

Any object which has mass and occupy spaces is called matter. State of matter can be classified as

State of Matter

- Solid
- Fluid
  - Liquid
  - Gas

**Basic Properties of Solid:**

1. Incompressible
2. Inflexible
3. Have mechanical strength
4. Has specific space

**Why is solid incompressible and have specific space?**

Intermolecular distance is minor between atoms, so atoms are closely packed, that's what intermolecular force is higher resulting solid to be incompressible.

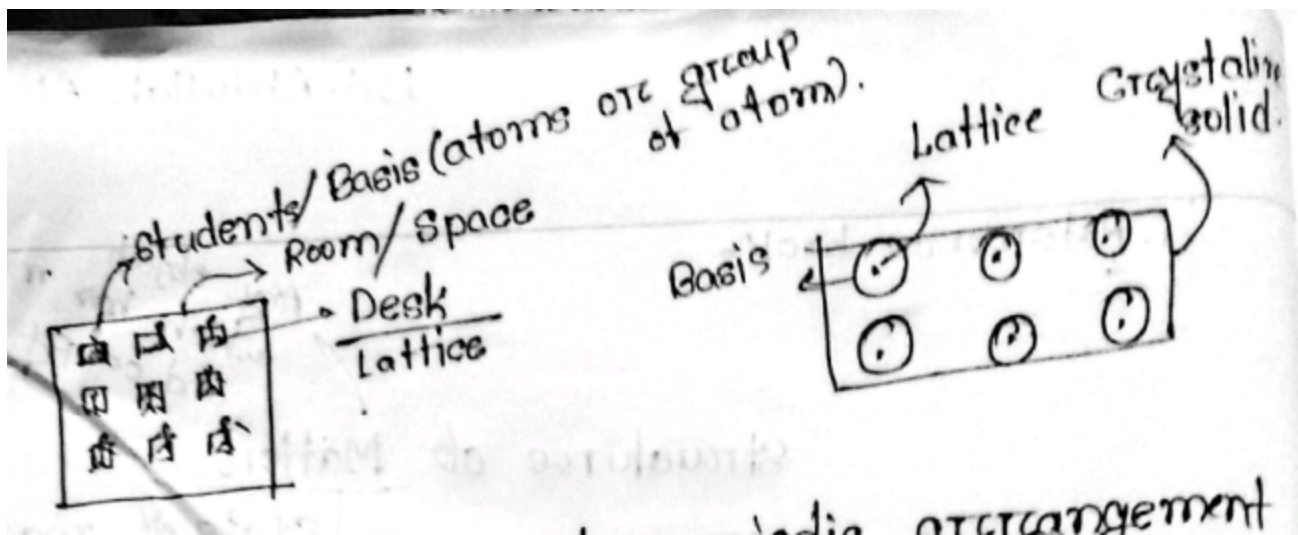
## Solid

Solid can be broadly divided into three categories

- Crystalline Solids
- Poly-crystalline solids
- Non-crystalline solids / Amorphous

## Crystalline Solids

The constituents (atoms, molecules, or ions) are arranged in an orderly manner in a definite geometric shape (long range)



**Lattice:** Regular and Periodic arrangement of points in space

**Basis:** Atoms or group of atoms.

Lattice + Basis -> Crystal Structure

Example: Salt, Diamonds

## Poly-Crystalline Solid

Solids that occur as powder resemble amorphous but properties are just like crystalline solids

## Crystalline Vs. Amorphous

Crystalline	Amorphous
If heat energy is provided the atoms gain kinetic energy and converts to liquid and vice versa	Generally in liquid state in room temperature
Have definite geometric shape	Does not have definite geometric shape
Sharp melting point	Exponential Melting Point
Long range order	Short range order
Higher intermolecular force	Lower intermolecular force
Isotropic	Anisotropic

## Metal

Metal is a crystalline solid. In the structure of metal, positive ion are floating in the sea of electron. Metal has unsaturated bond between electrons and positive ions. As electron moves

freely through the whole crystal and does not belong to any specific atom.

**Isotropic:** Does not change based on the direction. (Amorphous)

**Anisotropic:** Changes based on the direction. (Crystalline)

Classification of a crystal is dependent on its unit cell

**Unit Cell:** Unit cell is the smallest repeating unit that forms the total symmetry of a crystal.

Lattice parameter indicates physical dimension of unit cell and unit cell indicates crystal.

Lattice parameters determines the unit cell.

Lattice parameters

- Axial Length  $\rightarrow a, b, c$
- Axial Angle  $\rightarrow \alpha, \beta, \gamma$

Lattice parameter refers to the physical dimension of unit cell. If lattice parameter of two unit cell are same, then they are considered as same crystal.

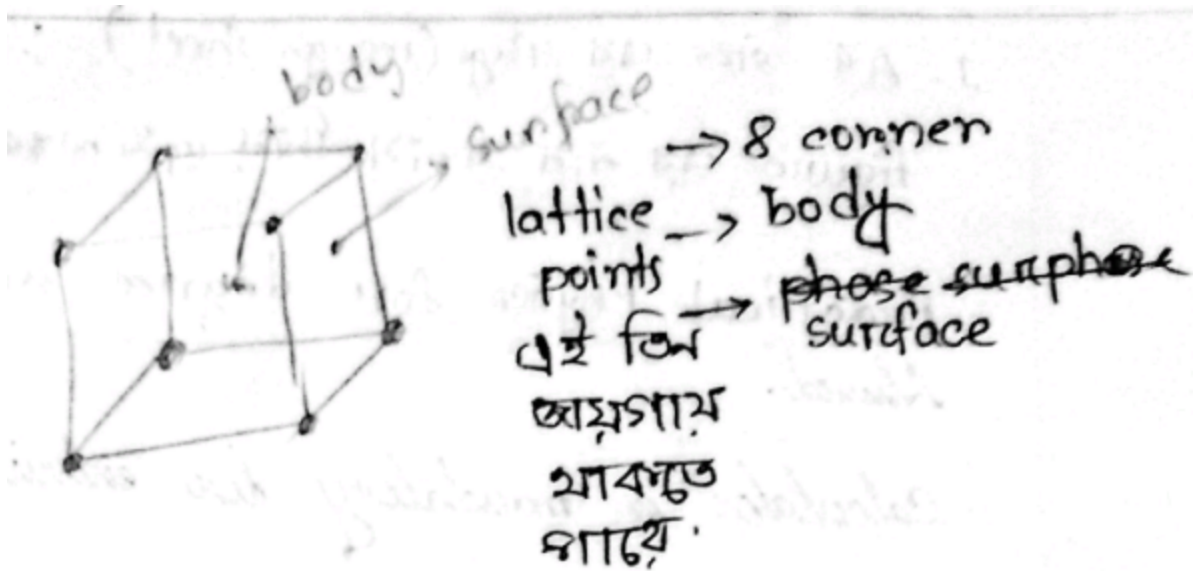
**Lattice Defects:** Little bit of disorder in the crystal but it will be considered as the part of the same crystal category.

Crystal System	Lattice Parameter
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ \neq$
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	$a = b \neq c$ $\alpha = \beta = \gamma = 120^\circ$
Hexagonal	$a = b \neq c$ $\alpha = \beta = 120^\circ$ $\gamma = 120^\circ$

Two unit cell of a same crystal can be different. Unit cell can be categorized in two parts

Unit Cell

- Primitive(Simple)
- Non-primitive



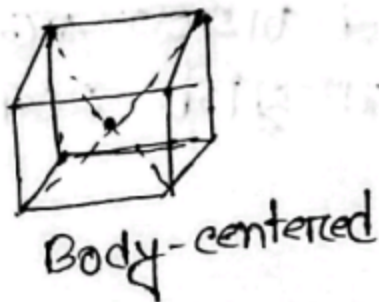
These classifications are based on the position of lattice points in the crystal. Lattice points can be placed in 8 corners, body or in the surface of the crystal

**Primitive:** Lattice points lie at only 8 corners

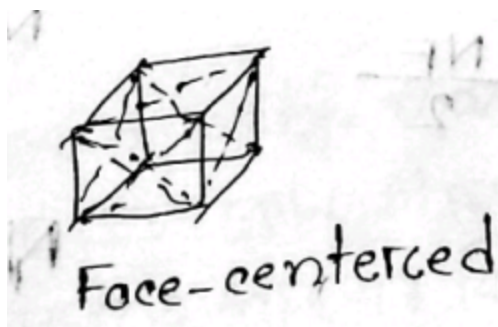
**Non-primitive:** Lattice points lie not only at the corners, but also at the body or at the surface.

Some examples of non-primitive unit cells:

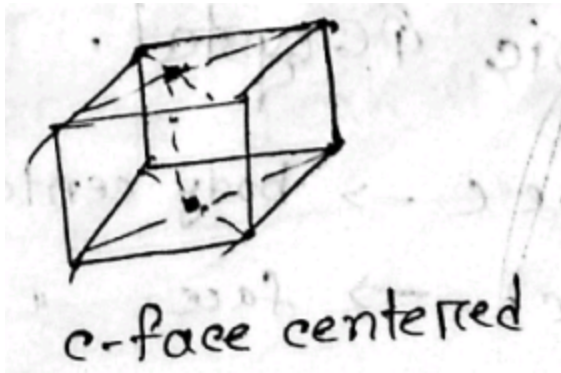
**Body-centered:** One lattice point at center



**Face-centered:** In the middle of each 6 faces



**Base-centered / c-face centered:** 8 corners + middle of one axis



**Law of determining effective lattice point:**

$$\frac{N_C}{8} + N_i + \frac{N_F}{2}$$

Where,

$N_C$  = of lattice point at corner

$N_i$  = of lattice point inside the body

$N_F$  = of lattice point at the face

**Number of Effective Lattice Point:**

- Primitive Unit Cell =  $\frac{1}{8} \times 8 = 1$
- Body-centered Unit Cell =  $1 + \frac{1}{8} \times 8 = 2$
- Face-centered Unit Cell =  $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$

When inter-molecular distance reduces, interaction increases, but this is true up to a limited distance which is called bond length. If inter-molecular distance reduce beyond, then repulsion force will be created resulting in a system collapse.

If a body-centered unit cell is the type cubic then it might be called body-centered cubic crystal. or *bcc* in short

*bcc* → body centered cubic

*fcc* → face centered cubic

**Density of Crystal Matter**

$$\rho = \frac{\text{mass per unit cell}}{\text{volume per unit cell}}$$

Let us consider a cuboidal where each side is of length  $a$ . Then the volume of that cuboidal is  $a^3$

mass per unit cell = of atoms  $\times$  mass of one atom

$$= n \times \frac{M}{N_a}$$

where,

$n$  = of atoms

$M$  = molecular weight

$N_a$  = Avogadro number

$$\therefore \rho = \frac{nM}{N_a \times V}$$

where,

$V$  = volume

**Packing Factor:** It indicates how atoms are closely packed in a unit cell.

$$\text{Packing factor} = \frac{\text{volume of all atoms in a unit cell}}{\text{volume of unit cell}}$$

**For Simple Cubic,**

$$V = a^3$$

Volume of one atom,  $v = \frac{4}{3}\pi r^3$

Volume of all atoms,  $v_n = \frac{4}{3}\pi r^3 n$

$n$  = number of effective atoms

$$\therefore P.F. = \frac{n \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

**For Simple Cubic Crystal,**

$$r = \frac{a}{2}$$

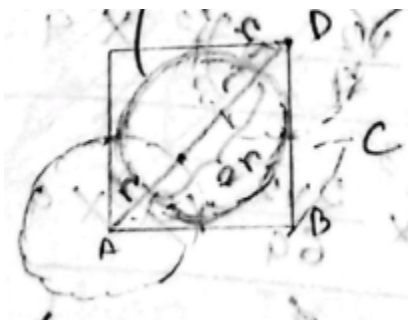
$$n = 1$$

$$\therefore P.F. = \frac{\frac{4}{3}\pi \left(\frac{a}{2}\right)^3}{a^3}$$

$$= \frac{\pi}{6} \times 100 = 52$$

$$\therefore \text{empty space} = 48$$

**For Base-centered cubic:**



$$AD^2 = AB^2 + BC^2 + CD^2 = 3a^2$$

$$\Rightarrow AD = \sqrt{3}a$$

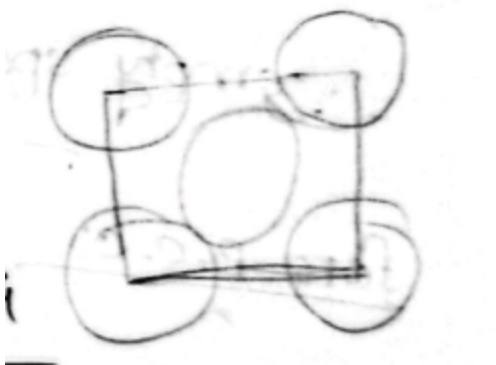
$$\Rightarrow 4r = \sqrt{3}a$$

$$\therefore r = \frac{\sqrt{3}}{4}a$$

$$\text{Packing Factor} = \frac{2 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} \times 100 = 68$$

$$\therefore \text{empty space} = 32$$

For **Face-centered cubic**:



$$AC^2 = AB^2 + BC^2 = 2a^2$$

$$\Rightarrow AC = 4r = \sqrt{2}a$$

$$\Rightarrow r = \frac{\sqrt{2}}{4}a$$

$$\text{P.F.} = \frac{\frac{4}{3} \times \pi \times \left(\frac{\sqrt{2}}{4}a\right)^3 \times 4}{a^3} = 74$$

Lattices are always in a vibrational motion

**Crystal Plane:** Crystal planes are some imaginary plane inside a crystal in which large concentration of atoms are present

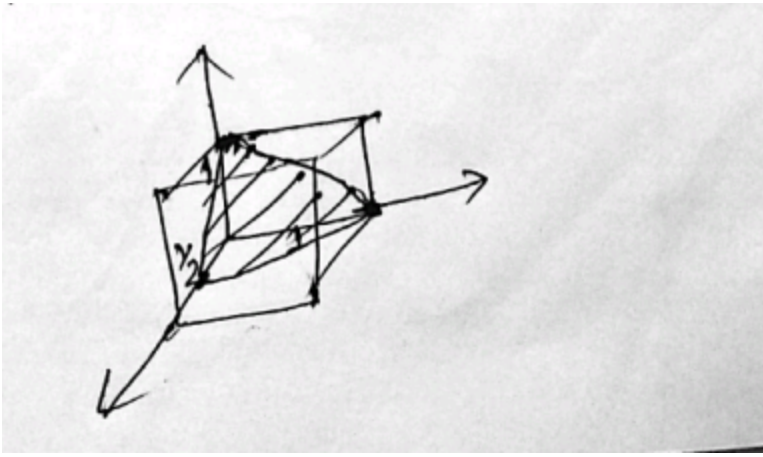
**Miller Indices:** The position and orientation of crystal plane is described by three integers  $h$ ,  $k$  and  $l$ , these are called Miller indices

Miller indices are expressed in the form  $(h, k, l)$

If,  $(2, 1, 1)$  then it should be converted into its reciprocal form as the maximum intersection is 1

$$\left(\frac{1}{2}, 1, 1\right)$$

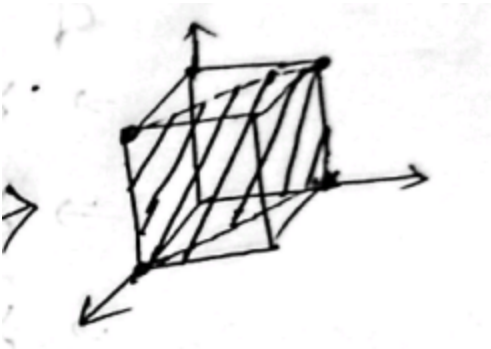
Here we will draw three points, one at the  $\frac{1}{2}$  mark of  $x$ -axis, other two at the full mark of  $y$ -axis and  $z$ -axis.



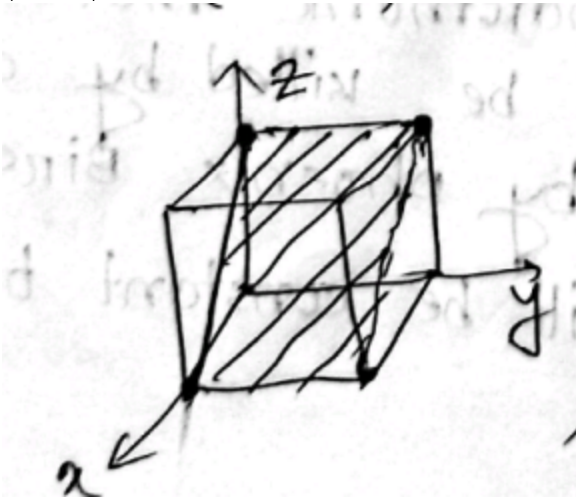
$(1, 1, 0)$

Reciprocal  $(1, 1, \infty)$

Indicating the plane will point at infinity at  $z$ -axis. Therefore, the plane will be something like this

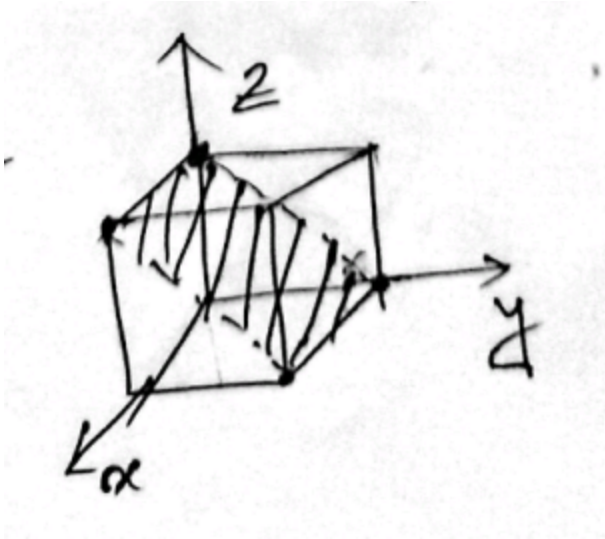


$(1, 0, 1)$

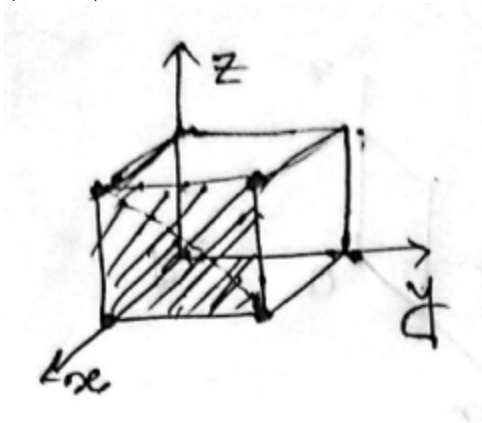




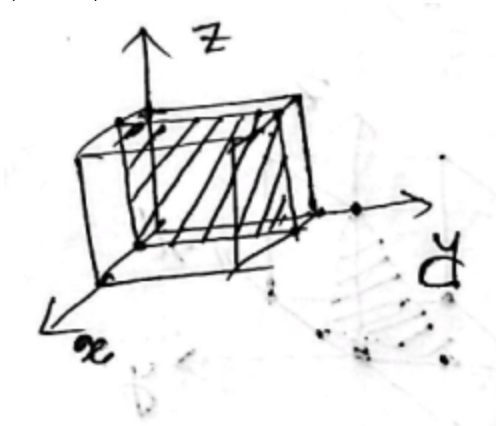
$(0, 1, 1)$



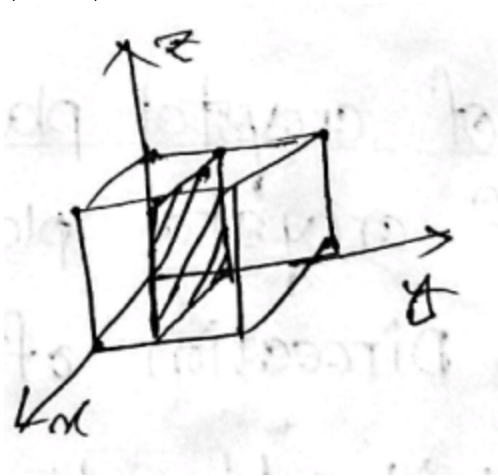
$(1, 0, 0)$



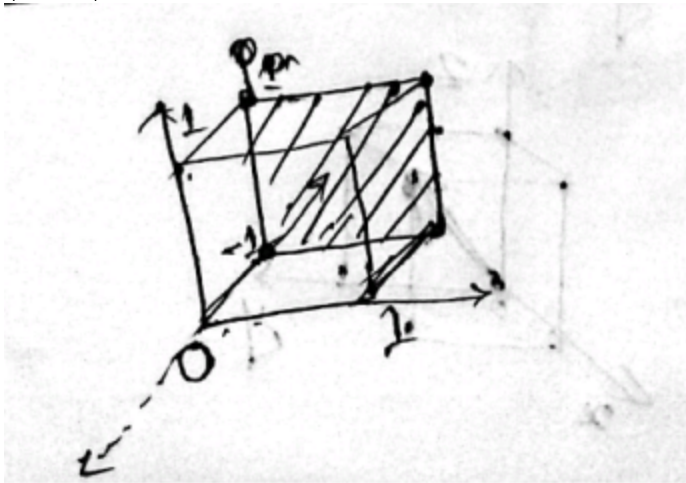
$(3, 0, 0)$



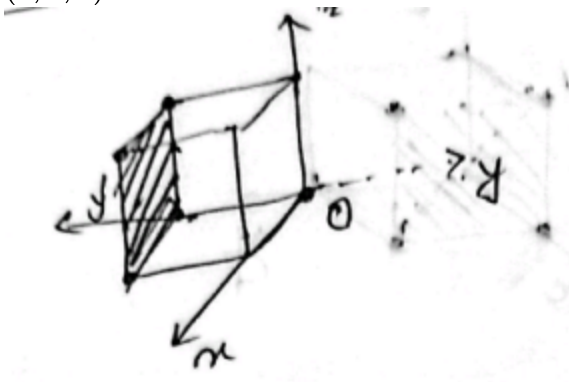
$(0, 2, 0)$



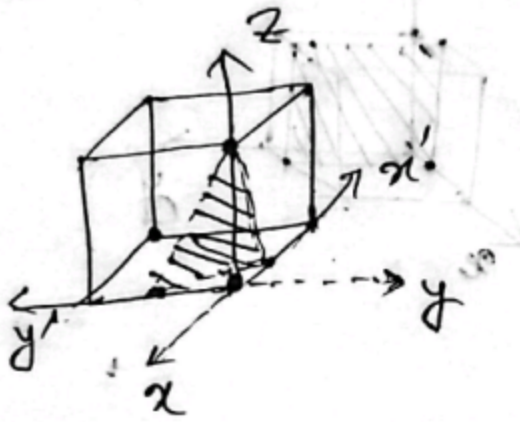
$(1, 0, 0)$



$(0, 1, 0)$



(3, 2, 1)



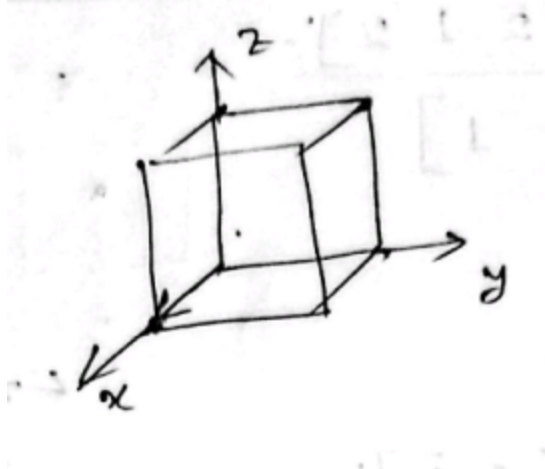
### Direction of Crystal Plane:

Direction of crystal plane in continuous.

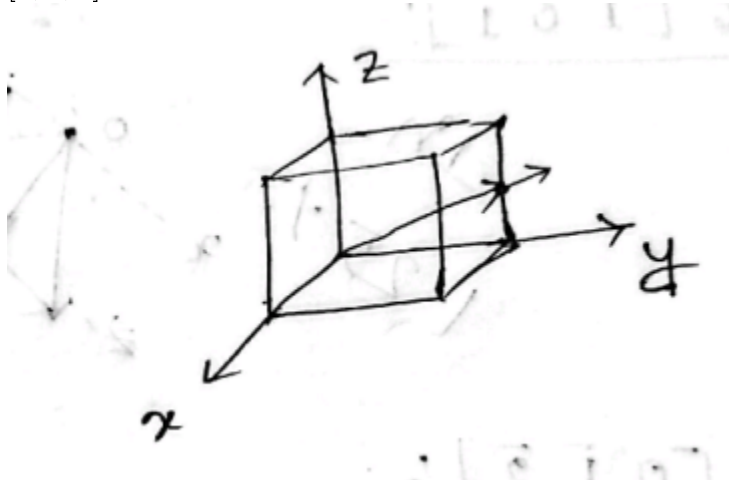
$[1, 1, 1]$  indicates the direction of the crystal plane  $(1, 1, 1)$

We find the direction of crystal plane  $[a, b, c]$  by dividing  $a, b, c$  by  $\max(a, b, c)$ . Then from the origin we get to that point and draw the direction

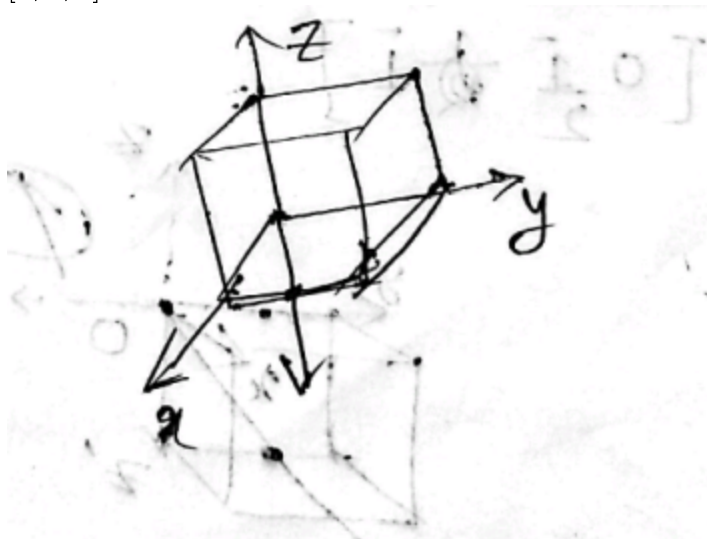
$[2, 0, 0]$



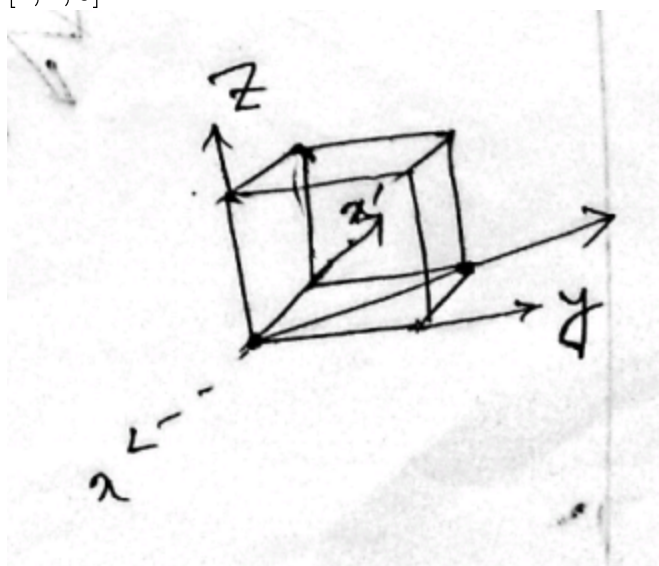
$[0, 2, 1]$



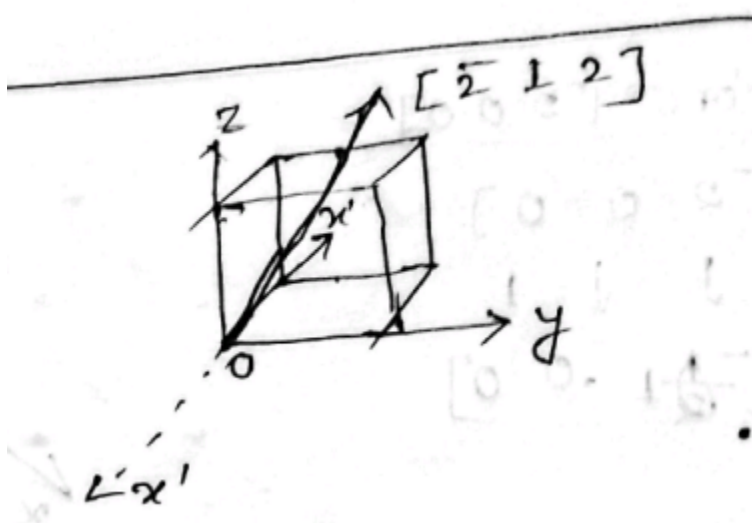
$[2, 1, 0]$



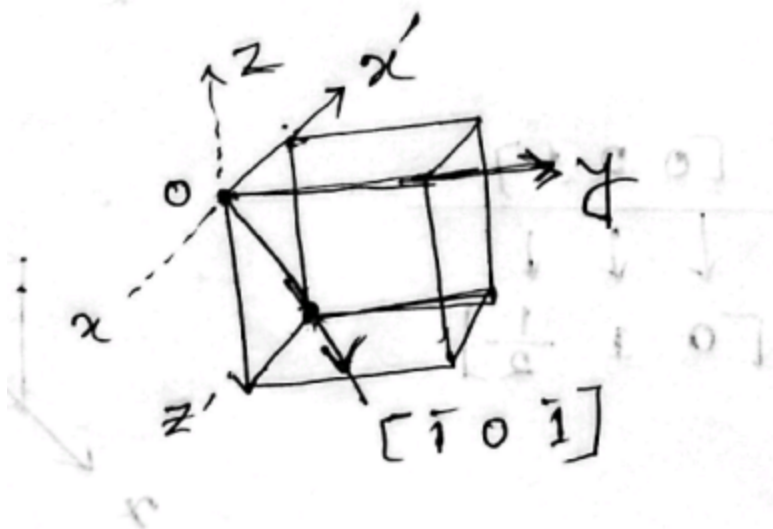
$[1, 1, 0]$



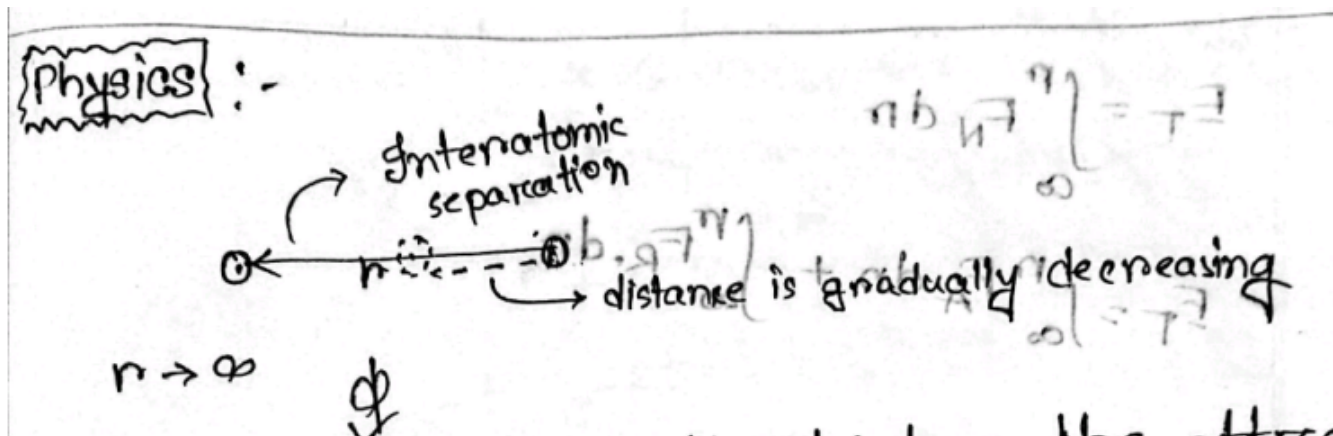
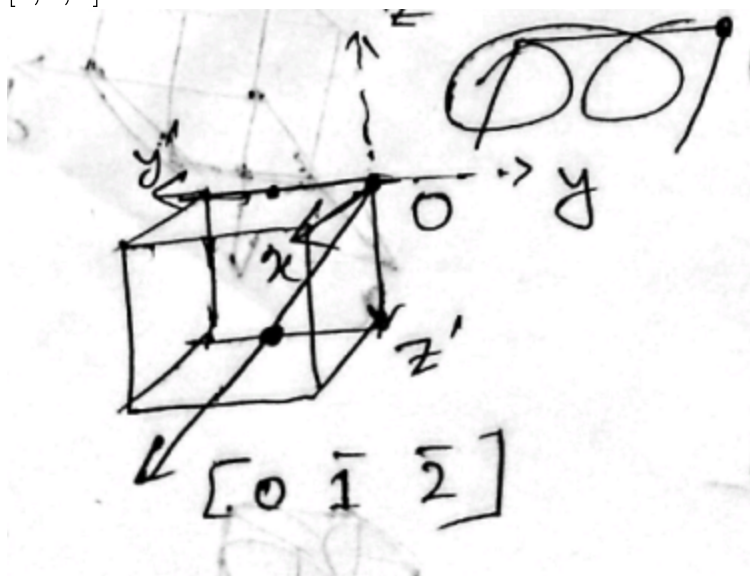
$[2, 1, 2]$



[1, 0, 1]

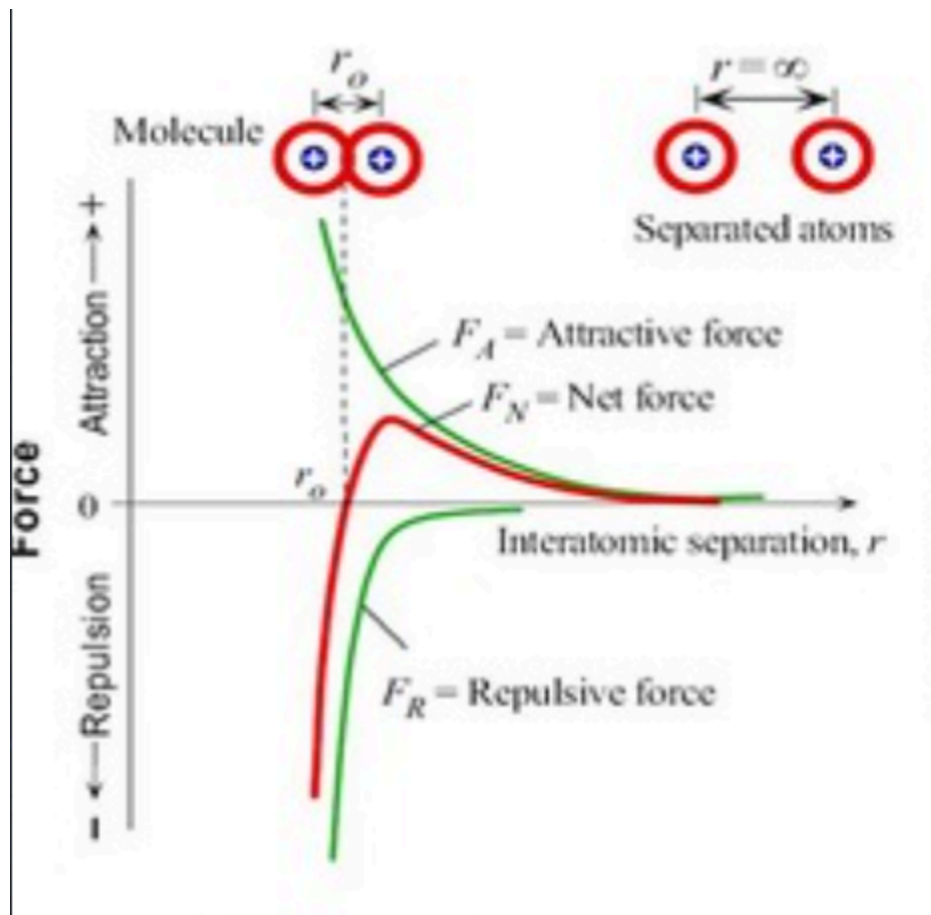


[0, 1, 2]



The less the distances the higher the attraction force, but if they come too close, their outer shell overlaps, as a result, there is an arise of repulsion force

So, we need to determine a distance where there will be zero net force, and the distance will be considered as bond length.



$r_o$  = bond length

For stabilizing a bonding, the energy should be minimum, and that is zero.

$$E_T = \int_{\infty}^r F_N dr = \int_{\infty}^r F_A dr + \int_{\infty}^r F_R dr$$

Now, we know that,

$$\frac{dE_T}{dr} = F_N$$

when  $r = r_o$ ,  $F_N = 0$  then  $E_T$  posses minimum

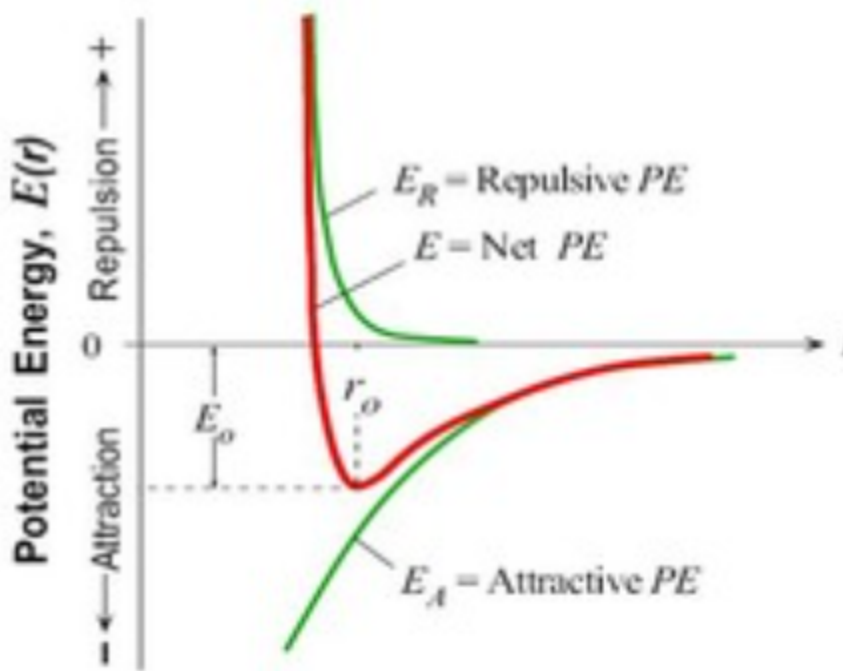
$$\frac{dE_T}{dr} = 0$$

Now,

$$E_A = \frac{-e^2}{4\pi r} = \frac{-A}{r}$$

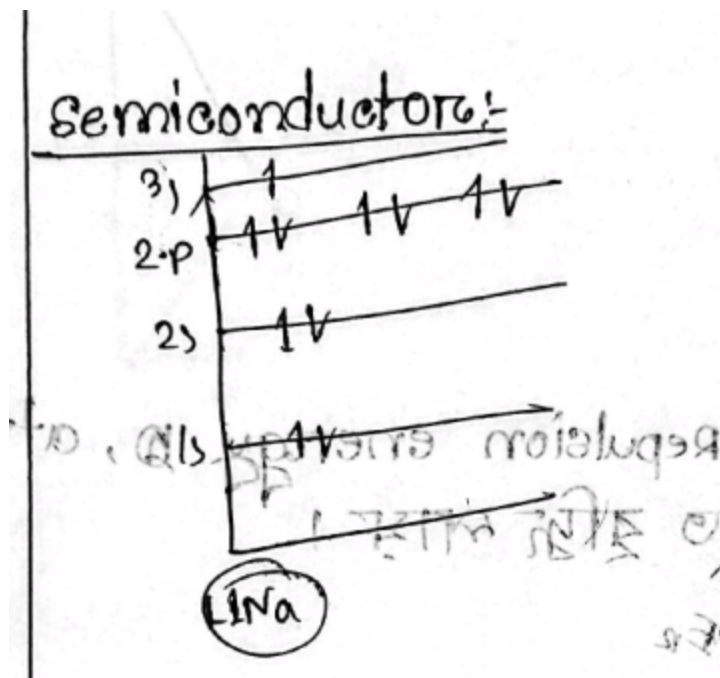
$$E_R = \frac{B}{r^m}$$



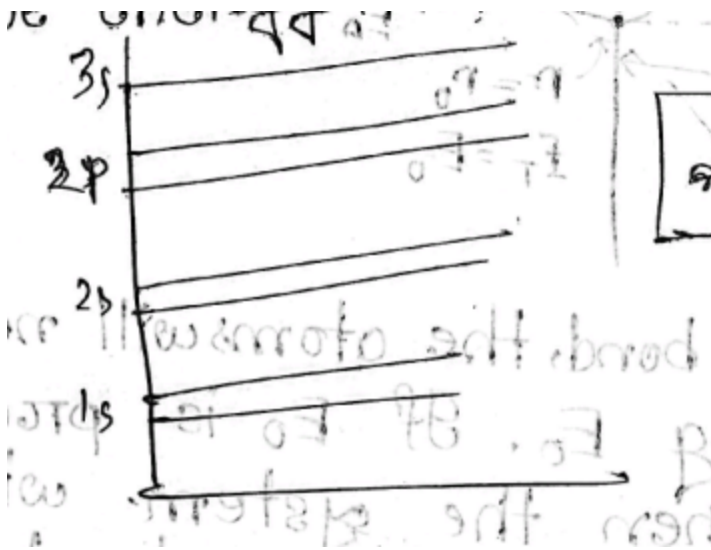


(b) Potential energy vs  $r$

## Semiconductors



While two atoms are closely packed, then the energy levels are split. Pauli's exclusion principle shows that no two atoms can have the same quantum state.

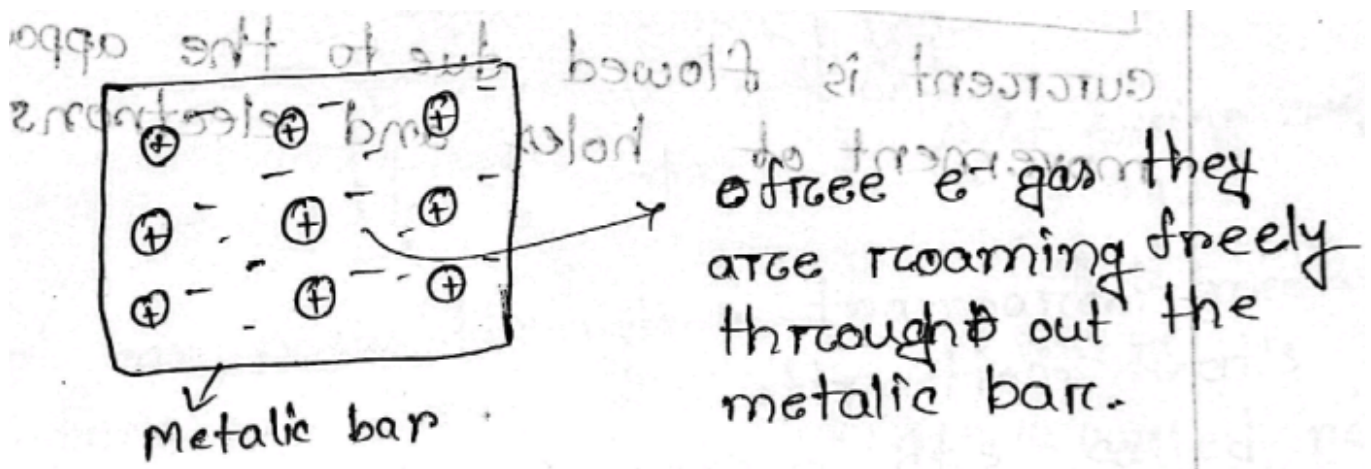


Similarly when many atoms are closely packed, then there will be lots of line or spectra energy which cannot be separated anymore creating a band. It will now act as band (where there is lower limit and upper limit)

**Valence Band:** The energy band that contains the energy levels of valence electrons, electrons are loosely bound

**Conduction Band:** The energy band that contains the energy levels of free electrons

### Metallic Bond



Electrons create unsaturated metallic bonds with the metallic ions.

If a little bit of electric field is provided then these electrons start to flow, while flowing, they collide with each other. If heat(thermal energy) increases, then resistivity increases for this reason.