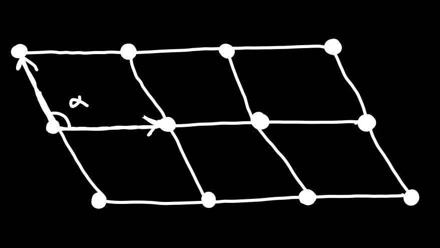
#Lecture: 8

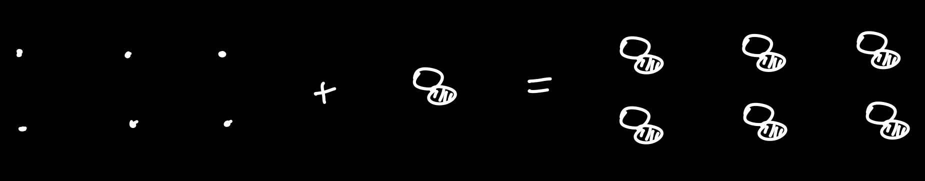
→ CRYSTAL LATTICE

replacing each atom by a geometrical point because only their geometry is of use.



POLYCRYSTALLINE → finite array of points in space

Crystal Structure = Crystal lattice + Basis



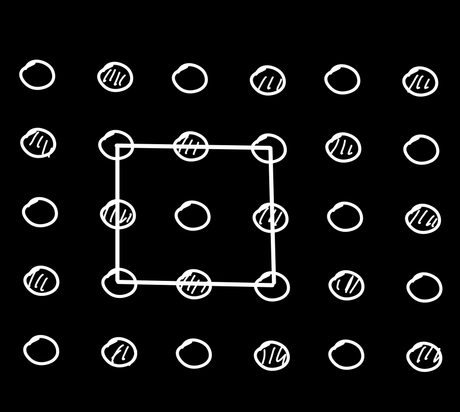
Crystal structures can be obtained by attaching atom, group of atoms, molecules which are called basis (motif) to the latice sides of the lattice point.

Unit Cell

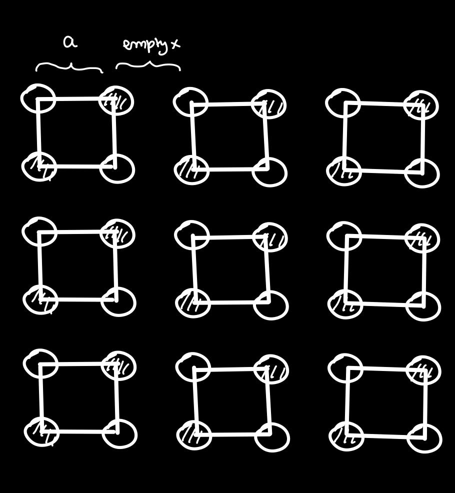
fundamental building block which repeats its own dimensions in various directions and gives crystal structure.

unit cell size should be constant throughout the crystal structure

eg: 2dimensional NaCl



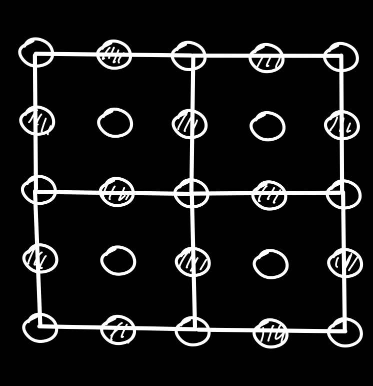
eg2:



→ Empty space is not allowed

→ periodicity not maintained in context of translational and rotational symmetry.

eg3



valid ✓
no spaces ✓
full symmetry ✓
unit cells are linked up. ✓

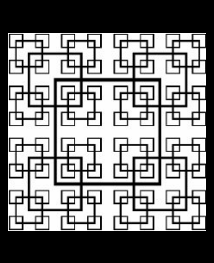
NOTE: A structure is a crystal if we can define its unit cell without violating the above rules.

→ no void space

→ fulfill rotational & translational symmetry (i.e. every unit cell should be linked up)

(≡ Periodicity implies translational symmetry)

eg)

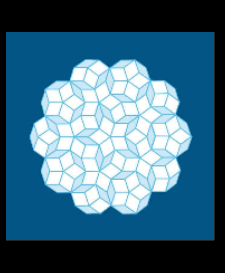


FRACTAL
self similarity
eg: silica aerogel

is this fractal a valid crystal structure ?

No, because even though we can find a repeating pattern, we cannot link up the unit cells. i.e. there is no translational symmetry

eg)



No, because even though it maintains rotational symmetry but it does not maintain translational symmetry

QUASI CRYSTAL
aperiodic, yet exhibits orientational Symmetry

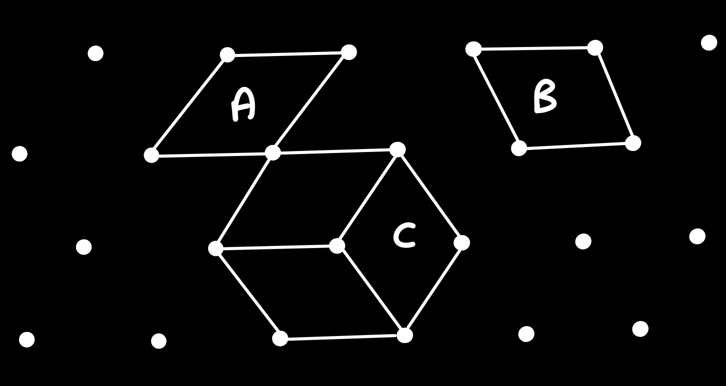
CONVENTIONAL/ PRIMITIVE UNIT CELL

→ minimum volume unit cell.

→ always consists of only ONE basis.

→ There can be multiple primitive unit cells in a single crystal structure.

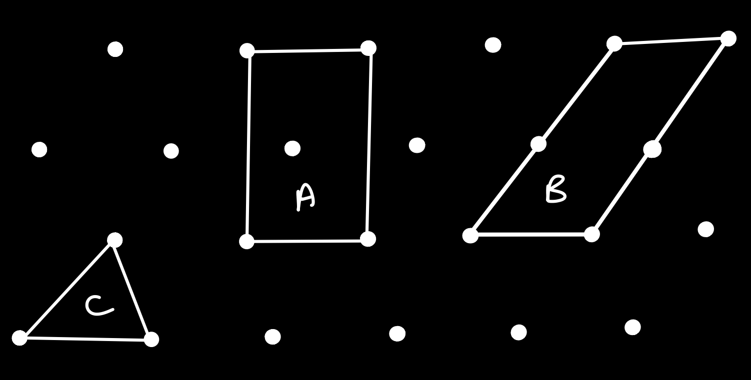
eg)



valid ✓

C ≡ SUPERCELL / CONVENTIONAL CELL

eg2)



invalid because A and B contain more than one basis and C contains empty space

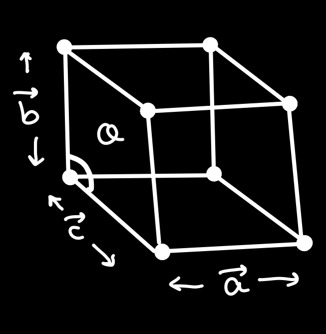
PRIMITIVE UNIT CELL VECTOR

$$\bar{R} = u\bar{a} + v\bar{b} + w\bar{c}$$

u, v, w : integers

a, b, c : primitive, if the volume of cell is smallest possible

lattice constant



$\bar{a}$: along x axis

$\bar{b}$: along y axis

$\bar{c}$: along z axis

$$\boxed{V_c = \bar{a} \cdot (\bar{b} \times \bar{c})}$$

RULES

→ $\bar{a}$ should be the shortest period of the lattice

→ $\bar{b}$ to shortest period and non-parallel to $\bar{a}$

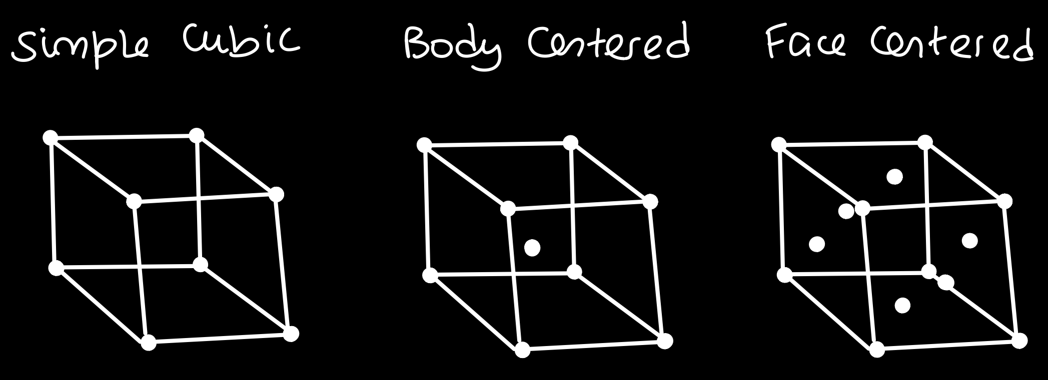
→ $\bar{c}$ to shortest period and non-parallel to ($\bar{a}$ & $\bar{b}$)

BRAVAIS LATTICE

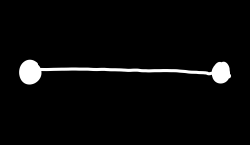
There are just 14 3d crystal lattices out of which 7 are main and other are subdivision of those main.

Seven main dimensions:

Cubic, Tetragonal, Orthorhombic, Hexagonal, Trigonal, Monoclinic, Triclinic

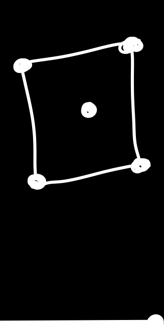

Simple Cubic — Body Centered — Face Centered

In 1D, we have just one Bravais Lattice

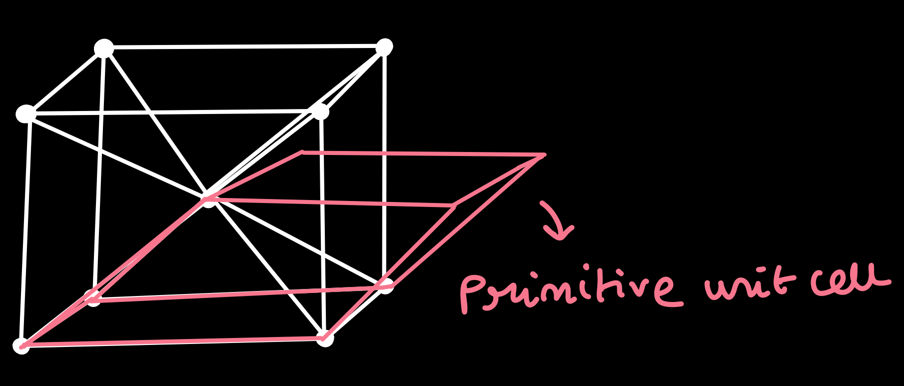


In 2D, we have 5 main divisions.

→ Square : $a = b$, $\theta = 90°$
→ Rectangle : $a \neq b$, $\theta = 90°$
→ Rhombus : $a = b$, $\theta = 60°$
→ Parallelogram : $a \neq b$, $\theta = 60°$
→ Body centered cube



BCC



There are two atoms in the conventional unit cell in the Body Centered Cube.

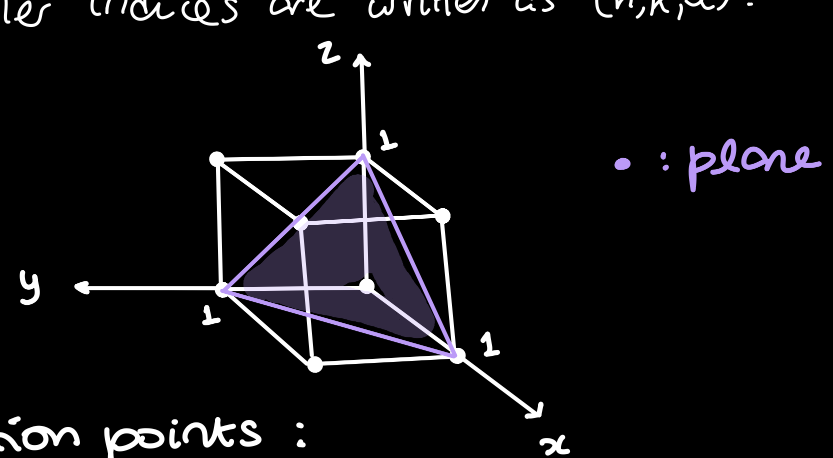
In case of FCC, we have 4 atoms in the conventional unit cell.

MILLER INDICES

Set of three integers that represent the orientation of a crystal plane or set of parallel planes.

miller indices are written as (h, k, l).

eg)

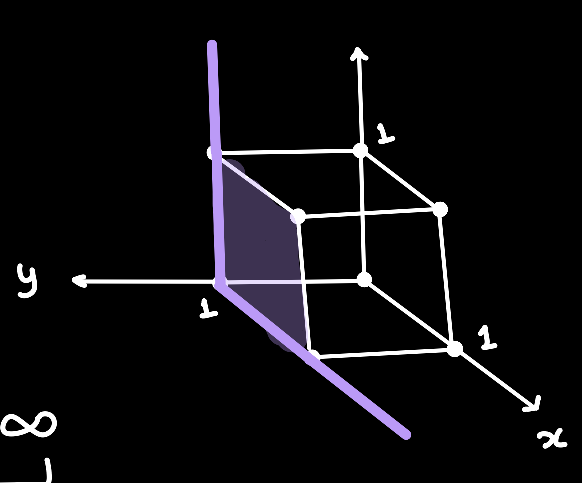


intersection points :

$$1 \quad 1 \quad 1$$
$$\Big\downarrow \text{reciprocal}$$
$$\frac{1}{1} \quad \frac{1}{1} \quad \frac{1}{1}$$
$$\downarrow$$

(1, 1, 1) → miller indices

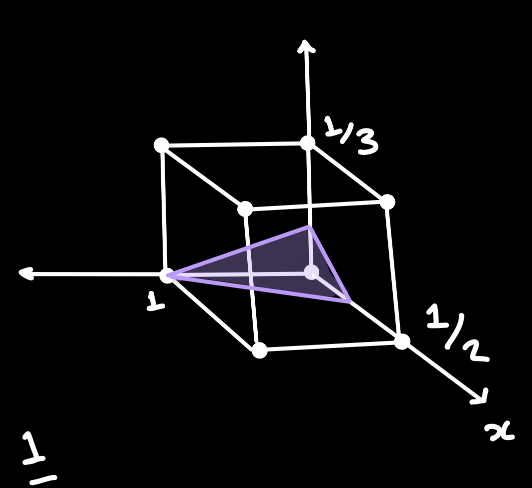
eg)



$$\underbrace{1 \quad \infty \quad \infty}$$
$$\downarrow$$
$$\underbrace{\frac{1}{1} \quad \frac{1}{\infty} \quad \frac{1}{\infty}}$$
$$\downarrow$$

(1, 0, 0) → miller indices

eg)



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

(1, 3, 2)