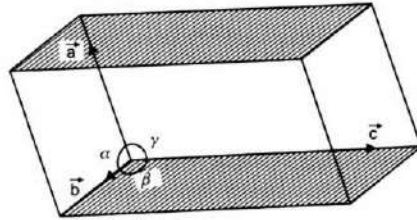
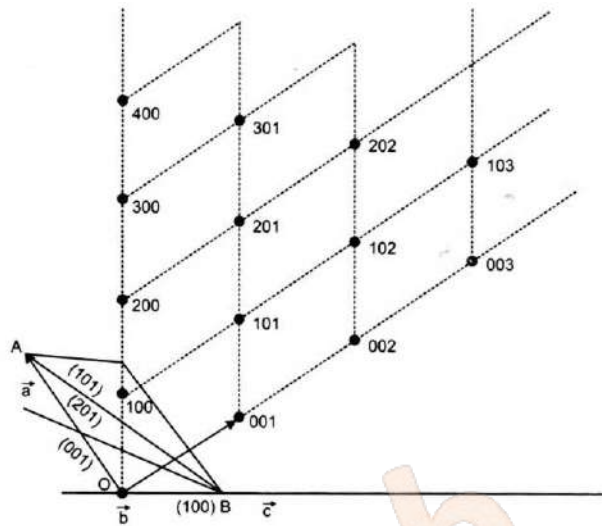


Fig.

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Now from a common origin (here point 0) erect normal to each plane. Set the length of each normal equal to 2π times the reciprocal of the interplanar spacing for a particular set of planes. Place points at the end of each normal. The coefficient of such points form a periodic array and is called the reciprocal lattice. It is to be noted that (002) planes lie mid way between (001) planes, so it is very easy to conclude that in the reciprocal lattice, the distance of (002) point is twice the distance of (001) point from the origin.

Q.10. Calculate the geometrical structure factor of a bcc lattice. Name two planes which will be missing from the X-ray diffraction spectrum.

Ans. Let us consider a unit cell (fig.) of a crystal, having n number of atoms per unit cell.

Let the position vector of the atom is given by

$$\vec{r}_j = u_j\vec{a} + v_j\vec{b} + w_j\vec{c} \quad \dots(2.33)$$

Here u_j, v_j and w_j are constants. Suppose that all the electrons of j th atom are concentrated at the position \vec{r}_j . Let f_j be the scattering power of j th atom relative to single electron when both are located at the same point.

Geometrical structure factor.

$$\therefore S = f \sum_j e^{-2\pi i[u_j + v_j k + w_j l]} \quad \dots(2.37)$$

The structure factor need not be real, the intensity involves the absolute value S i.e. S^*S , where S^* is the complex conjugate of S . The structure factor can cancel some of the reflections allowed by the space lattice, and the missing reflections help us in the determination of the structure. Let us calculate geometrical structure factor for some simple crystals and the intensity of various reflections associated with them. Enough, so that the intensity peaks may be seen.

(ii) Structure factor for b.c.c. lattice: A b.c.c. lattice has two identical atoms per unit cell, one contributed by the corner atoms of the cell $(0, 0, 0)$ and the

other at the centre of the cell $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

Hence from equation (2.37), put u_j, v_j and w_j equal to $(0, 0, 0)$ and $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

$$S = f \left[e^0 + e^{-2\pi i \left(\frac{h}{2} + \frac{k}{2} + \frac{l}{2} \right)} \right]$$

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$$\text{or} \quad S = f \left[1 + e^{-\pi i(h+k+l)} \right] \quad \dots(2.39)$$

Now it is obvious that

(i) $S = 0$ for $(h + k + l) = \text{odd integer}$ [$\therefore e^{-\pi i(h+k+l)} = -1$ for $(h + k + l)$ odd]

So in b.c.c. certain reflections are missing e.g.

(100), (300), (111), and (222)

(ii) $S = 2f$ for $(h + k + l) = \text{even integer}$ [$\therefore e^{-\pi i(h+k+l)} = 1$ for $(h + k + l)$ even]

So the reflection (200), (110), (222) are present

Reason for absence of (100) reflection and presence of (200) reflection.

The absence or presence of a reflection is considered only in terms of the first order reflection. The (100) reflection normally occurs when reflections

from the planes that bound the cubic cell differ in phase by 2π . In b.c.c. lattice there is an intervening plane (fig.) of atoms between the top and bottom cube faces due to body centre atoms of the unit cells. This intervening plane gives a reflection retarded in phase by π with respect to the first plane, hence cancelling the contribution from the plane. The phase difference between the radiations scattered from first plane (top plane) and the second plane (intervening plane due to body atoms) is π radians. Similarly, the phase difference between the second plane (intervening plane) and third plane (bottom plane) is π radians. Therefore, radiations from top and intervening plane and also from bottom and intervening plane interfere destructively to produce zero intensity. Hence (100) reflection is absent. The cancellations of (100) reflections occur in the b.c.c. lattice because the planes are identical in composition. A similar cancellation can easily be found in the hcp structure.

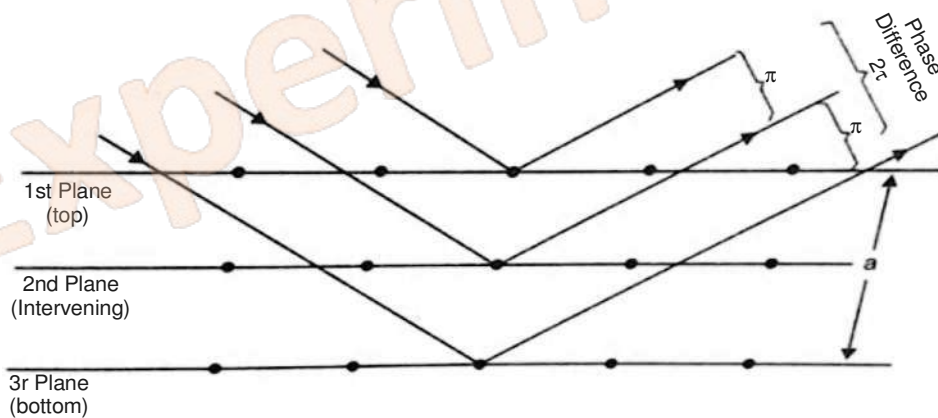


Figure. Explanation of the absence of a (100) reflection from a bcc lattice

For (200) reflection, the phase difference between top and bottom plane is 4π , hence the reflection from the middle plane would differ from the reflection from top and bottom planes by a phase of 2π resulting in constructive interference. Hence (200) reflection is present.

