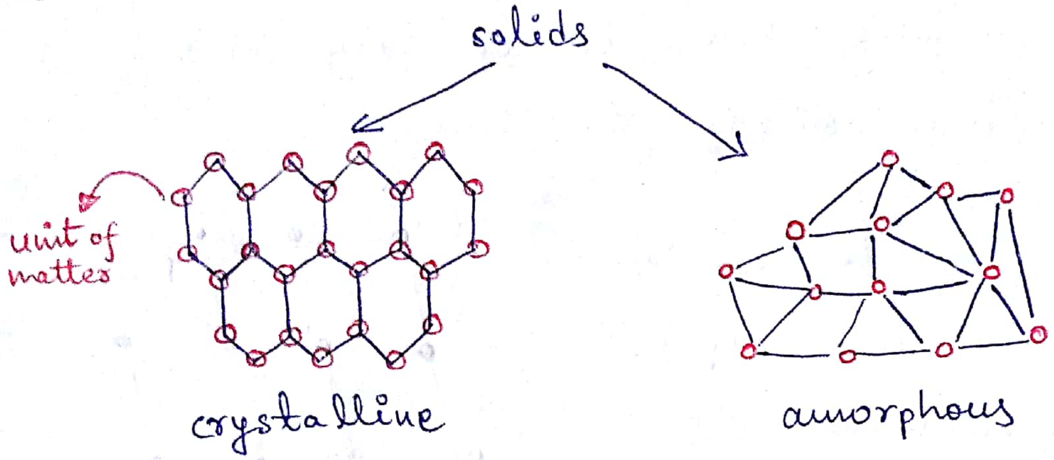
# SOLID STATE PHYSICS

## Crystal structure, direct lattice & (un)holy grail




(i) Amorphous solid : no order in arrangement of unit of matter (atoms, molecules etc). XRD shows "liquid like" property.

what's "solid"? → elasticity

stress $\sigma = K\frac{x}{\ell}$

$x$ = displacement

$\ell$ = length of lattice

$$F = -\ell^2 K \frac{x}{\ell} = -K\ell x = -kx,$$

But $\frac{1}{2}k\bar{x}^2 = \frac{1}{2}k_BT$ (equipartition theorem)

$$\therefore \bar{x}^2 = \frac{k_BT}{k} = \frac{k_BT}{K\ell}$$

So if $K \to 0$, $\bar{x}^2 \to \infty$ ⟶ "rigidity"

amorphous solids ⟷ highly viscous, supercooled liquids.

<u>Example</u> pitch, plastic, silicate glass.

SALIENT FEATURES

(i) molecular motion is irregular but distance is more or less same with elastic solid.

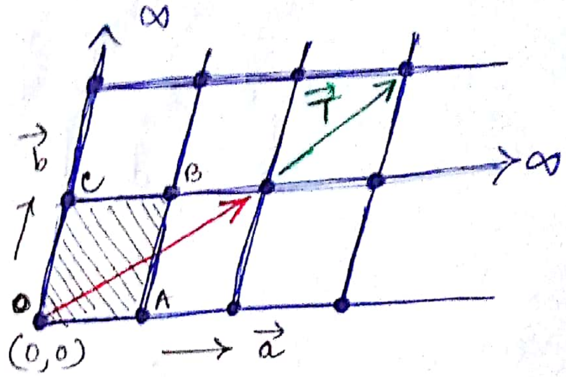
(ii) no regular shape → conductivity, elasticity, tensile strength is isotropic

(iii) no long range order. short range/medium range order possible.

(iv) no sharp melting point.

Scanned by CamScanner

There are polycrystalline substances which are composed of many small domains/regions of single crystals. Crystalline substances are distinguished from amorphous solids by their anisotropic behaviour (direction dependent).




<u>Ideal crystal</u> : infinite repetition of identical structure in space. Periodic arrangement of unit (atoms, molecules, ions) in a crystal is called the lattice, defined by three fundamental translation vectors $\vec{a}, \vec{b}, \vec{c}$. / basis vectors

Atomic position vector $\vec{r}' = \vec{r} + \vec{T}$

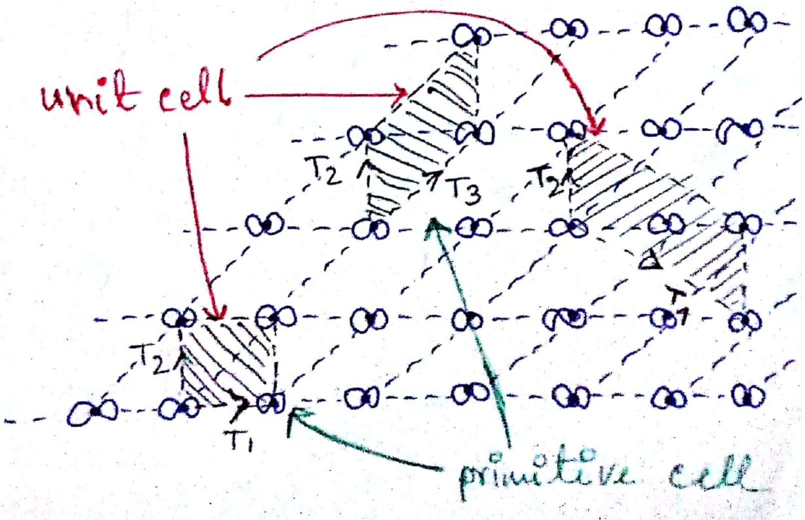
$$= \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

where $n_1, n_2, n_3$ are integers.

<u>primitive lattice & Unit cell</u>

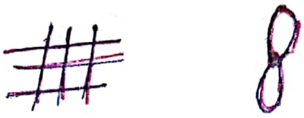
**Unit cell** is volume from which entire crystal can be constructed by translational repitition. ( OABC parallelogram)

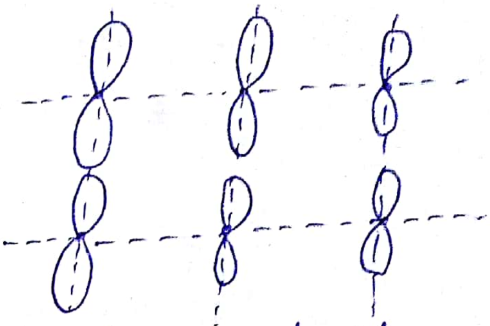
**primitive cell** is a type of unit cell that contain 1 lattice point at corners & minimum in volume $= |(\vec{a}\times\vec{b})\cdot\vec{c}|$



**Basis** In crystal structure, every lattice point is associated with an unit assembly of atoms/molecules/ions. This unit is called basis.

crystal structure = lattice + basis





Basis can contain even hundreds & thousands of molecules.

A translation operation leaves the crystal invariant.

$$f(\vec{r}) = f(\vec{r} + \vec{T})$$

**physical significance** : number density (point mass atom) $n(\vec{r}) = \sum_{\vec{T}} \delta(\vec{r} - \vec{T})$

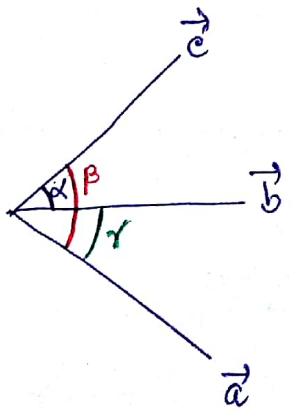
density $\rho(\vec{r}) = \sum_{\vec{T},\alpha} m_\alpha \, \delta(\vec{r} - \vec{T} - \vec{c}_\alpha)$

where $m_\alpha$ is mass of atom at lattice site $\vec{c}_\alpha$.

$$\rho(\vec{r}) = \rho(\vec{r} + \vec{T})$$

For cubic structure $|\vec{a}| = |\vec{b}| = |\vec{c}|$

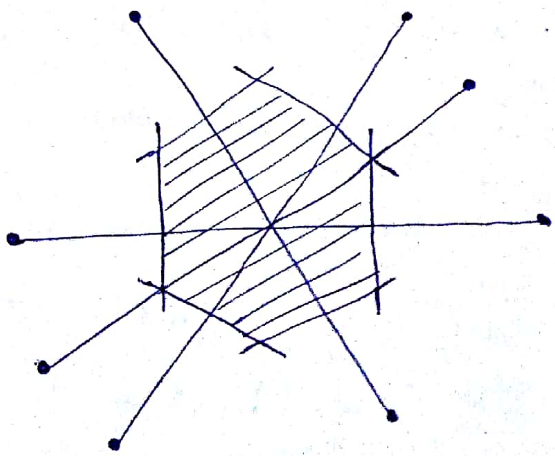
$\alpha = \beta = \gamma = \frac{\pi}{2}$



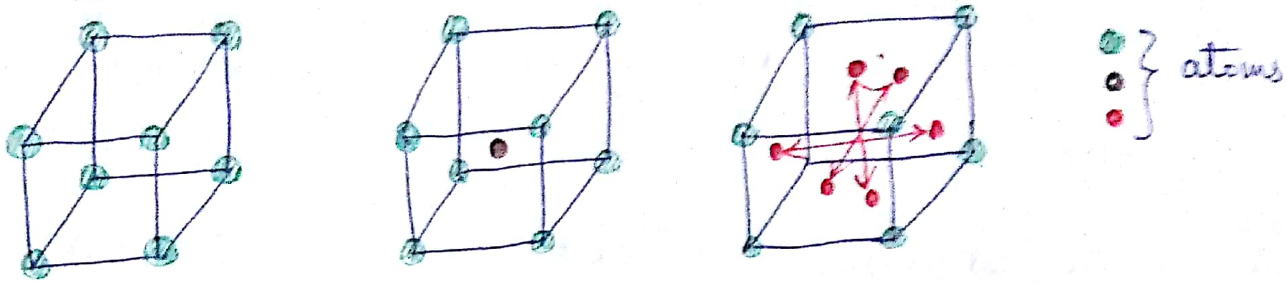

**Wigner-Sietz primitive cell**

1. Draw lines connecting nearby lattice points.
2. Draw planes/lines at midpoint of line & perpendicular to it.

This is WS primitive cell.



1 atom | 2 atom | 4 atom



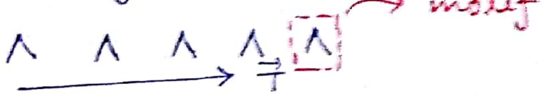

sc (primitive) | bcc | fcc

← unit cell →

## Elements of symmetry

A symmetry operation transforms the crystal to itself.

(i) Translation $\vec{r}' = \vec{r} + \vec{T}$




(ii) Rotation $n\phi = 2\pi$

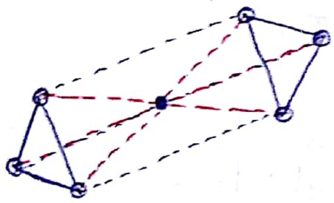
$\phi = 60^\circ$
$= \frac{2\pi}{6}$

$n$ = multiplicity of rotation axis.

= 1, 2, 3, 4, $\cancel{5}$, 6. A 2D square lattice has 4-fold rotational symmetry.

(iii) Reflection mirror image

(iv) Inversion
(only for 3D lattice)



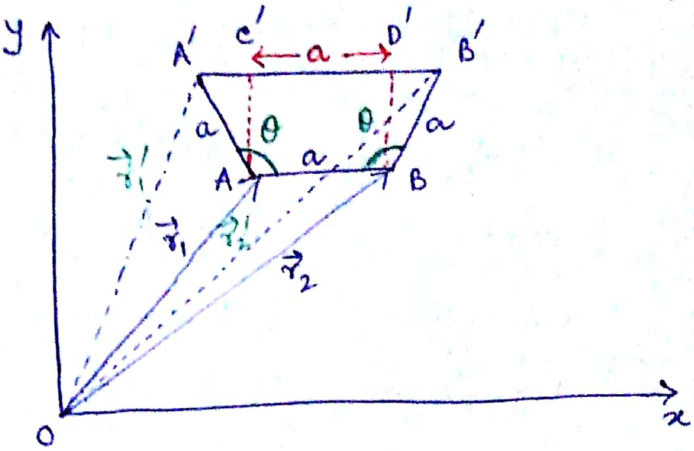
Symmetry operation performed about a point / line are called point group symmetry. 3 type of point group (i) plane of symmetry (reflection), (ii) axis of symmetry (rotation), (iii) centre of symmetry (inversion)

5-fold rotational symmetry : quasicrystals.

But why 5-fold rotational symmetry is not permissible in crystal structure ?

$AB = a = |\vec{a}| = |\vec{r}_1 - \vec{r}_2|$

$= AA' = BB'$




Suppose $A'B' = q|\vec{a}|$ ($q$ = integer)

$\angle A'AC' = \angle D'BB' = \theta - \pi/2$

$A'C' = D'B' = |\vec{a}| \cos\theta$

$\therefore A'B' = |\vec{a}| + |\vec{a}|\cos\theta + |\vec{a}|\cos\theta$

$q|\vec{a}| = |\vec{a}| + 2|\vec{a}|\cos\theta$ or $|\cos\theta| = \left|\frac{q-1}{2}\right|$

as $\cos\theta < 1$, allowed values of $q$ are $-1, 0, 1, 2, 3$

$\{q = -1, \theta = \frac{2\pi}{2}\}$, $\{q = 0, \theta = \frac{2\pi}{3}\}$, $\{q = 1, \theta = \frac{2\pi}{4}\}$

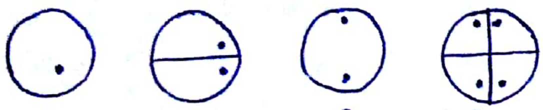
$\{q = 2, \theta = \frac{2\pi}{6}\}$, $\{q = 3, \theta = \frac{2\pi}{1}\}$.

So, $n = 1, 2, 3, 4, 6 \longrightarrow$ hexad.

diad (2), triad (3), tetrad (4)

## Point group & space group

[translation, rotation, reflection] (point) point group.



1    1m    2    2mm

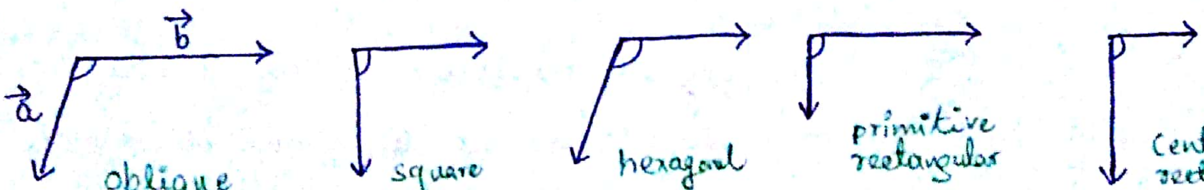
Total 32 point groups.

Group of all symmetry elements is space group.

In 2D : 17, 3D : 230.

## Bravais lattice :

$|\vec{a}|, |\vec{b}|, \phi$ 5 combination : symmetry operations are maintained.




| oblique | square | hexagonal | primitive rectangular | Centered rectangular |
|---|---|---|---|---|
| $\lvert\vec{a}\rvert \neq \lvert\vec{b}\rvert, \phi \neq \frac{\pi}{2}$ | $\lvert\vec{a}\rvert = \lvert\vec{b}\rvert, \phi = \frac{\pi}{2}$ | $\lvert\vec{a}\rvert = \lvert\vec{b}\rvert, \phi = \frac{2\pi}{3}$ | $\lvert\vec{a}\rvert \neq \lvert\vec{b}\rvert, \phi = \frac{\pi}{2}$ | $\lvert\vec{a}\rvert \neq \lvert\vec{b}\rvert, \phi = \frac{\pi}{2}$ |
| $\{\frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}\}$ rotation | $\{\frac{2\pi}{4}\}$ rotation | $\{\frac{2\pi}{6}\}$ rotation | $\{\frac{2\pi}{2}\}$ reflection | $\{\frac{2\pi}{2}\}$ inversion |