

(vii) Density, ρ :

The theoretical density of HCP cell is given by

$$\rho = \frac{ZM}{N_A V} = \frac{6M}{N_A (3\sqrt{2}a^3)} = \frac{\sqrt{2}M}{N_A a^3} \quad (26.27)$$

The characteristics of the three types of cubic unit cells and the HCP cell are summarized in Table-2.

Table - 2

Sr.No.	Characteristics	Unit Cell			
		SC	BCC	FCC	HCP
1.	Unit cell volume, V	a^3	a^3	a^3	$3\sqrt{2}a^3$
2.	Atoms per unit cell, Z	1	2	4	6
3.	Atomic radius, r	$a/2$	$a\sqrt{3}/4$	$a/2\sqrt{2}$	$a/2$
4.	Coordination number, CN	6	8	12	12
5.	Atomic packing fraction, APF	$\pi/6$ $= 0.52$	$\pi\sqrt{3}/8$ $= 0.68$	$\pi/3\sqrt{2}$ $= 0.74$	$\pi/3\sqrt{2}$ $= 0.74$
6.	Void space	48%	32%	26%	26%
7.	Density, ρ	$\frac{M}{N_A a^3}$	$\frac{2M}{N_A a^3}$	$\frac{4M}{N_A a^3}$	$\frac{\sqrt{2}M}{N_A a^3}$

It is seen from the above table that the SC cell is loosely packed and the FCC and HCP cells are the close packed cells among the four types of unit cells.

26.12 ATOM POSITIONS IN CUBIC UNIT CELLS

Let a rectangular right handed coordinate system be attached to the cubic lattice, as shown in Fig. 26.27. The position of a lattice site is described by three coordinates (x, y, z) which are expressed as

$$x = pa, \quad y = qb, \quad z = rc \quad (26.28)$$

where a , b and c are lattice constants in x , y and z directions respectively and p , q and r are integers. If the lattice constants a , b and c are taken as **unit** axial lengths, $a = 1$, $b = 1$, and $c = 1$, and the co-ordinates of the lattice site will be (p, q, r) . These are the indices of the lattice site and are written with commas separating the numbers and enclosed in parenthesis.

As an example, the indices of atomic sites in the BCC cell are shown in Fig. 26.27. The atom positions for the eight corner atoms are $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(1,1,1)$, $(1,1,0)$, $(1,0,1)$, and $(0,1,1)$. The body centre atom in the cell has the coordinates $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. By convention, the set of coordinates $(0,0,0)$ stands for the locations of all eight corners of cubic unit cell. Therefore, it is sufficient if the atom positions $(0,0,0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ are specified for the BCC cell.

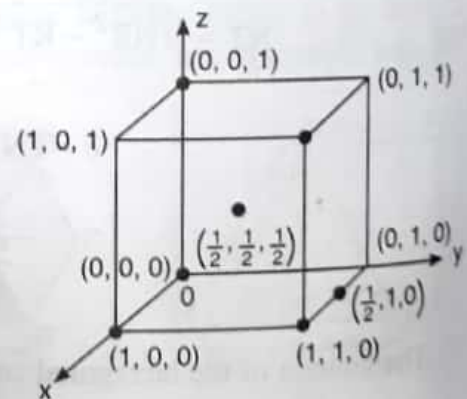


Fig. 26.27

The minimum number of coordinate sets necessary to specify the locations of all atoms in a unit cell are equal to the value of Z , the effective number atoms/cell.

26.13 INDICES OF CRYSTALLOGRAPHIC DIRECTION

Many crystals exhibit properties that are dependent on the direction in which they are measured and on the direction of the external stimuli, such as an electric field, magnetic field or mechanical stress, acting on the crystal. Therefore, it is essential that we know reference directions in crystals. To describe a direction in a crystal lattice, a straight line passing through the origin is chosen. The co-ordinates of the first lattice point lying on this line are utilized to denote the direction of the line. Thus, the indices of direction are the vector components of direction

resolved along each of the axes and reduced to the smallest integers.

The vector components are multiples of lattice constants. If the direction passes through the origin, then the indices of the lattice will also be the indices of direction.

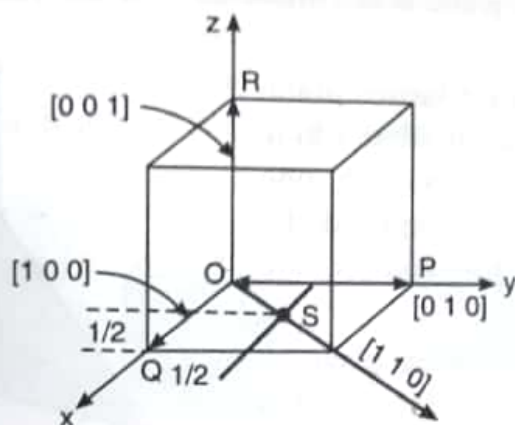


Fig. 26.28. Indices of direction

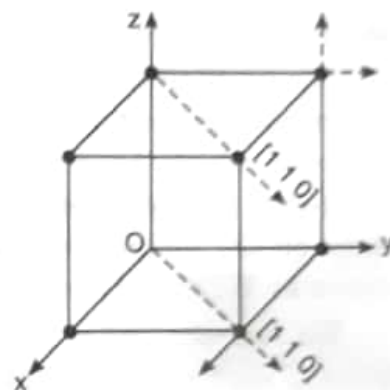


Fig. 26.29. Indices of parallel directions

The indices of direction are calculated by the following procedure.

- (i) First, find the coordinates of the lattice site nearest to the origin in a given direction.
- (ii) The coordinates are then divided by appropriate unit translations.
- (iii) If fractions are obtained, each of the fractions is multiplied by smallest common divisor.
- (iv) The integers obtained are the indices of direction written in square brackets, as $[p\ q\ r]$.

Thus, the indices of direction in a crystal are the set of smallest integers, which have the same ratios as the components of a vector in the desired direction, referred to the axes.

As an example let us consider a cubic cell shown in Fig. 26.28. Let the point 'O' be the origin. The point P is at the position $(0, b, 0)$. 'b' represents one unit distance. Therefore, the indices of the point P are $(0, 1, 0)$. The direction OP is given as $[0\ 1\ 0]$. On the other hand, the direction of PO is specified as $[0\ \bar{1}\ 0]$. A bar on the number indicates a negative direction.

Similarly, the directions OQ and OR are indicated as $[1\ 0\ 0]$ and $[0\ 0\ 1]$ respectively.

The direction of OS may be determined as follows. The position indices of the point S are $(\frac{1}{2}, \frac{1}{2}, 0)$. Then, using the instruction (iii), the direction of the line OS is obtained as

$$\left[2 \times \frac{1}{2}, 2 \times \frac{1}{2}, 0 \right] = [110].$$

All parallel directions have the same direction indices (Fig. 26.29) and the parallel directions are equivalent. $\langle pqr \rangle$ represents the family of directions $[0\ 1\ 0]$, $[0\ 0\ 1]$, $[1\ 0\ 0]$, $[0\ \bar{1}\ 0]$, $[0\ 0\ \bar{1}]$, $[\bar{1}\ 0\ 0]$. All of them are grouped as $\langle 1\ 0\ 0 \rangle$.

26.14 LATTICE PLANES AND MILLER INDICES

A crystal lattice may be regarded as an aggregate of a set of parallel, equally spaced planes passing through the lattice points. The planes are called **lattice planes** and the perpendicular distance between adjacent planes is called **interplanar spacing**. A given space lattice may have infinite sets of lattice planes, each having its characteristic interplanar spacing. In a crystal the geometrical location of a plane is not important. All the planes that are parallel to each other play a similar role.

The position and orientation of a lattice plane in a crystal are determined by three smallest whole numbers which have the same ratios with one another as the reciprocals of the intercepts of the plane on the three crystal axes. These numbers are known as **Miller indices** of that plane.

We find the Miller indices of a given plane as follows. We choose a set of coordinate axes parallel to unit cell edges at a convenient point. Let OX, OY and OZ be positive directions of the axes along the three edges of the unit cell, as shown in Fig. 26.30.

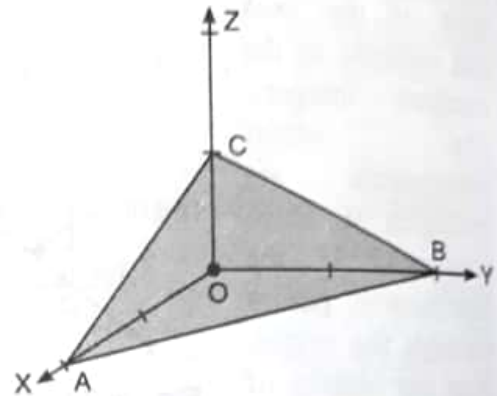


Fig. 26.30. A lattice plane intercepting the three crystallographic axes.

We consider a plane ABC oriented with respect to the coordinate axes and which intercepts the x -, y -, and z -coordinates at distances OA, OB and OC respectively. It will be seen that Miller indices for all the planes parallel to the plane ABC and containing similar type of atomic array are the same. The intercepts are not measured in metrical distances of cm or Å, but are measured in terms of respective unit lengths assigned to each edge of the cell, regardless the actual dimension of the edge. Thus, the intercepts OA, OB, and OC made by a plane such as ABC are expressed as multiples of the axial lengths.

For the plane of interest, we determine the intercepts x , y , and z on the coordinate axes.

- We express the intercepts in terms of the base vectors of the unit cell, pa , qb , and rc ; p , q and r are not necessarily integers but they do have rational ratios.
- We form the reciprocals $1/p$, $1/q$, and $1/r$.
- If the reciprocals are fractions, each fraction is multiplied by the least common denominator, D , and reduce them to the smallest set of integers. Thus, we obtain $D/p = h$, $D/q = k$ and $D/r = l$ respectively.
- We put the integers in parenthesis (hkl). These are the **Miller indices** of the given plane.

All the planes, having the same structure of atoms, which are parallel to each other and therefore have the same orientation with respect to the three edges of the unit cell belong to the same family of planes and are represented by the same Miller indices. Consider a plane, of a family of similar planes, lying within the unit cell and nearest to the origin. This plane cuts off intercepts equal to $(1/h)a$, $(1/k)b$, $(1/l)c$. This implies that the (hkl) plane divides " a " into h parts, " b " into k parts and " c " into l parts. Other members of the family cut off intercepts $2a/h$, $2b/k$, $2c/l$, ..., na/h , nb/k , nc/l so that the ratio between the intercepts is the same.

1. Parallel planes spaced equally have the same Miller indices. Thus, all the planes in a set parallel to a particular plane (hkl) are denoted by (hkl).
2. A plane parallel to one coordinate axis has Miller index 0 for that direction.
3. A plane passing through origin is denoted by Miller indices of a parallel plane having non-zero intercepts.
4. When the intercept of a plane is negative on an axis, a bar is placed on the corresponding Miller index.

26.14.1 Miller Indices of Principal Planes in a Cubic Cell

Any plane in the crystal containing some atoms is a crystal plane. However, the effect of the planes with small atomic density on the physical properties of the crystal is negligible. Hence, the planes with appreciable atomic density are called principal planes.

Fig. 26.31 depicts the principal crystallographic planes of cubic crystal structure. One of the faces of the cube is shown shaded in Fig. 26.31

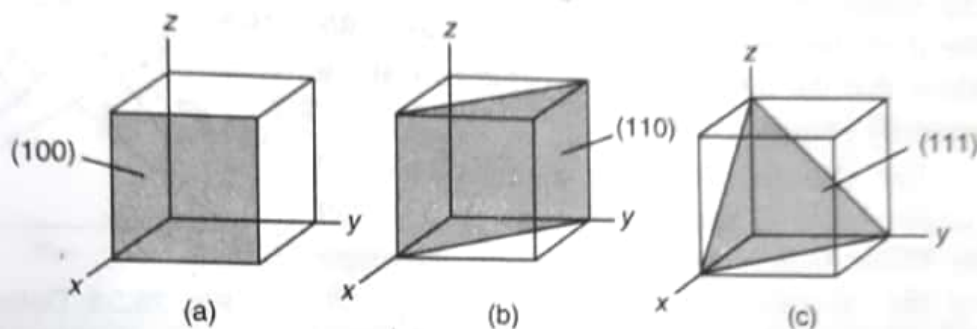


Fig. 26.31. The three principal Miller index planes in a cubic lattice.

(a). The shaded plane intercepts the axes x, y, z at $1, \infty, \infty$ respectively. The reciprocals of the intercepts are $1, 0, 0$. The Miller indices for this plane are (100) . The plane is called one-zero-zero plane. The plane in Fig. 26.31 (b) has the intercepts at $1, 1, \infty$. Therefore, the Miller indices are (110) and the plane is called one-one-zero plane. Finally, the plane in Fig. 26.31 (c) has intercepts at $1, 1, 1$ and hence the Miller indices are (111) . This plane is called one-one-one plane. These three planes are known as the **principal planes of cubic crystal system**.

26.14.2 Sketching a Lattice Plane (hkl)

The intercepts made by a plane can be found if the Miller indices of the plane are known.

- Let the Miller indices of a plane be (hkl).
- A unit cell (for e.g. a cube) is drawn with three coordinate axes.
- From the Miller indices, the reciprocals are obtained $\rightarrow \frac{1}{h}, \frac{1}{k}, \frac{1}{l}$

- The intercepts are marked on the coordinate axes.
- The three non-planar points are joined and the plane is obtained.

Example: Draw a plane (321)

Step (i): A cube having unit axial lengths ($a = 1$) along the three coordinate axes is drawn as shown in Fig. 26.32.

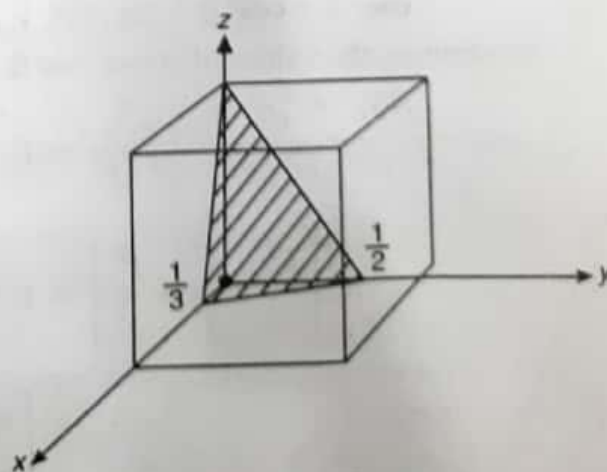


Fig. 26.32. (321) plane

Step (ii): The reciprocals of Miller indices are $p = \frac{1}{3}$, $q = \frac{1}{2}$ and $r = 1$.

Step (iii): The intercepts, $\frac{1}{3}$, $\frac{1}{2}$ and 1, are marked within the cube on x , y and z axes respectively.

Step (iv): A plane is drawn through the points and is shaded.

26.15 INTERPLANAR SPACING IN A CUBIC LATTICE

The distance ' d ' between successive lattice planes is known as the *interplanar distance*. The interplanar distance ' d ' involves the axial lengths of the unit cell and the Miller indices of the planes. We shall derive here an expression for d in the case of a cubic system only. We know that the three axes of a cubic crystal are mutually perpendicular.

Let ABC be one of the family of parallel lattice planes in the crystal (Fig. 26.33). Let its Miller indices be (hkl) and the intercepts on the crystallographic axes be $OA = a/h$, $OB = b/k$ and $OC = c/l$. The next plane of the set parallel to ABC passes through the origin of the coordinates O (which is not shown in the Fig. 26.33). Therefore, ON, the length of the normal from the origin to the plane is equal to ' d '. Let α , β , and γ be the angles ON makes with the three crystallographic axes respectively. Then the direction cosines of ON are

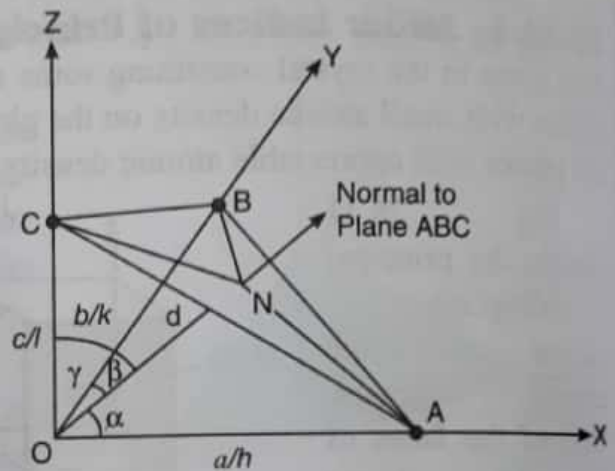


Fig. 26.33. Determination of interplanar distance in a cubic crystal

$$\cos \alpha = \frac{ON}{OA} = \frac{d}{a/h}$$

$$\cos \beta = \frac{ON}{OB} = \frac{d}{b/k}$$

$$\cos \gamma = \frac{ON}{OC} = \frac{d}{c/l} \quad (26.29)$$

The sum of the squares of the direction cosines of a line equals unity. Thus,

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1 \quad (26.30)$$

Substituting the values of $\cos \alpha$, $\cos \beta$, and $\cos \gamma$ in the above equation, we get

$$\frac{d^2}{a^2/h^2} + \frac{d^2}{b^2/k^2} + \frac{d^2}{c^2/l^2} = 1$$

$$d^2 \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

$$d = \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]^{-1/2} \quad (26.31)$$

\therefore

In case of cubic system, $a = b = c$. The above equation then reduces to

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (26.32)$$

Example 26.5. Determine lattice constant for FCC lead crystal of radius 1.746 \AA . Also find the spacing of (i) (111) planes, (ii) (200) planes and (iii) (220) planes.

Solution: The lattice constant is related to the atomic radius in FCC structure through

$$a = 2\sqrt{2}r = 2 \times 1.414 \times 1.746 \text{ \AA} = 4.938 \text{ \AA}.$$

The interplanar spacing is given by $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$(i) \quad d_{111} = \frac{4.938}{\sqrt{1^2 + 1^2 + 1^2}} \text{ \AA} = 2.851 \text{ \AA}$$

$$(ii) \quad d_{200} = \frac{4.938}{\sqrt{2^2 + 0^2 + 0^2}} \text{ \AA} = 2.469 \text{ \AA}$$

$$(iii) \quad d_{220} = \frac{4.938}{\sqrt{2^2 + 2^2 + 0^2}} \text{ \AA} = 1.746 \text{ \AA}$$

Example 26.6. The density of copper is 8980 kg/m^3 and unit cell dimension is 3.61 \AA . Atomic wt. of copper is 63.54 . Determine crystal structure. Calculate atomic radius and interplanar spacing of (1 1 0) plane.

Solution: (i) The effective number atoms per unit cell is given by $Z = \frac{\rho N_A a^3}{M}$

$$\therefore Z = \frac{8980 \text{ kg/m}^3 \times 6.02 \times 10^{26} / \text{k.mol} \times (3.61 \times 10^{-10} \text{ m})^3}{63.54 \text{ kg/k.mol}} = \frac{254.32}{63.54} = 4 \text{ atoms/unit cell.}$$

\therefore Copper exhibits FCC structure.

(ii) The lattice constant is related to the atomic radius in FCC structure through $a = 2\sqrt{2}r$

$$r = \frac{a}{2\sqrt{2}} = \frac{3.61 \text{ \AA}}{2 \times 1.4142} = 1.276 \text{ \AA}$$

(iii) The interplanar spacing is given by $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$d = \frac{3.61 \text{ \AA}}{\sqrt{1^2 + 1^2 + 0^2}} = 2.553 \text{ \AA}.$$

Example 26.7. A crystal with primitives 1.2 \AA , 1.8 \AA and 2 \AA has a plane (231) which cuts an intercept 1.2 \AA along x-axis. Calculate the intercepts along y- and z-axes.

Solution: Intercept on X-axis, $pa = 1.2 \text{ \AA}$

$$\therefore p = \frac{1.2 \text{ \AA}}{1.2 \text{ \AA}} = 1.$$

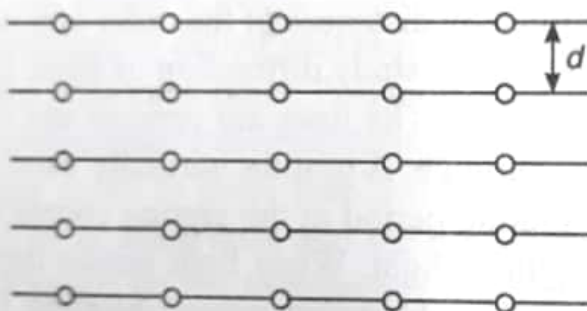
$$\text{L.C.M, } D = hp = 2 \times 1 = 2.$$

$$\therefore q = \frac{D}{k} = \frac{2}{3} \text{ and } r = \frac{D}{l} = \frac{2}{1}.$$

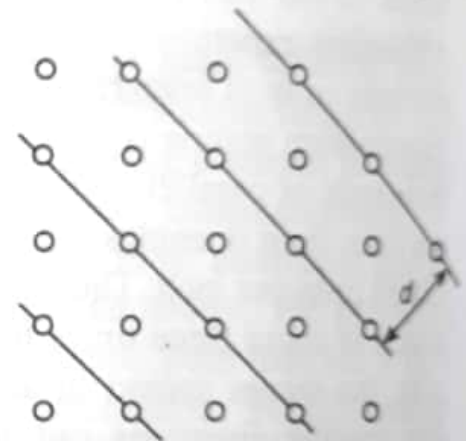
26.24 BRAGGS' LAW

In 1912 W.H.Bragg and W.L.Bragg discovered that X-rays can be regularly reflected by the cleavage planes of the crystals. The cleavage planes are successive atomic planes in the crystal (Fig. 26.48).

They are also known as Braggs' planes. Thus, a crystal may be regarded as consisting of a stack of several parallel planes of



(a)



(b)

Fig. 26.48. Two different sets of Bragg planes

atoms. Each plane in a given set has the same distribution of atoms. When an X-ray beam is incident on the crystal, each atom in the crystal scatters a portion of the incident beam. The scattered waves travel in all directions. It is convenient to consider the net scattering by atoms in terms of the diffraction (scattering) by the crystal planes. Each family of planes gives rise to scattering but only a certain family scatters constructively in a given direction. W.H.Bragg and W.L.Bragg derived a relation between the wavelength of X-rays and the angular positions of the scattered beam and the separation of atomic planes in the crystal.

Braggs made the following simplifications regarding the diffraction of X-rays from a crystal:

1. Any crystal may be viewed as a regular stack of atomic planes;
2. The atomic planes act like semitransparent mirrors for X-rays;
3. X-rays reflected from the successive atomic planes would interfere constructively or destructively depending upon the path difference between the rays;
4. Whenever the path difference between the rays is an integer multiple of wavelength (λ), the rays interfere constructively and produce a bright spot in that direction.

Thus, the complex phenomenon of diffraction of X-rays by the atoms was converted into the problem of reflection of X-rays by the parallel atomic planes. Hence, the words 'diffraction' and 'reflection' are mutually interchangeable in Braggs' treatment. Based on these considerations, Braggs derived a simple mathematical relationship that serves as a condition for the Bragg reflection to occur. This condition is known as Braggs' law.

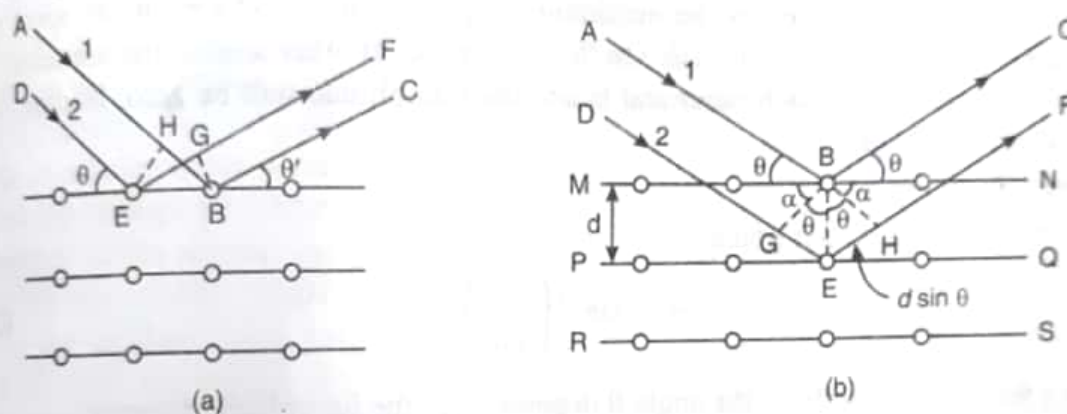


Fig. 26.49. Determination of path difference between X-rays diffracted by consecutive lattice planes

Let us consider a set of parallel atomic planes with interplanar spacing d . We represent the row of atoms as a single horizontal line, as shown in Fig. 26.49. Let a parallel beam of monochromatic X-rays of wavelength λ , represented by the parallel lines AB and DE, be incident on these planes at a glancing angle θ (Fig. 26.49 a). The scattered beam emerges along BC and EF. The contributions of two adjacent atoms in the same plane are considered in the Fig. 26.49 (a).

The rays BC and EF are coherent and reinforce each other, if they are in phase. It requires that the path lengths BK and EL are equal. They will be equal when $\theta = \theta'$. This is the condition of reflection.

We consider next the contributions of two adjacent atoms to the reflection from successive planes MN and PQ are considered (see Fig. 26.49 b). The path difference Δ between the reflected rays BC and EF is

$$\Delta = GE + EH \quad (26.35)$$

$$\angle ABG = \theta + \alpha = 90^\circ \quad (26.36)$$

$$\text{BE is normal to the plane MN. Therefore,} \quad (26.37)$$

$$\angle MBE = \alpha + \angle GBE = 90^\circ$$

From equ. (26.36) and (26.37) we get

$$\angle GBE = \theta$$

Similarly,

$$\angle EBH = \theta$$

In the $\triangle BGE$, $BE = d$

$$\therefore GE = d \sin \theta$$

Similarly, in the $\triangle EBH$, $EH = d \sin \theta$

$$\therefore \text{The path difference } \Delta = GE + EH = d \sin \theta + d \sin \theta = 2d \sin \theta \quad (26.38)$$

The rays BC and EF will constructively interfere only when $\Delta = m\lambda$, where $m = 1, 2, 3, \dots$

\therefore The condition for reinforcement of scattered waves is

$$2d \sin \theta = m\lambda \quad (26.39)$$

The above equation is called **Bragg's equation** or **Braggs' law**.

The meaning of the above equation is that the reinforcement of reflected waves will take place only at certain values of θ , corresponding to specific values of λ and d . In these directions the resultant wave has the maximum amplitude and produces bright spots on the photographic plate placed in their path. On the other hand, at other angles, the scattered waves may not be in phase with each other and hence their amplitude will be zero, leading to dark spots in those directions.

Order of reflection:

The reflection angle θ is given by

$$\theta = \sin^{-1} \left(\frac{m\lambda}{2d} \right) \quad (26.40)$$

For a fixed wavelength, λ , the angle θ depends d_{hkl} , the interplanar distance.

When the lattice planes of indices (hkl) give rise to x-ray reflection, the path difference between the rays reflected from successive planes is one wavelength. For example, if the reflection from (100) planes of the lattice occurs, say, at an angle θ_1 , then the path difference between the reflections will be λ and the order of reflection $m = 1$. When the path difference between the reflected rays is 2λ , the reflection will occur at an angle θ_2 and the Bragg equation is satisfied with $m = 2$. Thus, as θ is increased gradually, a number of positions will be found at which the reflections are intense. These positions correspond to $m = 1, 2, 3, \dots$ values. The diffraction lines appearing for $m = 1, 2$ and 3 are called first, second, third order diffraction lines respectively. Thus, m denotes the **order of reflection**. The highest possible order is determined by the condition that $\sin \theta$ cannot exceed unity.

If the value of θ is determined experimentally, and knowing the wavelength λ , the interplanar spacing ' d ' can be determined with the help of Bragg law.

Example 26.8. X-rays of unknown wavelength give first order Bragg reflection at glancing angle 20° with (212) planes of copper having FCC structure. Find the wavelength of X-rays if the lattice constant for copper is 3.615 \AA .

Solution: The interplanar spacing is given by $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$\therefore d = \frac{3.615 \text{ \AA}}{\sqrt{2^2 + 1^2 + 2^2}} = 1.205 \text{ \AA}.$$

According to Bragg's law

$$2d \sin \theta = m\lambda.$$

$$\lambda = \frac{2d \sin \theta}{m} = \frac{2 \times 1.205 \text{ \AA} \times \sin 20^\circ}{1} = 0.824 \text{ \AA}.$$

26.25 BRAGGS' SPECTROMETER

W.H. Bragg and W.L. Bragg devised an X-ray spectrometer in which a crystal is used as a reflection grating. It is used to measure glancing angle θ .

Construction: Bragg's spectrometer is very much similar in construction to the optical spectrometer. The schematic diagram of the Bragg's spectrometer is shown in Fig. 26.50. X-rays from an X-ray tube are collimated into a narrow beam by two slits S_1 and S_2 cut in lead plates. The beam is then allowed to

be incident at a glancing angle on the face of the crystal D , which is mounted in wax on the turntable of the spectrometer. The turntable is capable of rotation about a vertical axis passing through its center and the position of the crystal can be read from the circular scale, C . Most of the incident beam passes straight through the crystal. Some of the X-rays are however scattered by the regularly arranged atoms in different crystal planes. The scattered X-rays can be regarded as having been reflected from the

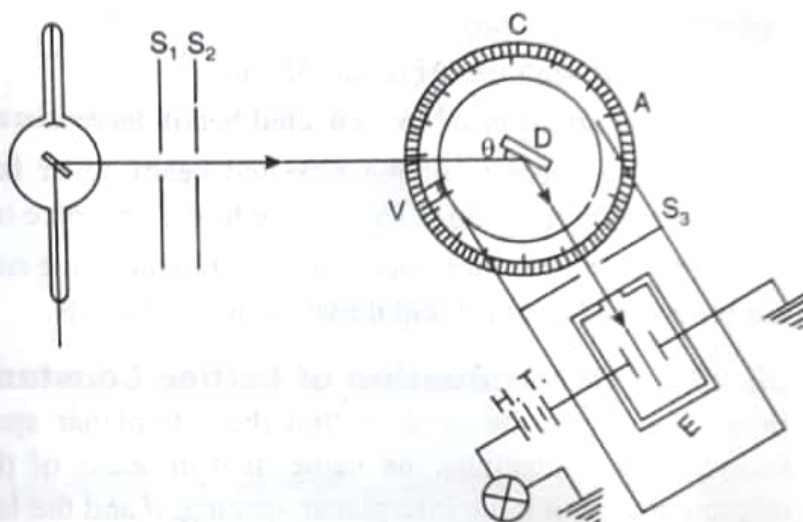


Fig. 26.50. The schematic diagram of the Bragg's spectrometer

crystal planes rich in atoms. The reflected X-ray beam enters an ionization chamber carried by the spectrometer arm, which is capable of rotation about the same axis as the turntable. The turntable and the arm are so linked together that when the turntable rotates through an angle θ , the arm turns through an angle 2θ . In this way, the X-ray beam is always reflected into the ionization chamber whatever its incidence angle is at the crystal face. The ionization current produced by the reflected beam is measured by a sensitive electrometer E or recorded on a photographic plate.

Working: Initially, the single crystal under investigation is mounted on the turntable such that the glancing angle $\theta = 0^\circ$ and the ionization chamber is adjusted to receive X-rays. Then the crystal is moved in small angles and the corresponding deflection obtained in the electrometer is noted down. A graph is plotted for glancing angle versus intensity of diffracted X-rays.

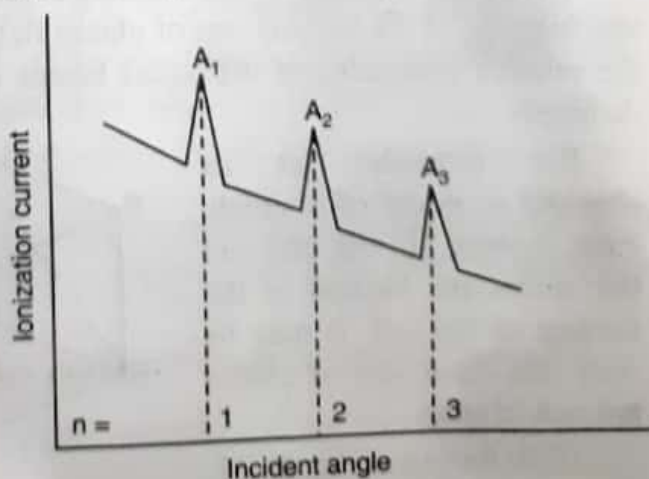


Fig. 26.51. A typical diffraction spectrum produced by a monochromatic X-rays scattered from a crystal.

X-ray spectrum: Fig. 26.51 shows a typical diffraction spectrum produced by a monochromatic X-rays scattered from a crystal. The diffraction spectrum is a graph plotted between the intensity of ionization and the glancing angle. It is seen from the graph that the intensity of ionization current increases abruptly for certain values of glancing angle. The peaks A_1, A_2, A_3 etc. in intensity occur whenever the Braggs' equation is satisfied. If θ_1, θ_2 and θ_3 are the angles of incidence where intense peaks occur, then they correspond to the different orders of reflection with $n = 1, 2$ and 3 respectively for a given wavelength. Using Braggs' law

$$2d \sin \theta_1 = \lambda, \quad 2d \sin \theta_2 = 2\lambda \quad \text{and} \quad 2d \sin \theta_3 = 3\lambda$$

That is, $2d \sin \theta_1 : 2d \sin \theta_2 : 2d \sin \theta_3 = \lambda : 2\lambda : 3\lambda$

$$\therefore \sin \theta_1 : \sin \theta_2 : \sin \theta_3 = 1 : 2 : 3 \quad (26.41)$$

The above ratio indicates that the peaks correspond to first, second and third order reflections respectively.

It may be seen from Fig. 26.51 that

- the intensity of the reflected beam decreases as the order of the spectrum increases.
- The intensity of the reflected beam never falls to zero. It reaches down only to a minimum value. This is due to the presence of continuous spectrum.

At a given time more than one set of planes give rise to reflections. Usually, the reflections are produced due to principal planes in the crystals.

26.25.1 Determination of Lattice Constant:

Bragg's law may be used to find the interplanar spacing, if the wavelength of X-rays is known. If we substitute the value of d in terms of the Miller indices of the planes in the relation connecting the interplanar spacing, d and the lattice constant, a , we can determine the lattice constant of the crystal. Thus, in case of a cubic crystal, the relation between d and a is given by

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (26.42)$$

Knowing the value of d , the lattice constant a can be calculated from the above equation.

26.25.2 Determination of Crystal Structure

The Braggs' method of determining crystal structure consists in finding out the interplanar spacing, d_{hkl} of the various sets of planes rich in atoms. From the knowledge of d_{hkl} and from the relative intensities of diffracted beams of different orders, the crystal structure can be deduced.

For example, let us consider a crystal of a simple cubic system. In the unit cell the atoms are located at the corners of the cell. It may be seen that three sets of planes are rich in atom.

(i) Referring to Fig. 26.52, we see that the set of planes ABFE, CDHG, ADHE, BCGF, ABCD and EFGH are all alike. Let the d_2 distance between the consecutive planes be d_1 . These planes are known as (100) planes.

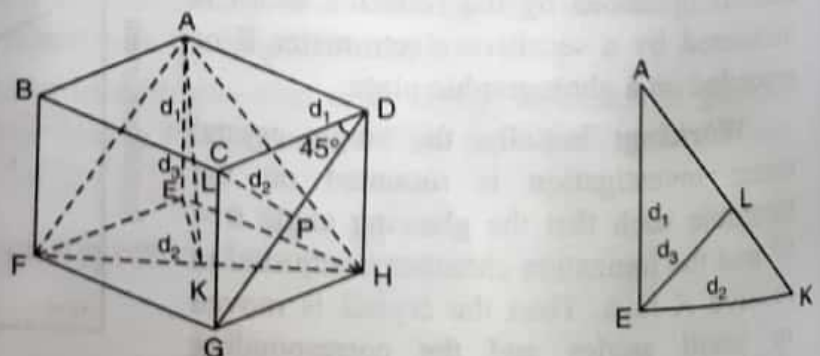


Fig. 26.52

(ii) The second set of planes consists of parallel planes like ADGF, inclined at an angle of 45° to the planes mentioned in (i). Let d_2 be the spacing between the second set of planes, as shown in Fig. 26.52 by CP. Note that a plane parallel to ADGF contains the line BC. Then, from the $\triangle CDP$, we find that

$$\frac{d_2}{d_1} = \sin 45^\circ = \frac{1}{\sqrt{2}}$$

$$\frac{d_2}{d_1} = \frac{1}{\sqrt{2}}$$

(26.43)

These planes are known as (110) planes.

(iii) The third set of planes consists of planes like AFH. Let us draw EK perpendicular to FH and join AK to complete the triangle AEK. The perpendicular EL denoted by d_3 represents the distance between the plane AFH and a parallel plane passing through E. In $\triangle AEK$, $AE = d_1$, $EK = d_2$ and $AK = \sqrt{d_1^2 + d_2^2}$. Further,

$$\sin A = \frac{d_3}{d_1} \quad \text{and also} \quad \sin A = \frac{d_2}{\sqrt{d_1^2 + d_2^2}}$$

$$\therefore d_3 = \frac{d_1 d_2}{\sqrt{d_1^2 + d_2^2}} = \frac{d_1 d_2}{\sqrt{2d_2^2 + d_2^2}} = \frac{d_1}{\sqrt{3}} \quad (26.44)$$

These planes are known as the (111) planes. The interplanar distances are in the ratio

$$d_1 : d_2 : d_3 = 1 : 1/\sqrt{2} : 1/\sqrt{3} \quad (26.45)$$

Using a KCl crystal, Bragg found the values of θ for reflections from the faces ABCD, ADGF and AHF respectively as

$$\theta_1 = 5^\circ 22', \theta_2 = 7^\circ 36' \quad \text{and} \quad \theta_3 = 9^\circ 25'.$$

Hence for the first order spectrum,

$$\begin{aligned} d_1 : d_2 : d_3 &= 1/\sin 5^\circ 22' : 1/\sin 7^\circ 36' : 1/\sin 9^\circ 25' \\ &= 1/0.0936 : 1/0.1323 : 1/0.1636 \\ &= 1/1 : 1/1.410 : 1/1.748 \end{aligned}$$

These ratios, within the limits of experimental error, are

$$d_1 : d_2 : d_3 = 1 : 1/\sqrt{2} : 1/\sqrt{3}$$

Hence it is concluded that KCl crystal has a simple cubic structure. On the other hand, NaCl crystal which is very much similar to KCl is found to have the ratio of interplanar distances as

$$d_1 : d_2 : d_3 = 1 : 1/\sqrt{2} : 2/\sqrt{3}$$

which agree with the theoretical values for a face centred cubic system. The observed dissimilarity between the conclusions on these similar crystals can be resolved once we determine the relative intensities of the diffracted beams. From such a study, it has been confirmed that both the KCl and NaCl crystals have face centred cubic crystal structure.