## Elements of Crystallography

## Introduction

The matter is usually regarded to exist in solid state or fluid state. All the materials are composed of atoms and molecules. A solid is an essentially an ordered array of atoms, bound together by electric forces to form a very large molecule. There are three different types of solids. Crystalline, poly crystalline and amorphous.

In a crystal, atoms are arranged into a regular periodically repeated structure that extends throughout the whole sample. The atoms are said to have long range order. Poly crystalline material is composed of many small crystals or grains of somewhat irregular size. In an amorphous solid a long range order is absent. (i.e.,) they have short range order. There is no periodicity in which atoms are arranged in space. They are also regarded as super cooled liquids.
Examples : metallic crystals : copper, silver, aluminum etc.,
Non metallic crystals: Germanium, silicon
Amorphous or non crystalline materials: glass, rubber, plastic


Difference between crystalline and amorphous material.

| S.No | Crystalline | Amorphous |
| :--- | :--- | :--- |
| $\mathbf{1}$ | Regular arrangement of atoms <br> gives definite and geometric shape. | Random arrangement of atoms does not <br> give definite and Geometrical shape. |
| $\mathbf{2}$ | They are anisotropic | They are isotropic |
| $\mathbf{3}$ | They have sharp Melting Point | They do not have sharp Melting Point |
| $\mathbf{4}$ | They possess internal symmetry | They do not possess internal symmetry |

Crystal Physics' or 'Crystallography' is a branch of physics that deals with the study of all possible types of crystals and the physical properties of crystalline solids by the determination of their actual structure by using X-rays, neutron beams and electron beams.

## CLASSIFICATION OF SOLIDS

Solids can broadly be classified into two types based on the arrangement of units of matter.
The units of matter may be atoms, molecules or ions.
They are,

- Non-crystalline (or) Amorphous solids


## CRYSTALLINE SOLIDS

- A substance is said to be crystalline when the arrangement of units of matter is regular and periodic.
- A crystalline material has directional properties and therefore called as anisotropic substance.
- A crystal has a sharp melting point.
- It possesses a regular shape and if it is broken, all broken pieces have the same regular shape.
- A crystalline material can either be a single (mono) crystal or a polycrystal.
- A single crystal consists of only one crystal, whereas the polycrystalline material consists of many crystals separated by well-defined boundaries.
- Examples
- Metallic crystals - $\mathrm{Cu}, \mathrm{Ag}, \mathrm{Al}, \mathrm{Mg}$ etc,
- Non-metallic crystals - Carbon, Silicon, Germanium,
- In amorphous solids, the constituent particles $t$ arranged in an orderly manner. They are randomly distributed.
- They do not have directional properties and so they are called as 'isotropic' substances.
- They have wide range of melting point and do not possess a regular shape.
- Examples: Glass, Plastics, Rubber etc.,
- SPACE LATTICE
- A lattice is a regular and periodic arrangement of points in three dimensions.
- It is defined as an infinite array of points in three dimensions in which every point has surroundings identical to that of every other point in the array.
- The Space lattice is otherwise called the Crystal lattice

- Consider the points $\mathrm{P}, \mathrm{Q}$ and R .
- Let us join the points P and Q by a straight line, and the point P and R by another straight line.
- The line PQ is taken as X -axis and the line PR is taken as Y -axis.
- The distance between any two successive lattice points in the X-direction is taken as `a'.
- Similarly, the distance between any two successive lattice points along the Y-direction is taken as ' $b$ '.
- Here a and b are said to be lattice translational vectors. Consider a square lattice in which $\mathrm{a}=\mathrm{b}$.
- Consider two sets of points $\mathrm{A}, \mathrm{B}, \mathrm{C}, \mathrm{D}, \mathrm{E}, \mathrm{F}$ and $\mathrm{A}^{\prime}, \mathrm{B}^{\prime}, \mathrm{C}^{\prime}, \mathrm{D}^{\prime}, \mathrm{E}^{\prime}, \mathrm{F}^{\prime}$.
- In these two sets, the surrounding environment looks symmetrical; i.e. the distances AB and $\mathrm{A}^{\prime} \mathrm{B}^{\prime}, \mathrm{AC}$ and $\mathrm{A}^{\prime} \mathrm{C}^{\prime}, \mathrm{AD}$ and $\mathrm{A}^{\prime} \mathrm{D}^{\prime}, \mathrm{AE}$ and $\mathrm{A}^{\prime} \mathrm{E}^{\prime}$ and AF and $\mathrm{A}^{\prime} \mathrm{F}^{\prime}$ are equal.
- Therefore, in the arrangement of points, if the surrounding environment looks the same when the arrangement is viewed from different lattice points, then that arrangement is said to be a space lattice.
- BASIS:
- A crystal structure is formed by associating every lattice point with an unit assembly of atoms or molecules identical in composition, arrangement and orientation. This unit assembly is called the 'basis'.
* When the basis is repeated with correct periodicity in all directions, it gives the actual crystal structure. The crystal structure is real, while the lattice is imaginary.

CRYSTAL STRUCTURE


## UNIT CELL:

A unit cell is defined as a fundamental building block of a crystal structure, which can generate the complete crystal by repeating its own dimensions in various directions.
CRYSTALLOGRAPHIC AXES:

* Consider a unit cell consisting of three mutually perpendicular edges OA, OB and OC as shown in figure.
* Draw parallel lines along the three edges.
* These lines are taken as crystallographic axes and they are denoted as $\mathrm{X}, \mathrm{Y}$ and Z axes.



## LATTICE PARAMETERS

Consider the unit cell as shown in figure. Let OA, OB and OC are the intercepts made by the unit cell along $\mathrm{X}, \mathrm{Y}$ and Z axes respectively.

* These intercepts are known as primitives. In crystallography the intercepts OA, OB and OC are represented as $\overrightarrow{\mathrm{a}, \mathrm{b}}$ and c .
The angle between X and Y axes is represented as $\gamma$.
* Similarly the angles between Y and Z and Z and X axes are denoted by ' $\alpha^{\prime}$ and ' $\beta^{\prime}$ respectively as shown in the above figure. These angles $\alpha, \beta$ and $\gamma$ are called as interaxial angles or interfacial angles.
* To represent a lattice, the three interfacial angles and their corresponding intercepts are essential. These six parameters are said to be lattice parameters.


## PRIMITIVE CELL:

* It is the smallest unit cell in volume constructed by primitives. It consists of only one full atom
A primitive cell is one, which has got the points or atoms only at the corners of the unit cell. If a unit cell consists of more than one atom, then it is not a primitive cell.
Example for primitive cell: Simple Cubic unit cell.
Examples for non-primitive cell: BCC and FCC unit cell.


## CRYSTALS SYSTEMS:

* A three dimensional space lattice is generated by repeated translation of three translational vectors $\mathrm{a}, \mathrm{b}$ and c
* Crystals are grouped under seven systems on the basis of the shape of the unit cell
* The seven crystal systems are distinguished from one another by their lattice parameters. The seven systems are,

1. Cubic 2. Tetragonal 3. Orthorhombic 4.Trigonal (rhombohedral) 5. Hexagonal 6. Monoclinic and 7. Triclinic
The space lattices formed by unit cells are marked by the following symbols.

* Primitive lattice: $\mathrm{P} \rightarrow$ having lattice points only at the corners of the unit cell.
* Body centred lattice: $\mathrm{I} \rightarrow$ having lattice points at the corners as well as at the body centre of the unit cell.
* Face centred lattice: $\mathrm{F} \rightarrow$ having lattice points at the corners as well as at the face centres of the unit cell.
* Base centred lattice: $\mathrm{C} \rightarrow$ having lattice points at the corners as well as at the top and bottom base centres of the unit cell.


## BRAVAIS LATTICES

Bravais in 1948 showed that 14 types of unit cells under seven crystal systems are possible. They are commonly called as `Bravais lattices'
S.No. Crystal system Axial length Interfacial angles Example

| 1. | Cubic | $\mathrm{a}=\mathrm{b}=\mathrm{c}$ | $\alpha=\beta=\gamma=90^{\circ}$ | $\mathrm{NaCl}, \mathrm{CaF}_{2}, \mathrm{Au}, \mathrm{Cu}$ |
| :---: | :---: | :---: | :---: | :---: |
| 2. | Tetragonal | $a=b \neq c$ | $\alpha=\beta=\gamma=90^{\circ}$ | Ordinary white, tin, |
|  |  |  |  | Indium, $\mathrm{SnO}_{2}$ |
| 3. | Orthorhombic | $a \neq b \neq c$ | $\alpha=\beta=\gamma=90^{\circ}$ | Sulphur, Topaz, BaSO4, |
|  |  |  |  | KNO3 |
| 4. | Monoclinic | $a \neq b \neq c$ | $\alpha=\beta=90^{\circ} ; \gamma \neq$ | Na2So4, FeSo4, Gypsum |
|  |  |  | $90^{\circ}$ |  |

$$
\begin{array}{ll}
\alpha \neq \beta \neq \gamma \neq 90^{\circ} & \text { CuSo4, K2Cr2O7 } \\
\alpha=\beta=\gamma \neq 90^{\circ} & \text { Calcite, } \mathrm{Sb}, \mathrm{Bi} . \\
\alpha=\beta=90^{\circ} ; & \text { Quartz, } \mathrm{Zn}, \mathrm{Mg} .
\end{array}
$$

6. Rhombohedral $\mathrm{a}=\mathrm{b}=\mathrm{c}$
7. Hexagonal $a=b \neq c$

MILLER INDICES: The crystal lattice may be regarded as made up of an infinite set of parallel equidistant planes passing through the lattice points which are known as lattice planes. Miller indices are defined as the reciprocals of the intercepts made by the plane on the three crystallographic axes. In simple terms, the planes passing through lattice points are called 'lattice planes’.

- For a given lattice, the lattice planes can be chosen in a different number of ways.
- The orientation of planes or faces in a crystal can be described in terms of their intercepts on the three axes. Miller introduced a system to designate a plane in a crystal.
- He introduced a set of three numbers to specify a plane in a crystal.
- This set of three numbers is known as 'Miller Indices' of the concerned plane.
- Miller indices are set of three possible integers represented as (h, k, l) which is used to designate plane in the crystal, is the reciprocal of the intercept made by the planes on the crystallographic axes.



## Procedure for finding Miller Indices

Step 1: Determine the intercepts of the plane along the axes $X, Y$ and $Z$ in terms of the lattice constants a,b and c.
Step 2: Determine the reciprocals of these numbers.
Step 3: Find the least common denominator ( $l c d$ ) and multiply each by this $l c d$.
Step 4: The result is written in parenthesis. This is called the 'Miller Indices' of the plane in the form (h k l). This is called the `Miller Indices' of the plane in the form (hkl).


Plane ABC has intercepts of 2 units along X -axis, 3 units along Y -axis and 2 units along Z-axis.

## DETERMINATION OF 'MILLER INDICES'

Step 1: The intercepts are 2,3 and 2 on the three axes.
Step 2: The reciprocals are $1 / 2,1 / 3$ and $1 / 2$.
Step 3: The least common denominator is ' 6 '. Multiplying each reciprocal by
lcd, we get 3,2 and 3 .
Step 4: Hence Miller indices for the plane ABC is (3 23 )

## IMPORTANT FEATURES OF MILLER INDICES

For the cubic crystal especially, the important features of Miller indices are,

* A plane which is parallel to any one of the co-ordinate axes has an intercept of infinity ( $\infty$ ). Therefore the Miller index for that axis is zero; i.e. for an intercept at infinity, the corresponding index is zero.

EXAMPLE ( 100 ) plane (Plane parallel to $Y$ and $Z$ axes)

In the above plane, the intercept along X axis is 1 unit.


* The plane is parallel to $Y$ and $Z$ axes. So, the intercepts along $X$ and $Z$ xixes are ' $\infty$ '.
* Now the intercepts are $1, \infty$ and $\infty$.
* The reciprocals of the intercepts are $=1 / 1,1 / \infty$ and $1 / \infty$.
* Therefore the Miller indices for the above plane is (100).


## 1. Body centered cubic structure (BCC):



## 2. Face centered cubic structure (FCC):



## Properties of the Unitcell (Cubic)

1. Volume of a unit cell:

The general expression for finding the volume a unit cell is
$\left.V=a b c 1-\cos ^{2} \alpha-\cos ^{2} \beta-\cos ^{2} \gamma+2 \cos \alpha \cos \beta \cos \gamma\right]^{1}$
Where a,b,c, $\alpha, \beta$ and $\gamma$ are called lattice parameters.
For cubic system $a=b=c$ and $\alpha=\beta=\gamma=90^{\circ}$.
Therefore $V=a^{3}$.

## 2. Co-ordination number:

It is the number of nearest neighbors directly surrounding a given atom well within a crystal.
The co-ordination number for an atom in simple cubic structure is $=6$
The co-ordination number for an atom in body centered cubic structure is $=8$
The co-ordination number for an atom in face centered cubic structure is $=12$

## 3. Number of atoms per unit cell:

In a unit cell atoms are at the corners, at the center of the faces and at the center of the body.
An atom situated at the corner share $1 / 8^{\text {th }}$ part to a unit cell.
An atom situated at the face share $1 / 2$ part to a unit cell.
An atom situated at the center of the body share one full part to a unit cell.

1. In a simple cubic structure there are 8 corner atoms.
$\therefore$ Total share of all the corner atoms/unit cell $=(1 / 8) \times 8=1$
$\therefore$ The number of atoms/unit cell in simple cube $=1$
2. In a body centered cubic structure there are 8 corner atoms and an atom at the center of the unit cell.
$\therefore$ Total share of all the corner atoms per unit cell $=(1 / 8) \times 8=1$
The share of an atom at the center of the body $=1$
$\therefore$ The number of atoms per unit cell in body centered cube $=1+1=2$
3. In a face centered cubic structure there are 8 corner atoms and 6 face centered atoms in a unit cell.
$\therefore$ total share of atoms at the corner/unit cell= $(1 / 8) \times 8=1$
Total share of atoms at all the faces/unit cell $=(1 / 2) \times 6=3$
$\therefore$ The number of atoms/unit cell in face centered cube $=1+3=4$

## 4. Atomic packing factor (APF)

The fraction of the space occupied by atoms in a unit cell is known as atomic packing factor. It is the ratio of the total volume occupied by the atoms in the unit cell to the total available volume of the unit cell.

1. Simple cubic structure (SC):

There is only one lattice point at each of the eight corners of the unit cell. In a simple cubic structure an atom is surrounded by six equidistant neighbours. Hence the co-ordination number is 6 . Since each atom in the corner is shared by 8 unit cells, the total number of atoms in one unit cell is $(1 / 8) \times 8=1$

The nearest neighbour distance ' 2 r ' is the distance between the centers of two nearest neighbouring atoms.

The nearest neighbour distance $2 \mathrm{r}=\mathrm{a}$
The number of lattice points per unit cell $=1$
Volume of all the atoms in a unit cell $\mathrm{v}=\frac{4}{3} \pi \mathrm{r}^{3}$
Volume of unit cell $=\mathrm{V}=\mathrm{a}^{3}=(2 \mathrm{r})^{3}$

$$
\text { v } \quad 4 \pi r \quad \pi
$$

Packing factor is P.F $=\frac{}{V}=\frac{}{3 \times 8 r^{3}}=\frac{}{6}=0.52=52 \%$
2. Body centered cubic structure (BCC): In a BCC structure eight atoms are present at eight corners and one atom is at the center. The co-ordination number is 8 . The number of atoms per unit cell is $=[(1 / 8) \times 8]+1=2$

The lattice constant is
$(A B)^{2}=a^{2}+a^{2}=2 a^{2}$
$(\mathrm{AC})^{2}=(\mathrm{AB})^{2}+(\mathrm{BC})^{2}$
$(4 r)^{2}=2 a^{2}+a^{2}=3 a^{2}$
Lattice constant $a=4 \mathrm{r} / \sqrt{ } 3$
Volume of all the atoms per unit cell $\mathrm{v}=2 \times\binom{\left(\frac{4}{-} \pi r^{3}\right)}{3}$
Volume of the unit cell $\mathrm{V}=\mathrm{a}^{3}=\frac{64 r^{3}}{3 \sqrt{3}}$
Atomic packing factor $=\frac{\mathrm{v}}{\mathrm{V}}=\frac{8 \pi r^{3} \times 3 \sqrt{3}}{3 \times 64 r^{3}}=\frac{3 \pi}{8}=0.68=68 \%$

## 3. Face centered cubic structure (FCC):

In a FCC structure eight atoms are at the corners of the unit cell and six atoms are present at the center of the six faces. The center atom is surrounded by 12 points. The co-ordination number is 12 . Each corner atom is shared by 8 unit cells and the face centered atom is shared by 2 surrounding unit cells.
$\therefore$ The number of atoms per unit cell is $=\frac{1}{8} \times 8+6 \times \frac{1}{2}=4$
Atomic radius of face centered cube
$\mathrm{AB}=4 \mathrm{r}$
$(\mathrm{AB})^{2}=\mathrm{a}^{2}+\mathrm{a}^{2}$
$(4 \mathrm{r})^{2}=2 \mathrm{a}^{2}$
Lattice Constant $\mathrm{a}=\frac{4 r}{\sqrt{2}}$


Nearest neighbor distance $2 \mathrm{r}=\frac{a \sqrt{2}}{2}$
Volume of all the atoms in unit cell $\mathrm{v}=4 *(4 / 3) \pi r^{3}$
Volume of unit cell $V=a^{3}=64 r^{3} / 2 \sqrt{ } 2$
$\therefore$ The packing factor $=\mathrm{v} / \mathrm{V}=\sqrt{ } 2 \pi / 6=74 \%$

| Parameters | SC | BCC | FCC |
| :--- | :--- | :--- | :--- |
| Co-ordination number | 6 | 8 | 12 |
| Atomic Radius (r) | $a / 2$ | $\sqrt{ } 3 a / 4$ | $\sqrt{ } 2 a / 4$ |
| Atoms per unit cell | 1 | 2 | 4 |
| Atomic packing factor | $\pi / 6$ | $3 \pi / 8$ | $2 \pi / 6$ |
|  |  |  |  |

## HEXAGONAL CLOSED PACKED STRUCTURE



- It consists of three layers of atoms.
- The bottom layer has six corner atoms and one face centred atom.
- The middle layer has three full atoms.
- The upper layer has six corner atoms and one face centred atom.
- Each and every corner atom contributes $1 / 6$ of its part to one unit cell.
- The number of total atoms contributed by the corner atoms of both top and bottom layers is $1 / 6 \times 12=2$.
- The face centred atom contributes $1 / 2$ of its part to one unit cell.
- Since there are 2 face centred atoms, one in the top and the other in the bottom layers, the number of atoms contributed by face centred atoms is $1 / 2 \times 2=1$.
- Besides these atoms, there are 3 full atoms in the middle layer.
- Total number of atoms present in an HCP unit cell is
$2+1+3=6$.


## CO-ORDINATION NUMBER (CN)

- The face centered atom touches 6 corner atoms in its plane.
- The middle layer has 3 atoms.
- There are three more atoms, which are in the middle layer of the unit cell.
- Therefore the total number of nearest neighbours is $6+3+3=12$.


## ATOMIC RADIUS (R)

- Consider any two corner atoms.
- Each and every corner atom touches each other. Therefore $\mathrm{a}=2 \mathrm{r}$. i.e., The atomic radius, $\quad \mathrm{r}=\mathrm{a} / 2$


## Bragg's Law:

Consider a set of parallel planes called Bragg's planes. Each atom is acting as a scattering center. The intensity of the reflected beam at certain angles will

bemaximum when the path difference between two reflected waves from two adjacent planes is an integral multiple of $\lambda$.
Let‘d' be the distance between two adjacent planes, ' $\lambda$ ' be the wavelength of the incident x-ray, ' $\theta$ ' be the glancing angle. The path difference between the rays reflected at $\mathrm{A} \& \mathrm{~B}$ is given by

$$
\begin{aligned}
& =C B+B D \\
& =d \sin \theta+d \sin \theta=2 d \sin \theta
\end{aligned}
$$

For the reflected light intensity to be maximum, the path difference $2 \mathrm{~d} \sin \theta=\mathrm{n} \lambda$, where ' $n$ ' is the order of scattering. This is called Bragg's law.

## Bragg's x-ray spectrometer:

The schematic diagram of Bragg's x-ray spectrometer is shown in fig. It is used to determine lattice constant and inter-planar distance‘d’. It has 1) x-ray source 2) A Crystal fixed on a circular table provided with scale and vernier. 3) Ionization chamber.


BRAGG'S X-RAY SPECTROMETER
A collimated beam of x-rays after passing the slits $S_{1}$ and $S_{2}$ is allowed to fall on a crystal $C$ mounted on a circular table. The table can be rotated about vertical axis. Its position can be measured by vernier $\mathrm{V}_{1}$. An ionization chamber is fixed to the longer arm attached to the table. The position of which is measured by vernier $\mathrm{v}_{2}$. An electrometer is connected to the ionization chamber to measure the ionization current produced by diffracted x-rays from the crystal. $\mathrm{S}_{3}$ and $\mathrm{S}_{4}$ are the lead slits to limit the width of the diffracted beam. Here we can measure the intensity of the diffracted beam.

If x-rays incident at an angle ' $\theta$ ' on the crystal, then reflected beam makes an angle $2 \theta$ with the incident beam. Hence the ionization chamber can be adjusted to get the reflected beam till the ionization current becomes maximum.

A plot of ionization current for different incident angles to study the x-ray diffraction spectrum is shown in fig.


VARIATION OF IONIZATION CURRENT

The rise in Ionization current for different values of ' $\theta$ ' shows that Bragg's law is satisfied for various values of ' $n$ '. i.e. $2 d \sin \theta=\lambda$ or $2 \lambda$ or $3 \lambda$ etc. Peaks are observed at $\theta_{1}, \theta_{2}, \theta_{3}$ etc. with intensities of $\mathrm{P}_{1}, \mathrm{P}_{2}, \mathrm{P}_{3}$ etc.
i.e. $2 d \sin \theta_{1}: 2 d \sin \theta_{2}: 2 d \sin \theta_{3}=\lambda: 2 \lambda: 3 \lambda$

The crystal inter-planer spacing 'd' can be measured using $2 d \sin \theta=\mathrm{n} \lambda$ If $d_{1}, d_{2}, d_{3}$ be the inter-planar spacing for the planes (100), (110) \& (111) respectively.
It can be shown -
For cubic crystal: $\mathrm{d}_{1}: \mathrm{d}_{2}: \mathrm{d}_{3}=1: \frac{1}{\sqrt{2}}: \frac{1}{\sqrt{3}}$
For FCC

$$
: \quad \mathrm{d}_{1}: \mathrm{d}_{2}: \mathrm{d}_{3}=1: \frac{1}{\sqrt{2}}: \frac{2}{\sqrt{3}}
$$

For BCC

$$
: \quad \mathrm{d}_{1}: \mathrm{d}_{2}: \mathrm{d}_{3}=1: \frac{2}{\sqrt{2}}: \frac{1}{\sqrt{3}}
$$

METALS, SEMICONDUCTORS AND INSULATORS

| S.No | Conductors | Semiconductors | Insulators |
| :---: | :---: | :---: | :---: |
| 1 | Easily conducts the electrical current. | Conducts the electric current less than conductor and greater than insulator. | Does not conduct any current. |
| 2 | Has only one valence electron in its outermost orbit. | Has four valence electron in its outermost orbit. | Has eight valence electron in its outermost orbit. |
| 3 | Conductor formed using metallic bonding. | Semiconductors are formed due to covalent bonding. | Insulators are formed due to ionic bonding. |
| 4 | Valence and conduction bands are overlapped. | Valence and conduction bands are separated by forbidden energy gap of 1.1 eV . | Valence and conduction bands are separated by forbidden energy gap of 6 to 10 eV . |
| 5 | Resistance is very small | Resistance is high | Resistance is very high |
| 6 | It has positive temperature coefficient | It has negative temperature coefficient | It has negative temperature coefficient |
| 7 | Ex: copper,aluminium,etc | Ex: silicon, germanium, etc | Ex: Mica, Paper, etc |

## Energy Bands in Solids:

The electrons of an isolated atom have discrete energy levels. When a large number of atoms are brought closer, then the valence electrons of all these atoms interact with each other. Due to this, the discrete energy levels of all the valence electrons of all these atoms come very close to each other. These closely spaced energy levels form the Energy Bands.
Consider a Silicon Crystal with N -atoms.


The electronic configuration of $\mathbf{S i}(\mathbf{z}=\mathbf{1 4})$ is $1 s^{2} 2 s^{2} 2 p^{6} 3 s^{2} 3 p^{2}$. In this case, the 1st and 2 nd orbits are completely filled with electrons. Here 3 S subshells is completely filled with 2 electrons whereas 3 p subshell contains only 2 electrons. However, it can accommodate 6 electrons.
In Silicon Crystal, there are $\mathbf{1 4 N}$ electrons (or 14 N Energy Levels). In this case, the 1 st and 2 nd orbits are completely filled with energy levels. Here 3 s subshell is completely filled with 2 N energy levels whereas the 3 p subshell contains only 2 N Energy levels. However, it can accommodate 6 N energy levels.

## Let us discuss the different situations-

- If the interatomic distance of the atom is very large (i.e. $\mathrm{r}=\mathrm{d}$ ), then there is no interatomic interaction.
- When the interatomic distance is equal to ' $c$ ', the interactions between the valence electrons of various Silicon atoms becomes appreciable.
- When the interatomic distance is equal to ' $b$ ', the energy gap between 3 s and 3 p levels completely disappears. Now the energy levels of 3 s subshell and 3p
subshell mix with each other. In such a situation, it is not possible to distinguish between the electrons belonging to 3 s and 3 p subshell. We can only say that there are 8 N energy levels in which 4 N energy levels are filled and 4 N energy levels are empty.
- When the interatomic distance ' $r$ ' is equal to ' $a$ ', (the actual interatomic distance in the crystal), then the energy band containing 4 N filled energy levels is separated from the energy band which contains 4 N empty energy levels. The energy gap between the filled energy band and the empty energy band is called the forbidden gap. The lower completely filled band is called the valence band and the upper unfilled band is called the conduction band.


## Introduction to X-ray

X rays, which were first discovered in 1901, have revolutionized modern medicine. Wilhelm Conrad Röntgen, a German physicist, was even given the Nobel Prize for his discovery of electromagnetic radiation. An X-ray is a painless, rapid exam that creates images of the inside components of your body, notably your bones. X -rays are electromagnetic radiation that can see through a person's skin and provide images of the bones beneath it. Technology advancements have resulted in more powerful and focussed X-ray beams, as well as a growing number of applications for these light waves. X-ray beams flow through your body, and depending on the density of the material they pass through, they are absorbed in varying amounts. On X-rays, dense materials like bone and metal appear white. Your lungs' air appears to be black. Fat and muscle appear as grayscale images.

## Types of X-rays

There are two types of X-ray spectrum:

1. Continuous - when high-speed electrons collide with a high-atomic-number target material, X-rays are created. The majority of the energy of the electrons is used to heat the target material in the creation of X-rays.A few fast-moving electrons penetrate deep into the interior of the target material's atoms and are drawn to their nuclei by their nuclei's attraction forces. The electrons are thrown from their initial route due to these forces. As a result, electrons slow down, and their energy reduces over time. The X-rays have a continuous frequency range up to a maximum frequency max or a minimum wavelength min. This is called Continuous X-rays. The minimum wavelength depends on the anode voltage. If $V$ is the potential difference between the anode and the cathode
$\mathrm{eV}=\mathrm{h} \nu_{\text {max }}=\mathrm{hc} / \lambda_{\text {min }}$
The minimum wavelength of the given radiation is,
$\lambda_{\text {min }}=\mathrm{hc} / \mathrm{eV}$
where h is Planck's constant, c is the velocity of light and e , the charge of the electron.
Substituting the known values in the above equation.
$\lambda_{\text {min }}=12400 / \mathrm{V} \mathrm{A0}$
For the given operating voltage, the minimum wavelength is the same for all metals.

2. Characteristic X-ray - Characteristic radiation is a sort of energy emission that is important in the creation of X-rays. When a fast-moving electron collides with a Kshell electron, the electron in the K-shell is ejected (if the incident electron's energy is larger than the K-shell electron's binding energy), leaving a 'hole' behind. An outer shell electron fills this hole (from the L-shell, M-shell, and so on) with the emission of a single X-ray photon with an energy level equal to the energy level difference between the outer and inner shell electrons engaged in the transition.


## TYPES OF BONDING

There are basically four classes into which the bonds can conveniently be divided, although the boundaries between them are not always distinct:

1. Ionic Bonding,
2. covalent bonding,
3. metallic, or unsaturated covalent bonding, and
4. van der Waals bonding.

The first three are primary bonds, whereas the fourth one is a secondary bond.

## Ionic Bond

- It is the simplest type of primary bond.
- Electrons break free of atoms with excess in their valence shell, producing positive ions, and unite with atoms having an incomplete outer shell to form negative ions.
- The positive and negative ions have a natural attraction to each other, producing a strong bonding force.
- The below Figure shows the process for a bond between sodium and chlorine.

- In Ionic-type bonding, however, the atoms do not unite in simple pairs. All positively charged atoms attract all negatively charged atoms.
- Thus, for example, sodium ions surround themselves with negative chlorine ions and chlorine ions surround themselves with positive sodium ions
- The attraction is equal in all directions and results in a three-dimensional structure, rather than the simple link of a single bond.
- For stability in structure, the total charge neutrality must be maintained, thereby requiring an equal number of positive and negative charges.
- Some other examples are bonds in $\mathbf{M g C l}_{2}, \mathbf{K}_{2} \mathbf{O}, \mathbf{C u O}, \mathbf{M o F} 2$, etc.
- General characteristics of materials joined by ionic bonds include moderate to high strength, high hardness, brittleness, high melting point, and electrically insulating properties.


## Covalent Bond

- In this type of bond, the atoms being linked find it impossible to produce a complete shell by electron transfer but achieve the same goal by electron sharing so that each attains a stable electronic structure.
- Moreover, the shared negative electrons locate between the positive nuclei to form the bonding link.
- The covalent bond is found in a wide variety of materials since it can be formed between atoms of the same or different elements.
- Some of the materials having covalent bonds are $\mathbf{C l}_{2}, \mathbf{N}_{2}, \mathbf{H F}$, diamond, etc.
- Like the ionic bond, the covalent bond tends to produce materials with high strength and high melting points.
- Atom movement within the material (deformation) requires the breaking of distinct bonds, thereby making the material characteristically brittle.
- Electrical conductivity depends upon bond strength, ranging from conductive tin (weak covalent bond) through semiconductive silicon and germanium to insulating diamond.
- Engineering materials possessing ionic and covalent bonds tend to be ceramic or polymeric in nature.


## Metallic Bond

- This type of bond is characteristic of the elements having a small number of valence electrons, which are loosely held so that they can be easily released to the common pool.
- The bonding results when each of the atoms of the metal contributes its valence electrons to the formation of an electron cloud that pervades the solid metal.
- In the metallic bonds, the highly mobile free electrons account for the observed well as the opaque optical properties (electrons can absorb light radiation energies).
- Electrons provide necessary bonding forces.
- Bond strength and, therefore, the material strength vary over a wide range.
- Positive ions can move without breaking distinct bonds.
- Materials bonded by metallic bonds, therefore, can be deformed by atom movement mechanisms and produce a deformed material every bit as strong as the original.
- This is the basis of metal plasticity, ductility, and many of the shaping processes used in metal fabrication.


## van der Waals bond

- Weak or secondary bonds known as van der Waals forces can link molecules that possess a non-symmetric distribution of charge.
- Some molecules, such as hydrogen fluoride and water, can be viewed as electrical dipoles in that certain portions of the molecules tend to be more positive or negative than others (an effect referred to as polarization).
- The negative part of one molecule tends to attract the positive part of another to form a weak bond.


Another weak bond can result from momentary polarization caused by the random movement of the electrons and the resulting momentary electrical unbalance. This random and momentary polarization leading to attractive forces is called the dispersion effect.

## Hydrogen bond

A hydrogen bond can be defined as the attractive force that binds one molecule's hydrogen atom with the electronegative atoms like fluorine, oxygen, and nitrogen of another molecule.


The magnitude of hydrogen bonding depends on the physical state of the compound, which
is maximum in a solid state and minimum in a gaseous state. This allows the hydrogen bond to influence the structure and properties of the compounds strongly.

Image
It is of two types;

1. Intermolecular hydrogen bond: Bond formed between two different molecules
2. Intramolecular hydrogen bond: Bond formed within a molecule
