

Class  $\Rightarrow$  B.Sc (Part II) Subsidiary

Subject  $\Rightarrow$  Chemistry

Chapter  $\Rightarrow$  Solid State

Topic  $\Rightarrow$  No. of atoms in a cubic unit cell, Bragg's Equation.

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### NO. of atoms in a cubic unit cell

The number of atoms in a unit cell is calculated by considering the following facts.

- ① An atom at the corner of a cubic unit cell is shared by eight unit cells. Hence each atom contributes  $\frac{1}{8}$  to the cubic unit cell.
- ② An atom at the face is shared by two unit cells, contributing  $\frac{1}{2}$  to the cubic unit cell.
- ③ An atom within the body of the unit cell is shared by no other unit cell. Hence each atom contributes 1 to the cubic unit cell.
- ④ An atom present on the edge is shared by four unit cells. Hence, each atom on the edge contributes  $\frac{1}{4}$  to the cubic unit cell.

### Primitive (simple) cubic unit cell.

Each cubic unit cell has eight atoms on its corner and  $\frac{1}{8}$  of each atom belongs to that cell.

The no. of atoms in a primitive (simple) cubic unit cell =  $8 \times \frac{1}{8}$

$$= 1 \text{ atom.}$$

### Body-centered cubic unit cell

Each atom present at corner of the unit cell contributes  $\frac{1}{8}$  to the cell, whereas the atom present in the

(2)

body centre belongs completely to the unit cell, thus.

The no. of atoms present in a body-centered cubic unit cell is calculated as -

Eight atoms at the corners  $= 8 \times \frac{1}{8} = 1$  atom

Atoms at the body centre = 1 atom

$\therefore$  Number of atoms in a body-centered cubic unit cell  $= 1 + 1 = 2$  atoms.

### face-centered cubic unit cell

Each atom present at corner of the unit cell contributes  $\frac{1}{8}$  th to the cell, whereas the atom present in each face is shared by two adjacent unit cells and hence contributes  $\frac{1}{2}$  to each unit cell.

Thus, the no. of atoms present in a face-centered cubic unit cell is calculated as -

One atom at each corner  $= (8 \times \frac{1}{8} \text{ each}) = 1$  atom

Atoms at each of the six face centers  $= (6 \times \frac{1}{2} \text{ each})$

$= 3$  atoms.

$\therefore$  Number of atoms in a face-centered cubic unit cell  $= 1 + 3$  atoms  $= 4$  atoms.

### Calculation of mass of the unit cell

Mass of the unit cell is calculated from the number of atoms in the unit cell. To calculate mass of the unit cell, multiply the mass of one atom by the number of atoms in the unit cell.

Thus,

The Mass of one atom = Molar Mass of the substance / Avogadro's Number

(3)

## Bragg's Equation

Bragg's derived a mathematical relation to determine interatomic distances from x-rays diffraction patterns and this relation is called Bragg equation.

They showed that

- ① The x-ray diffracted from atoms in crystal planes obey the laws of reflection.
- ② The two rays reflected by successive planes will be in phase if the extra distance travelled by the second ray is an integral number of wavelengths.

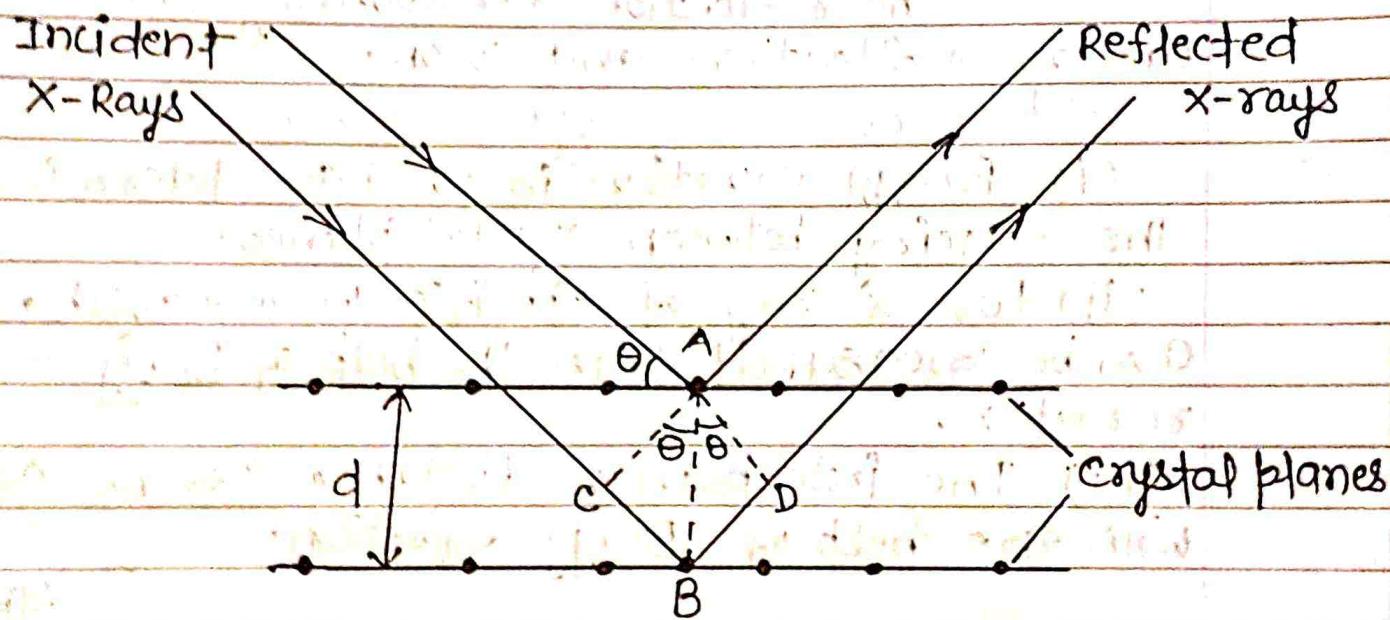


Fig:- Reflection of x-Rays from two different planes of a crystal

figure shows a beam of x-Rays falling on the crystal surface. Two successive atomic planes of the crystals are shown separated by a distance  $d$ . Let the x-rays of wavelength  $\lambda$  strike the first plane at an angle  $\theta$ . Some of the rays will be reflected at the same angle. Some of the rays will penetrate and get reflected from the second plane. These rays will reinforce those reflected from the first plane.

(4)

if the extra distance travelled by them ( $CB + BD$ ) is equal to integral number  $n$  of wave lengths.  
i.e.,

$$n\lambda = CB + BD \quad \text{--- (1)}$$

Geometry shows that,

$$CB = BD = AB \sin \theta \quad \text{--- (2)}$$

from (1) and (2) it follows that

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

$$\text{or } n\lambda = 2d \sin \theta$$

This is known as Bragg's equation.

The reflection corresponding to  $n=1$  (for a given series of planes) is called the first order reflection.

The reflection corresponding to  $n=2$  is the second order reflection and so on.

### Applications of Bragg's Equation

(i) Bragg equation is used for determination of the spacing between crystal planes.

(ii) for X-rays of specific wave length, the angle  $\theta$  can be measured with the help of Bragg X-ray spectrometer.

(iii) The interplanar distance can be calculated with the help of Bragg equation.