Sumedh

- X-Ray diffraction (XRD)

· Crystalline solid

A solid with regular - longrange - ordered arrangements of atoms / ions / molecules

↓ metallic solid

↓ Ionic solid

↓ Organic solids

· Diff b/w crysta & Amo

Crys	Amor
Regular arrangement	Irregular arrangement
Anisotropic	Isotrophic
Sharp MP	Soft over a range of temp
definite shape & geometry	Indefinite geometry and shape.
bound to have interfacial angles	No interfacial angles (No plane faces)

· Lattice

Array of img pts such that each pt has identical environment

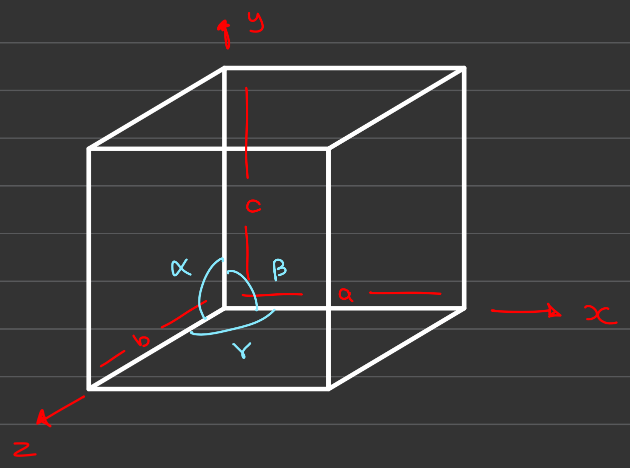
OR

A framework where whole crystal is built

· Unit cell

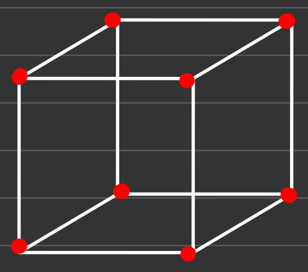
Smallest fundamental unit, which when repeated in all direction gives the whole crystal

(small size, high symm)

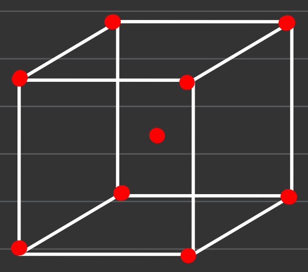


- Type of Unit cells

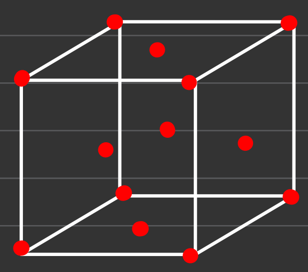
① Primitive Unit Cell



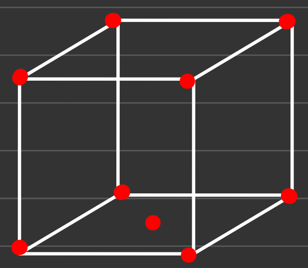
② Body Centered Unit cell



③ Face Centered



④ End base centered



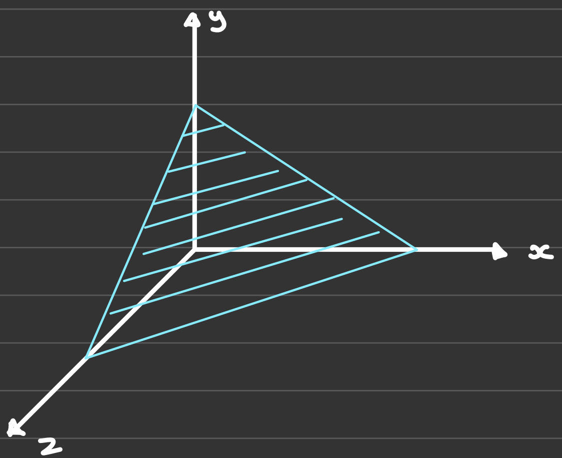
- 7 Crystal systems

① Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$		P, I, F
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$		P, I
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$		P, I, F, A
Rhombohedral / Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90$		P
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90$	$\gamma = 120°$	P
Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90°$	$\gamma \neq 90°$	P, A
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90$		P

- Lattice planes

A set of img planes in a crystal lattice having fixed interplanar dist.

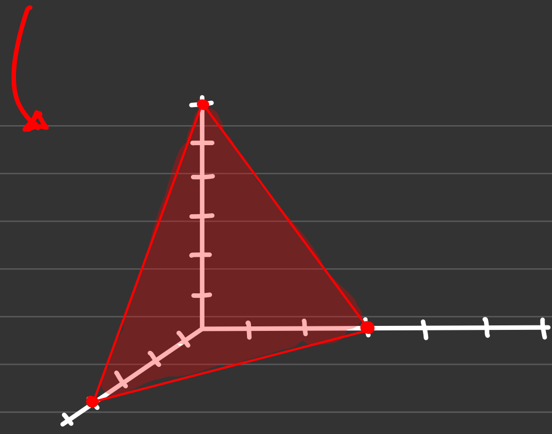
- Miller indices (hkl)



Miller indices are the reciprocals of intercepts made by a lattice plane on x, y & z axis and denoted by h, k, l resp.

They're used to label a lattice plane

		x	y	z	
eg	intercept	4	2	3	
	reciprocal	1/4	1/2	1/3	
	clr fractn	3	6	4	(HCM)
	M.I	(3 6 4)	$\equiv$ (h, k, l)		

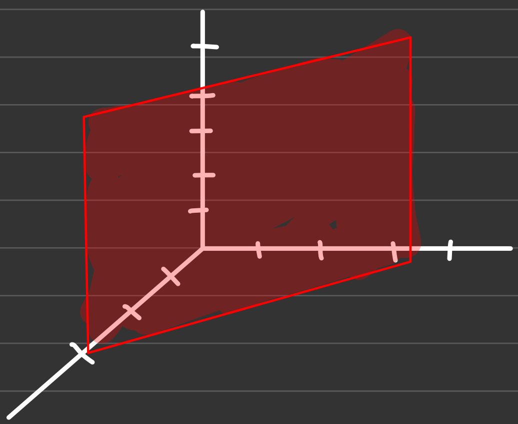


$3, 2, \infty$

$\frac{1}{2}\ \ \frac{1}{3}\ \ \frac{1}{\infty}$

$(2, 3, 0)$

eg

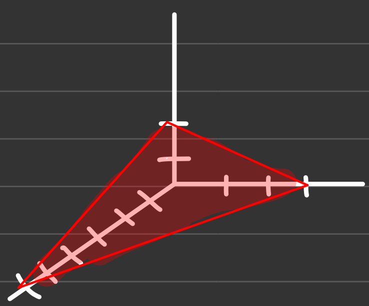


eg $(2a, 3b, c)$

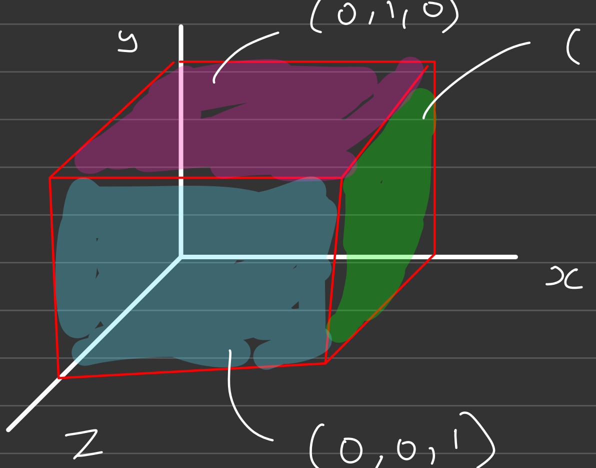
$2 \quad 3 \quad 1$

$\frac{1}{2} \quad \frac{1}{3} \quad \frac{1}{1}$

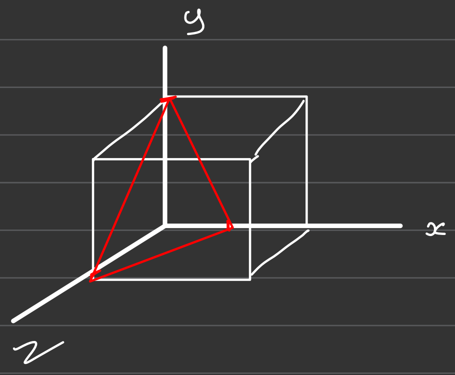
$(3 \quad 2 \quad 6)$



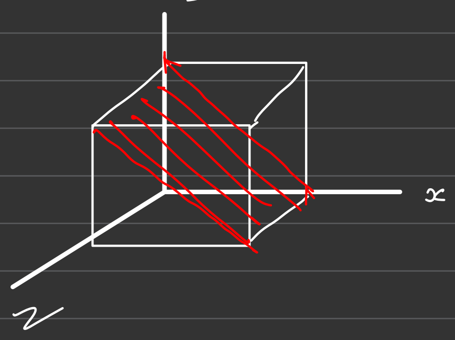
- For unit cell



eg $(2,1,1)$ index —— $(1/2, 1, 1)$ 'intercept'



eg $(1,1,0)$ index $\longrightarrow$ $(1,1,\infty)$



- Interplanar dist (d)

i) for ortho $(a \neq b \neq c)$ $\alpha = \beta = \gamma = 90°$

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

ii) for cubic $(a = b = c)$

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

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

eg The para. of orthorhom unit cell are $a = 50pm$, $b = 100pm$, $c = 150pm$ determine the spacing b/w $(1\ 2\ 3)$ plane

Sol^n

$$\frac{1}{d^2} = \frac{10000}{2500}\times10^{-8} + \frac{40000}{10000}\times10^{-7} + \frac{90000}{22500}\times10^{-8}$$

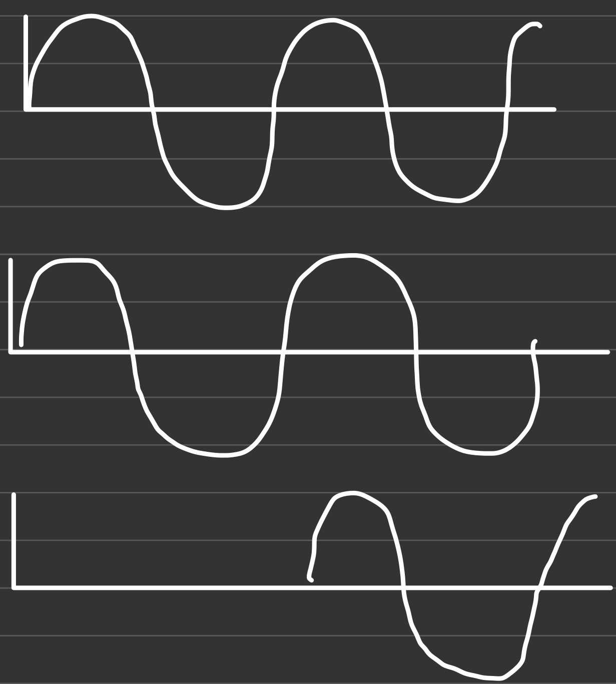
$$\frac{1}{d} = 4\times10^{-8} + 4\times10^{-7} + 4\times10^{-8}$$

$$\frac{1}{d^2} = 8.4 \times 10^{8}$$

$$d = 2.89 \times 10^{4} \ m$$

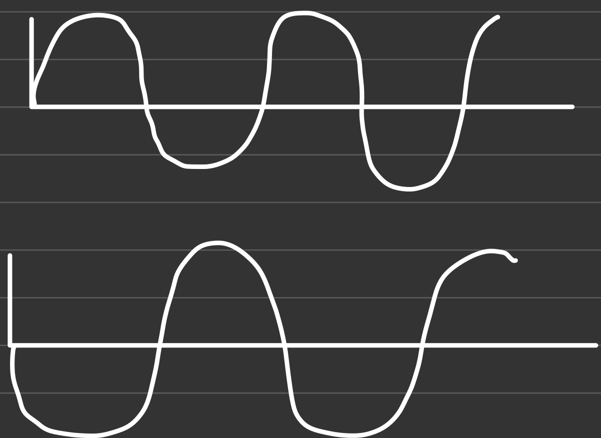
- X- Ray diffraction
  - double - slit exp

- Constructive interference



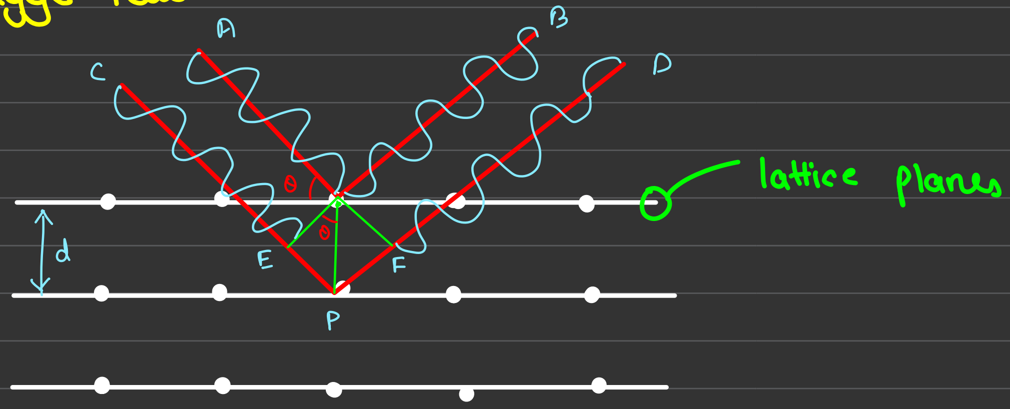
phase diff = $n\lambda$

- destructive law



phase diff = $(2n+1)\frac{\lambda}{2}$

- Bragg's law



The law gives the condⁿ at which a particular set of plane will show diffractⁿ

Path diff = PE + PF (extra dist travelled by lower wave)

In $\triangle OPE$

$$\sin\theta = \frac{PE}{OP} = \frac{PE}{d}$$

$$PE = d\sin\theta$$

"ly $PF = d\sin\theta$

$\therefore$ $PE + PE = 2d\sin\theta$ = Path diff

$\because$ wave AOB & CPD are constructive

Path diff = $n\lambda$

$$\therefore n\lambda = 2d\sin\theta$$

n = order of diffractⁿ
λ = wavelength of X-ray
d = interplanar dist
θ = Bragg's law

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

$$d = \frac{n\lambda}{2\sin\theta}$$

for d min, $\sin\theta$ max i.e 1 & $n=1$

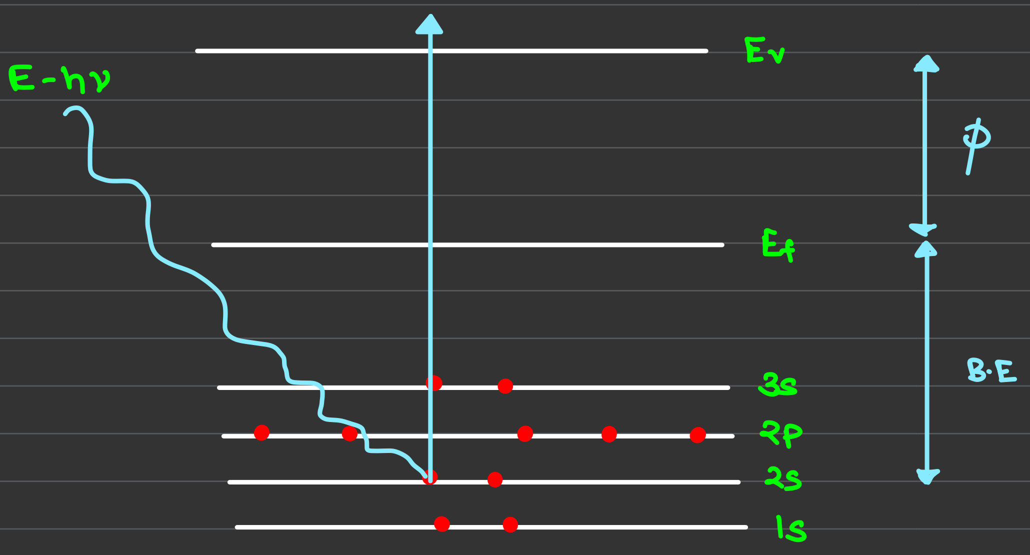
$$\therefore d\,min = \frac{\lambda}{2}$$

eg $\lambda = 100\,A^\circ$, $\theta = 90^\circ$, $n=1$

Soln $1 \times 100 \times 10^{-10} = 2d$

$$d = 50 \times 10^{-10}\,m$$

- XPS (X-ray photoelectron Spectroscopy)
  - (ESCA) - Electron spectroscopy for Chem analysis)



Ef : Fermi-height energy level occupied by e^- at absolute zero temp

Ev : Energy vaccum, i.e not attracted by Ef

When E is more than BE of the e^-, the e^- is released & it releases KE

$$KE = [h\nu - (BE + \phi)]$$

of the photoelectron

- Applications

① Qualitative Analysis

- Elemental Composition
- Empirical formula

2) Quantitative Analysis
3) Determination of OS / electronic ~~environ~~ environment.
4) Determination of contamination / impurities.

* XPS - Surface sensitive technique

eg in X-Ray diff of set of crystal planes having $d = 0.18\,nm$
$n = 1$, $\theta = 22°$

$$n\lambda = 2d\sin 22$$
$$\lambda = 2 \times 0.18 \times 10^{-9}$$

eg $\theta = ?$, $n = 1$, $\lambda =$, $d =$

Soln $n\lambda = 2d\sin\theta$

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

1.54×10^{-10}

0.77×10^{-10}

$$\sin^{-1}(0.191 \times 10^{-10})$$

eg wire with $r = 5\,mm$ is hung freely ceiling, a load of $F = 5N$ to free end, find elonga if vol. $= 7.85 \times 10^{-5}\ m^3$ & $Y = 10^{11}\ N/m^2$

Sol

$$\Delta l = \frac{Fl}{AY}$$

$$= 5 \times$$

$$10^{-5} \times 7.85 = \pi r^2 h$$

$$\Delta l = \frac{5 \times 1}{78.5 \times 10^{11}}$$

$$h = \frac{7.85 \times 10^{-5}}{3.14 \times 5 \times 10^{-3}}$$

$$\Delta l = 0.064 \times 10^{-11}$$

$$\Delta l = 6.4 \times 10^{-13}$$

$$= \frac{7.85 \times}{3.14 \times 5 \times 5} 10^{1}$$

$$\pi r^2 \times 10^{-3} \times 10^{-3}$$

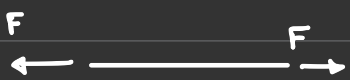
$$78.5 \times 10^{-6}$$

$$\frac{5 \times 1}{78.5 \times 10^{11} \times 10^{-6}}$$

$$0.064 \times 10^{-5}$$

eg $Y = 10^5\ N/m^2$, $l = 1\,m$, $r = 3 \times 10^{-3}\,m$, Assuming uni crx sec, find After $F = 1\,N$ from both ends

Sol



$$\Delta l = \frac{1 \times 1}{3.14 \times 9 \times 10^{-6} \times 10^{5}}$$

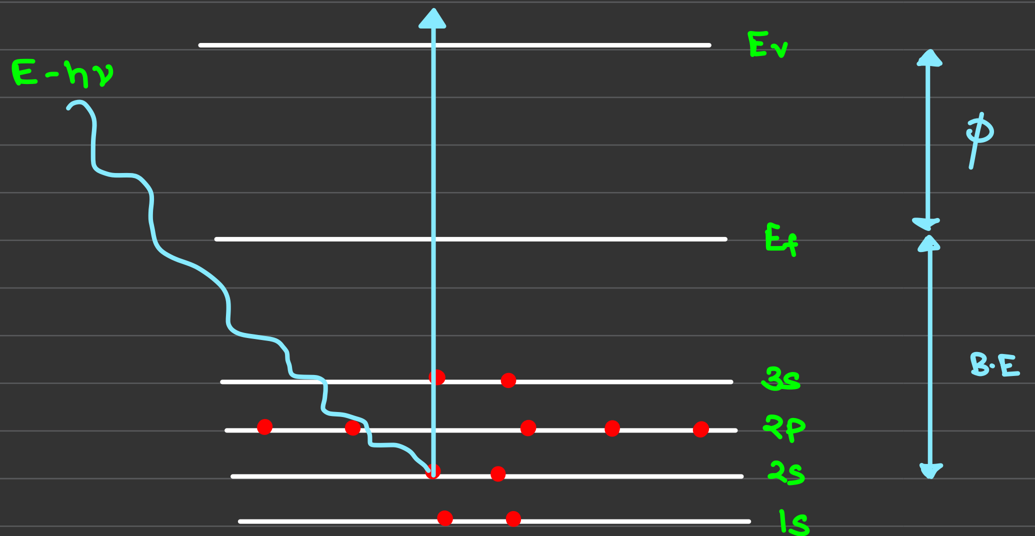
$$\simeq 0.35$$

$l = 1\,m$

$l' = 1.35\,m$

- XPS

(ESCA) - Electron spectroscopy for chem analysis)



E_f : Fermi-height energy level occupied by e^- at absolute zero temp

E_v : Energy vaccum, i.e not attracted by E_f

Principle : When the Energy is more than Binding energy of the e^-, the e^- is released with some KE

$$KE = h\nu - (BE + \phi)$$

- Theory

i) Electric gun beams e^-s to the X-ray anode
ii) X-ray annode of Mg Kα & Al Kα, and beams X-ray
iii) The X-ray then goes to crystal monochromator and shoots narrow X-ray
iv) The x-ray then on the sample is then analysed by the electric beam hemispherical analyser.
v) detector count e^-s

Applications

i) Qualitative – dictate the elements present.
ii) Quantitative – elemental composition
iii) OS – High OS, high BE
iv) depth profiling

Advantages :-

detect inorganic and organic materials, stainless steel passivation.

Disadvantages :-

size matterns, challenges with reproducing.

$$V_1 = V_2$$

$$\cancel{\pi} r_1^2 h_1 = \cancel{\pi} r_2^2 h_2$$

$$9 \times 10^{-6} \times 1 = r_2^2 \times 1.35$$

$$6.667 \times 10^{-6} = r_2^2$$

$$2.58 \times 10^{-3}$$

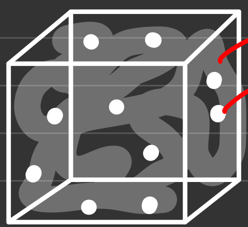
- Composites

Compu

Combination of 2 diff materials which r physically fixed with no chem rxn, they're called:-

Matrix - continuous phase (dispersion med)

Reinforcement - dispersion phase



Matrix (nm) nano

Reinforcement (µm) micro

Matrix

- Metal (MMC) — eg Al, Ti, Mg
- Polymer (PMC) — eg all type
- Ceramic (CMC) — eg Carbites, Nitrites

all have thermal stability

can be polymer

Reinforcement

- Particles
  - hollow
  - filled
- Fibres
  - Short
  - long
    Continuous
- Plates / Flakes
- Wiskers
- rods
- layers

eg FRP (Fibre Reinforced Plastic)

Fibre → Rein

Plastic → Poly matrix

Properties of composite materials:

- High **strength** per unit weight
- High **flexibility**
- Easy to **fabricate**
- Good **chemical** and **heat resistance**
- Good **corrosion resistance**
- **Low maintenance**
- High **toughness** and retain toughness even at low temperature
- **Low thermal conductivity**

- PMC

Polymer Matrix are made up of fibres that are embedded in a organic polymer matrix

Based on level of strength and stiffness into two different type :-

i) Reinforced plastics
ii) Advanced composites.

Composition :-

Matrix - Conti. phase
Reinforcement - dis conti phase
Interphase - The interphase b/w rein & matrix phase where load transmission takes place

Properties :-

1. Greater Toughness
2. Corrosion resistance
3. Cost reduction
4. density control

Applications

1. Biomedical : Medical implants , MRI scanners, X-ray tables.

2. Electrical : Panels, insulators, connectors.

eg : FRP
L GRC , CRP

- FRP (Fibre Reinforced Plastic)

Matrix : Plastic (Polymer)
Reinforcement : Fibre

Properties of FRP depend on

1. Fibre length
2. Fibre orientation & conc.
3. Prop of fiber & matrix.

Application

1. Paper industries
2. Air pollution
3. Medical apps.
4. Oil & gas industry.

PMC conti

Matrix - continuous phase

1. Thermoset resin

   i) Polyester
   ii) Epoxy

2. Thermoplastic resin
   i) Nylon
   ii) Polyproylene.

Reinforcement Fibre : dis cont. phase

1. Glass FR

   i) E, S, C -glass

2. Aramid (Kevlar) FR
3. Carbon FR

- Glass Reinf Plastic (GRP)

Matrix : Plastic (Polymer)
Reinforced phase : glass fibre

Types : E, R, S glass

Properties

1. High strength and stiffness
2. Inexpensive and easy to manufacture

Applications

1. Auto mobile industry
2. Industrial flooring

- Carbon Reinforced Plastic

Matrix : Plastic (Plastic)
Reinforced : carbon / graphite

Properties

1. Low or -ve coefficient of Thermal Expansion
2. High Thermal & electrical conductivity.

Application :

1. Sports equipment
2. air craft components

- Metal Matrix Composites (MMCs)

Matrix : metal
Reinforcement : Fibres / Particulates.

They are a class of materials comprised of a metal fused with another substance.

Properties

1. High Strength
2. High Heat Resistance
3. Fibre resistance
4. Radiation resistance

Examples

1. Aluminium MMC
2. Mg MMC
3. Titanium MMC

Applications

1. Sports
2. Aerospace Industry
3. Automative Application.

- Ceramic Matrix Composite (CMCs)

Matrix : Ceramic
Reinforcement : Carbon, alumina, silicon in the form of whiskers, particles, long sheet fibres, nano fibres.

Properties

1. Light weight
2. High Creep resistance
3. High Temp res.
4. Corrosion