Solid

Unit Cell

The smallest repeating unit of the crystal lattice is the unit cell, the building block of a crystal. The unit cells which are all identical are defined in such a way that they fill space without overlapping. The 3D arrangement of atoms, molecules or ions inside a crystal is called a ***crystal lattice.*** It is made up of numerous unit cells. One of the three constituent particles (atoms, ions and molecule) takes up every lattice point.

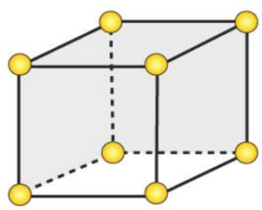
Types of Unit Cell

Numerous unit cells together make a crystal lattice. Constituent particles like atoms, molecules are also present. Each lattice point is occupied by one such particle.

1. ***Primitive Cubic Unit Cell***
2. ***Body-centered Cubic Unit Cell***
3. ***Face centered cubic unit cell***

1. Primitive Cubic Unit Cell

1. The atoms in the **primitive cubic unit cell** are present only at the corners
2. Every atom at the corner is shared among eight adjacent unit cells
3. Four unit cells are present in the same layer
4. Four unit cell in the upper/lower layer
5. Each small sphere in the following figure represents the center of a particle which occupies that particular position and not its size.



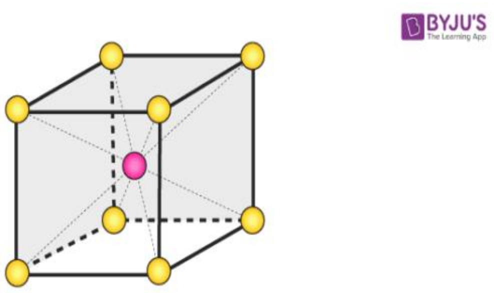
Simple cubic unit cell

In each cubic unit cell, there are 8 atoms at the corners. Therefore, the total number of atoms in one unit cell is

$$8 \times 1/8 = \mathbf{1\ atom}.$$

2. Body-centered Cubic Unit Cell (BCC)

1. **I**n BCC unit cell every corner has an atoms.
2. There is one atom present at the center of the structure
3. Below diagram is an open structure
4. According to this structure atom at the body centers wholly belongs to the unit cell in which it is present.



Body-centred Cubic Unit Cell (BCC)

In each BCC unit cell there are 8 atoms at the corner and 1 atom at the center, so

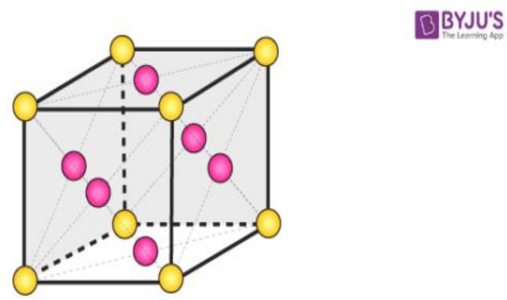
Atom at the corner = 8 × 1/8 = 1atom

Atom at the center = 1 atom

Total number of atom at BCC unit cell is 2.

3. Face-centered Cubic Unit Cell (FCC)

1. In FCC unit cell atoms are present in all the corners of the crystal lattice
2. Also, there is an atom present at the center of every face of the cube
3. This face-center atom is shared between two adjacent unit cells.



Face-centred Cubic Unit Cell (FCC)

In each face centered cubic unit cell, there are 8 atoms at the corner and 6 atoms at the faces so,

Atoms at corners = 8 × 1/8 = **1 atom**.

Atom at faces = 6 × 1/2 = **3 atom**.

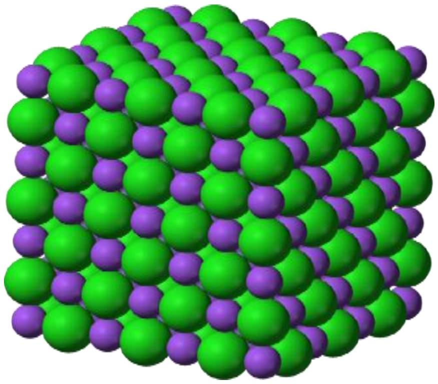
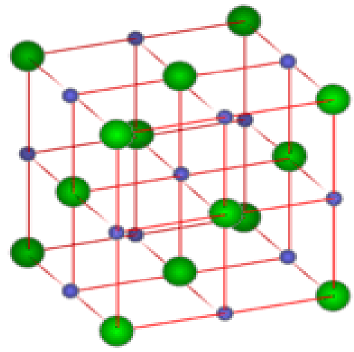
Total number of atom in FCC unit cell is 4.

Crystal structure of NaCl

Rock salt also known as NaCl is an ionic compound. It occurs naturally as white cubic crystals. The structure of NaCl is formed by repeating the unit cell. It has an organized structure and has a 1:1 ratio of Na:Cl. The structure of NaCl is formed by repeating the face centered cubic unit cell. It has 1:1 stoichiometry ratio of Na:Cl with a molar mass of 58.4 g/mol.

Structure

The smaller ions are the Na^+ with has an atomic radius of 102 pm, and the larger ions are the Cl^- with an atomic radium of 181 pm. Since NaCl are one to one ratio as a compound, the coordination numbers of Na and Cl are equal. The larger green ions represent Cl^- and the smaller purple ions represent Na^+. However, the structure of this molecule allows their positions to be switched since the coordination numbers are equivalent.

1- Chloride ions are present at the corners and at the center of each face of the cube.

   Chloride ions at corner of unit cell = 1/8 × 8 = 1

   Chloride ions at faces = 6 × 1/2 = 3

   Total chloride ions in a unit cell is 4.

2- Sodium ions are so located that there are six chloride ions around it. Sodium ions are present at edge center and body center.

   Sodium ions at edges of unit cell = 12 × 1/4 = 3

   Sodium ion at the center of unit cell is = 1

   Total sodium ions in a unit cell is 4.

3- Each sodium ion is surrounded by 6 chlorides ions and vice versa. So the coordination number of Na and Cl are six.

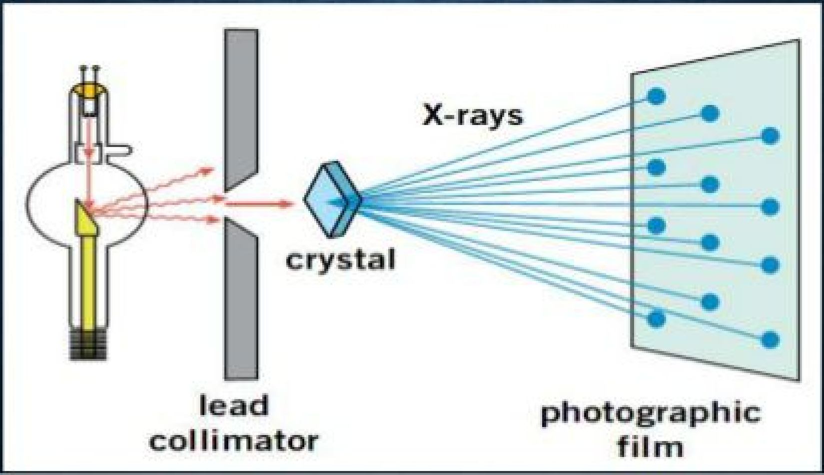
4- The structure of sodium chloride consists of eight ions a unit cell, four are Na^+ ions and the other four are Cl^- ions. So 4 NaCl are present in one unit cell.

X- ray diffraction

- X-ray crystallography works based on **X-ray diffraction** principle: It means that scattering of x-ray by crystal.

X-ray diffraction is based on constructive

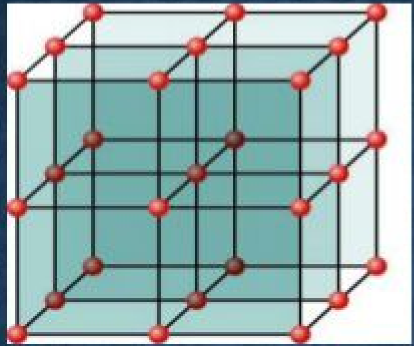
interference of monochromatic X rays and crystalline sample.



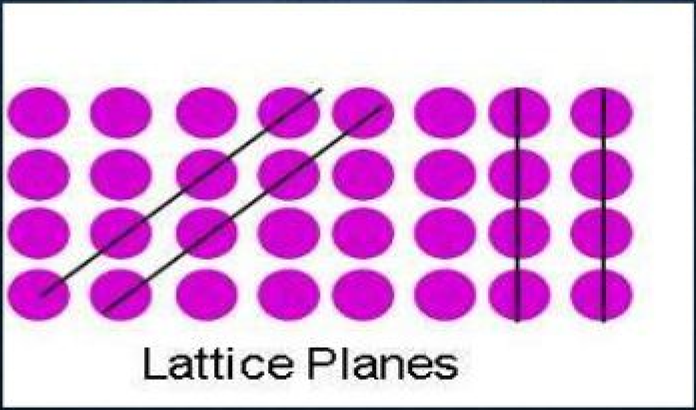
BRAGG'S LAW

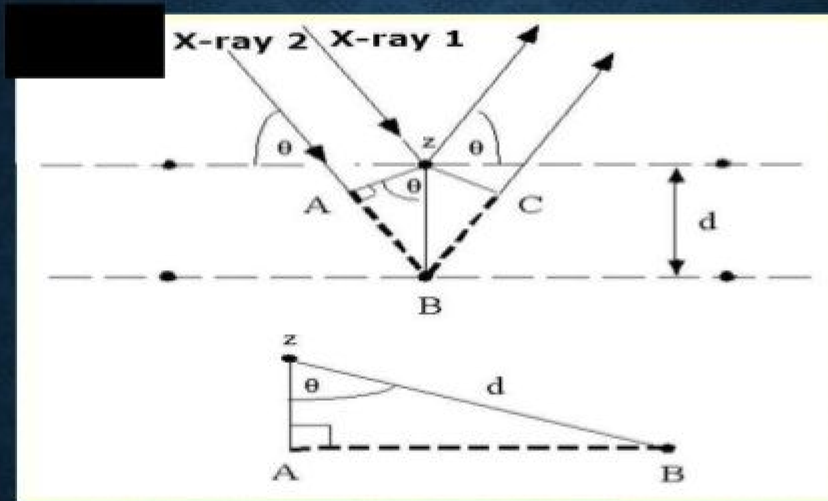
- Diffraction occurs only when Bragg's Law is satisfied.
- Bragg law identifies the angles of the incident radiation relative to the lattice planes for which diffraction peaks occurs.
- Bragg derived the condition for constructive interference of the X-rays scattered from a set of parallel lattice planes.
- When the X-rays strike a layer of a crystal, some of them will be reflected. These two x-ray beams travel slightly different distances.
- Connecting the two beams with perpendicular lines shows the

  difference between the top and the bottom beams.
- For a crystalline solid, the waves are scattered from lattice planes separated by the inter planar distance *d*.
- When the scattered waves interfere constructively, they remain in phase since the difference between the path lengths of the two waves is equal to an integer multiple of the wavelength.
- The path difference between two waves undergoing interference is given by $2d\sin\theta$, where θ is the scattering angle.



crystal





THE LENGTH AB IS THE SAME AS BC SO THE TOTAL DISTANCE TRAVELED BY THE BOTTOM WAVE IS EXPRESSED BY:

$$AB = D \sin\Theta$$

$$BC = D \sin\Theta$$

$$AB + BC = 2D \sin\Theta$$

$$N\Lambda = 2D \sin\Theta$$

CONSTRUCTIVE INTERFERENCE OF THE RADIATION FROM SUCCESSIVE PLANES OCCURS WHEN THE PATH DIFFERENCE IS AN INTEGRAL NUMBER OF WAVE LENGTHS. THIS IS THE BRAGG LAW.

4. POWDER CRYSTAL METHOD

- When an X-ray is shined on a crystal, it diffracts in a pattern characteristic of the structure. In powder X-ray diffraction, the diffraction pattern is obtained from a powder of the material.
- Powder diffraction is often easier and more convenient than single crystal diffraction since it does not require individual crystals be made. Powder X-ray diffraction (XRD) also obtains a diffraction pattern for the bulk material of a crystalline solid, rather than of a single crystal.

Powder crystal method