Day - 15

→ Alternative crystal structure description —

Atoms tend to arrange in close-packed configurations

→ hard spheres

close-packed structures : $\geq$ 6 nearest neighbours

↓

Simplest eg: Simple Cubic (6)

BCC → 8

FCC → 12

HCP → 12

→ Atomic Packing Fraction (APF) $= \dfrac{V_{atoms}}{V_{unit\,cell}}$

↓

only for hard sphere model.

for BCC : $V_{atoms} = 2 \times \frac{4}{3}\pi r^3 = \frac{8\pi r^3}{3}$

$V_{UC} = a^3$

so $APF = \frac{8\pi}{3}\left(\frac{r}{a}\right)^3$

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

so $APF = \frac{8\pi}{3} \times \frac{3\sqrt{3}}{64}$

$= \frac{\sqrt{3}\pi}{8}$

$\simeq 68\%$

for FCC : $V_{atoms} = 4 \times \frac{4}{3}\pi r^3$

$$= \frac{16\pi r^3}{3}$$

$$APF = \frac{16\pi}{3}\left(\frac{r}{a}\right)^3$$

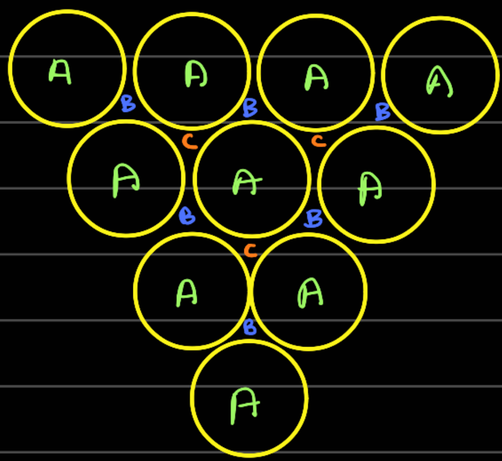
But $4r = \sqrt{2}a \Rightarrow \frac{r}{a} = \frac{1}{2\sqrt{2}}$

$$= \frac{16\pi}{3} \times \frac{1}{16\sqrt{2}} = \frac{\pi}{3\sqrt{2}} \simeq 74\%$$

$\downarrow$

Highest achievable APF (Kepler conjecture)

→ Closed Packed plane



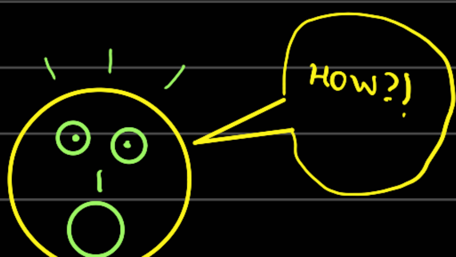
A-plane (arbitrarily labelled)

we can choose either B or C

Choose B, then stack on C. It can be repeated again (ABCABC....)

we can have ABAB.....

OR ABC ABABABC also!



But nature chooses — ABC — (CCP) → (111) plane of FCC

— AB — (HCP) → (001) plane (hP) with 2 atoms/u.c.

☆ Even though you can close-pack spheres in 3D, a max. of 74% of u.c can be occupied.

26% lost space → putting different-sized atoms

Locations where the centres of these different sized atoms can be arranged in a regular fashion → interstitial positions

↓

2 types: I finds itself no. of lattice atoms (L) coordinated to it

4 → tetrahedral interstice

6 → octahedral interstice

No. of interstitial position in one u.c. or per lattice atom.

<u>Octahedral:</u>

1 Body centre → 1

12 edge centres → $12 \times 1/4 = 3$

$1+3 = 4$ octahedral sites $\longrightarrow 1:1$
(4 lattice sites)

8 tetrahedral sites $\longrightarrow 2:1$

hcp: no. of lattice atoms $= 2$

octahedral $\longrightarrow 2$
tetrahedral $\longrightarrow 4$

BCC $\longrightarrow$ NO regular tetrahedral sites.