



Crystal Structure

Thapar Institute of Engineering & Technology
(Deemed to be University)

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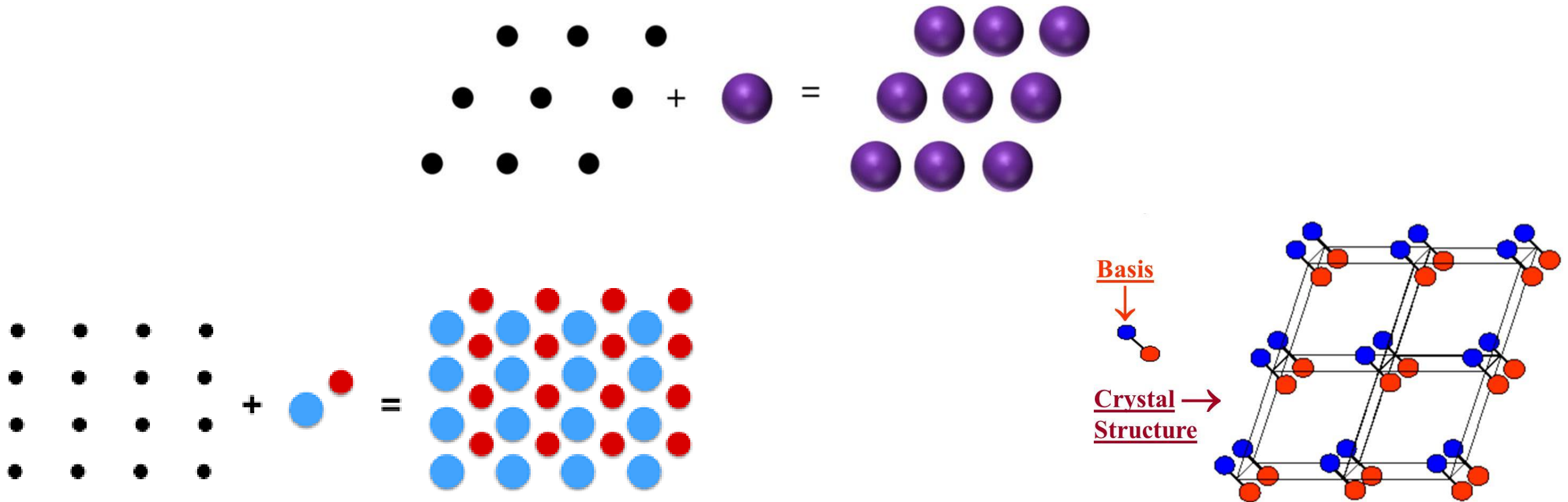
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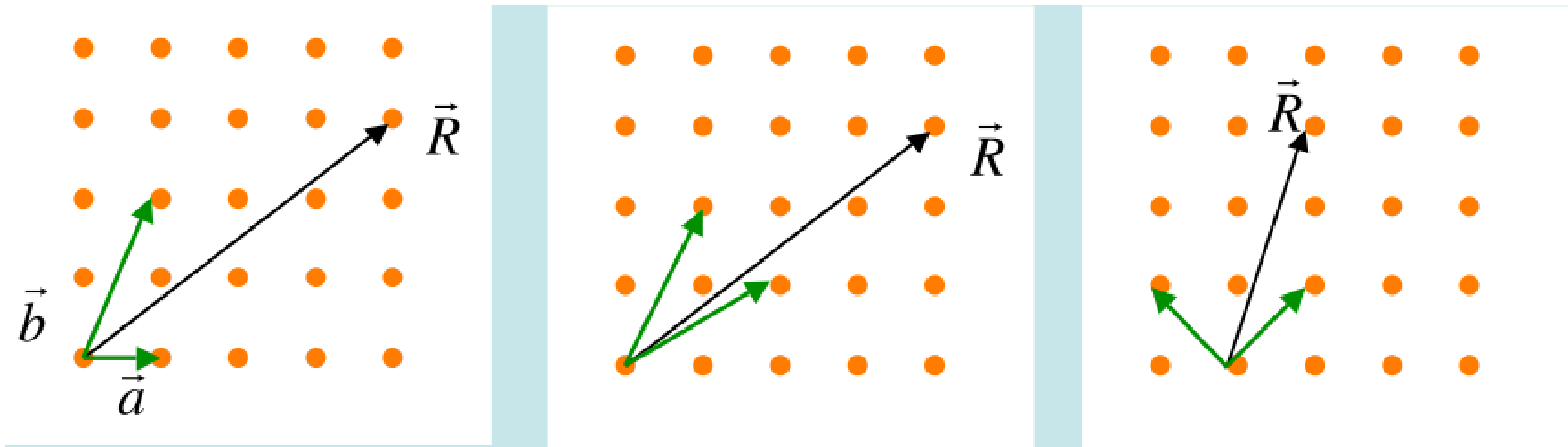
The atoms do not necessarily lie at lattice points !!



Lattice + Basis = Crystal Structure

We can have more than one atoms, ions and molecules at each lattice point.

$\vec{R} = n_1 \vec{a} + n_2 \vec{b}$, “a” and “b” are the repeating distance in 2-D

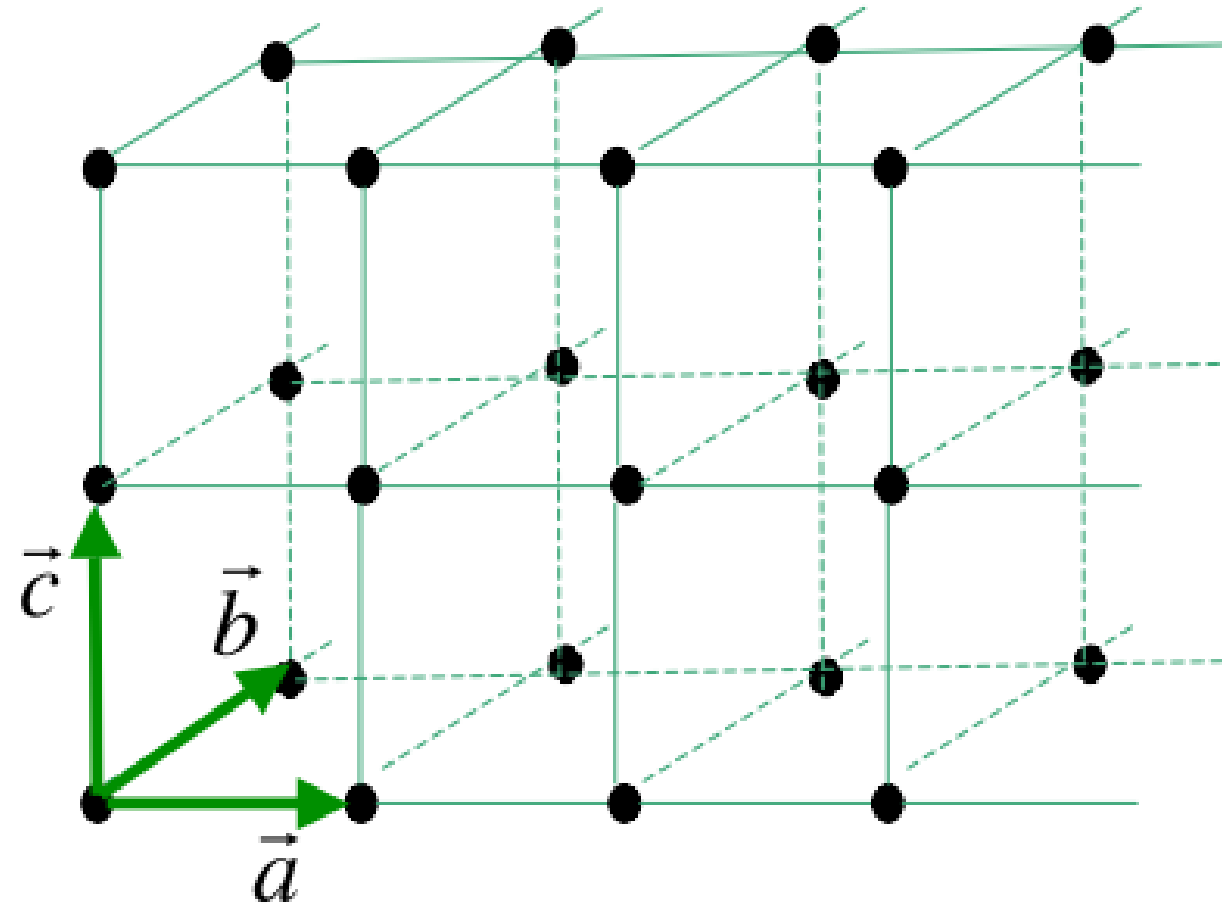


The repetition of translation vector \vec{R} gives the crystal structure in 2-D

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

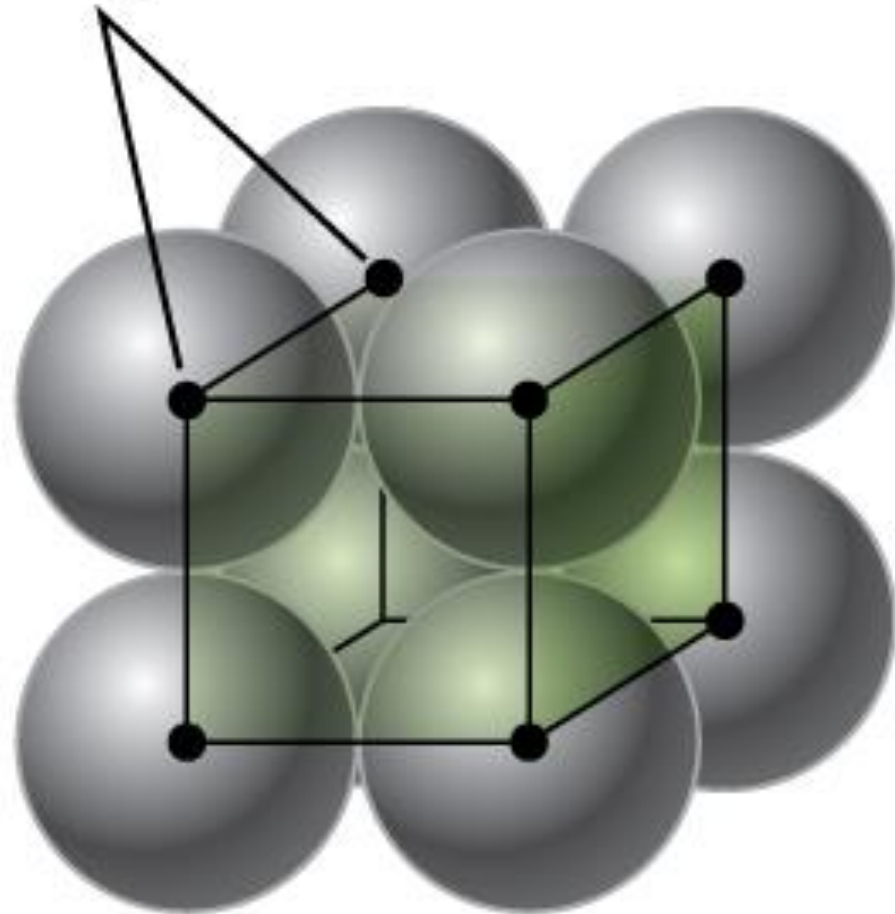
repeating distance in 2-D

“a” and “b” and “c” are the

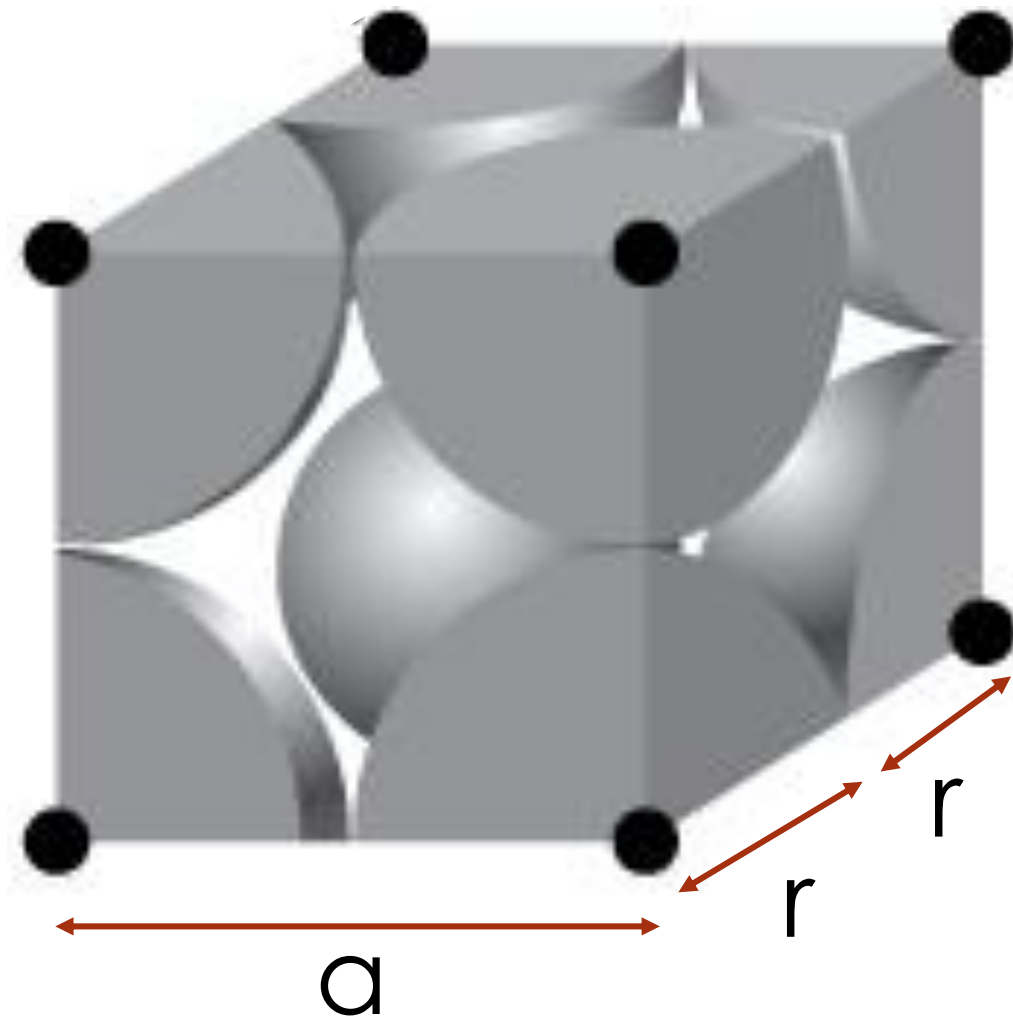


The repetition of translation vector R gives the crystal structure in 3-D

Lattice points

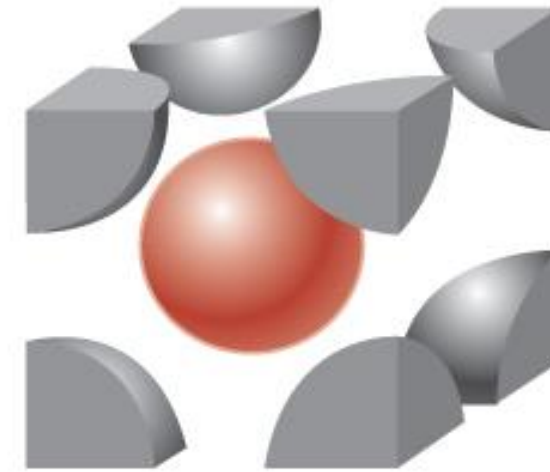
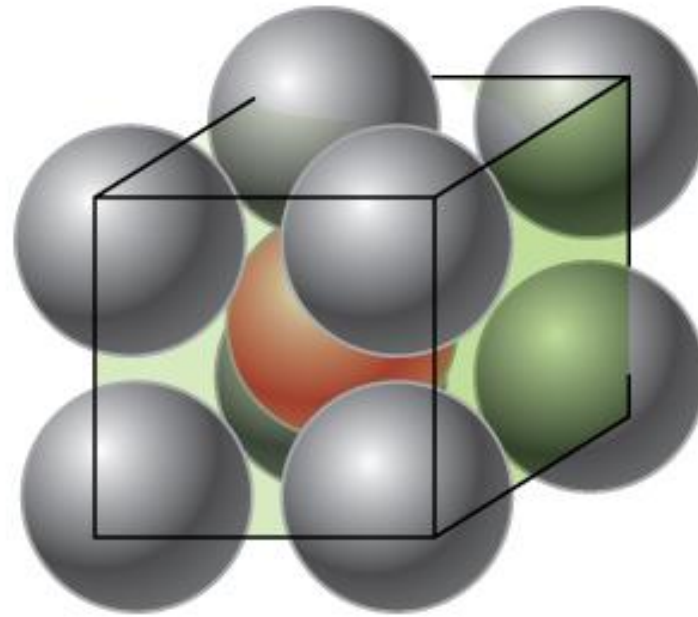
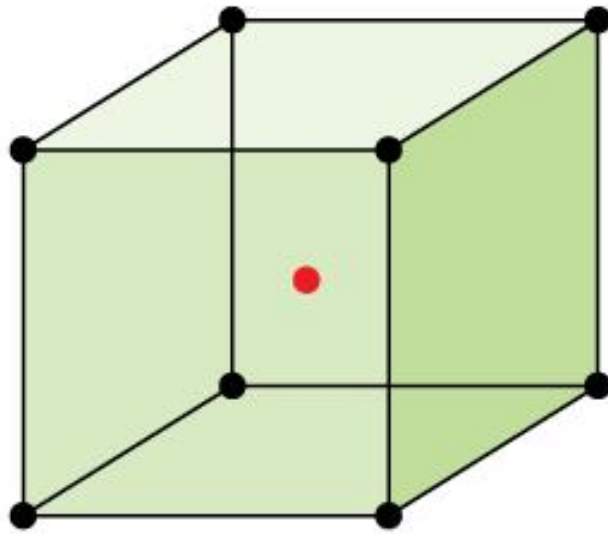


Simple cubic lattice cell



Lattice points in a unit cell : $\frac{1}{8} * 8 = 1$

Body centered cubic (BCC)

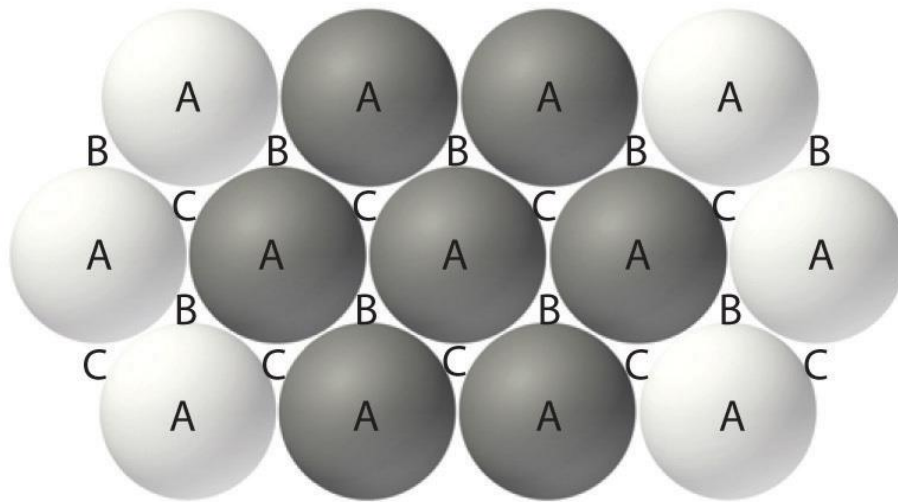


Body-centered cubic structure

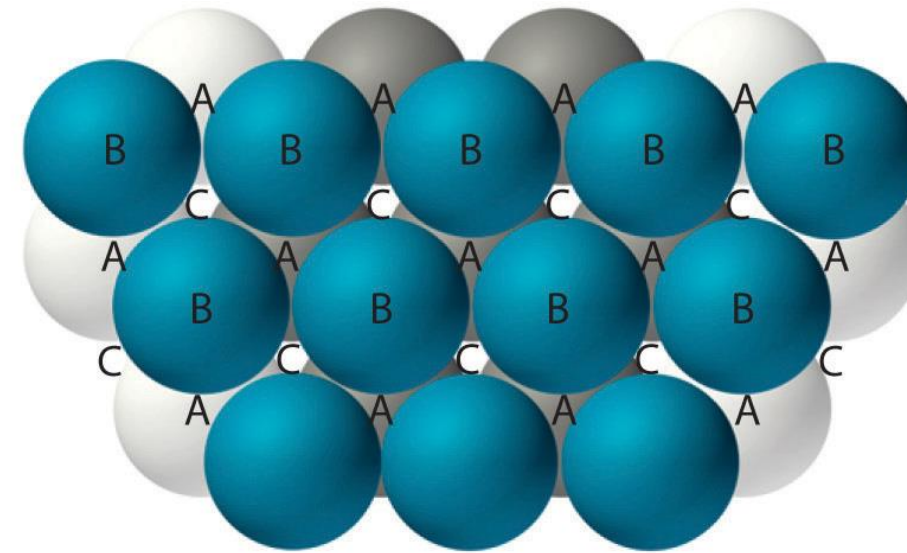
Lattice points in a unit cell : $\frac{1}{8} * 8 + 1 = 2$

Closed packed structures

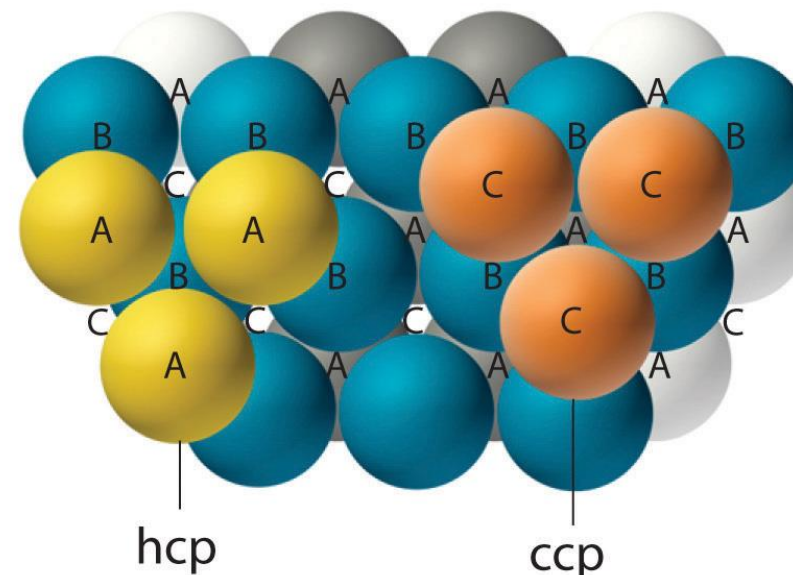
Closed packed structures have highest density in a unit cell



(a) Single layer



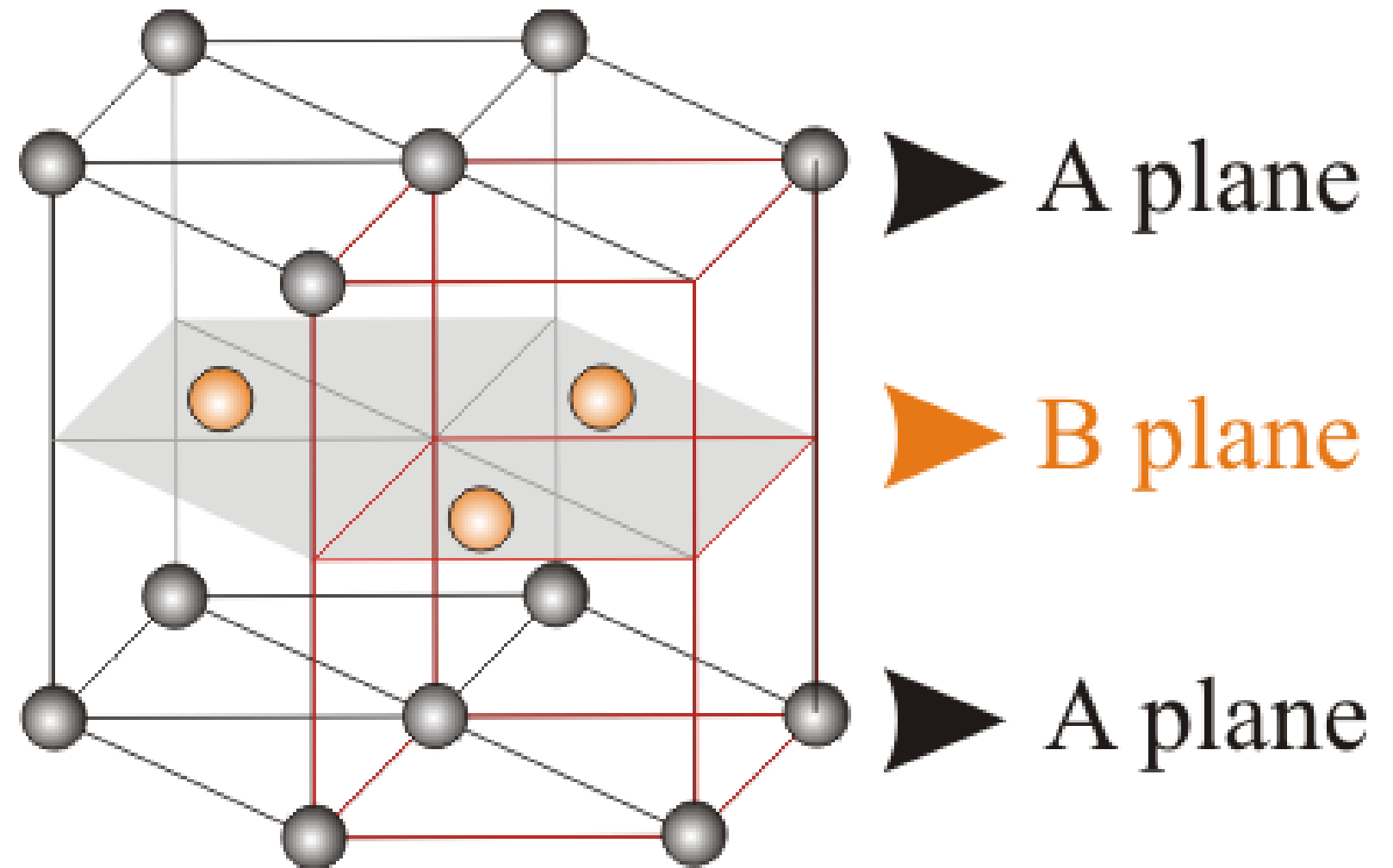
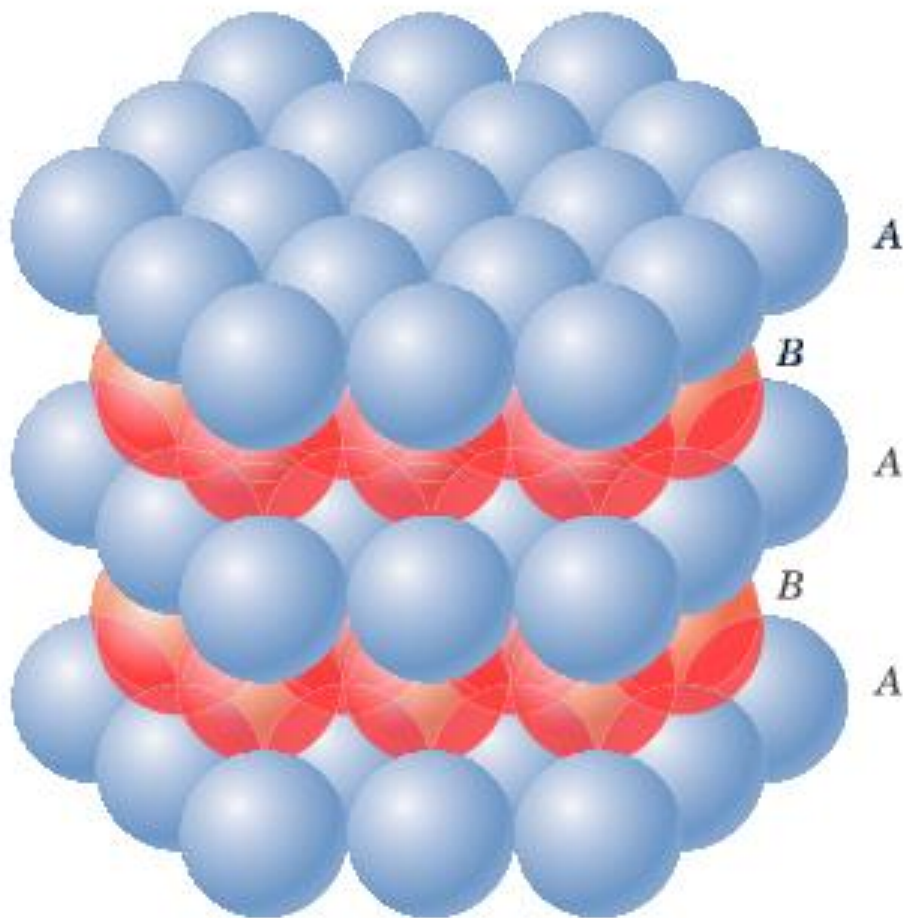
(b) Two layers



(c) Three layers

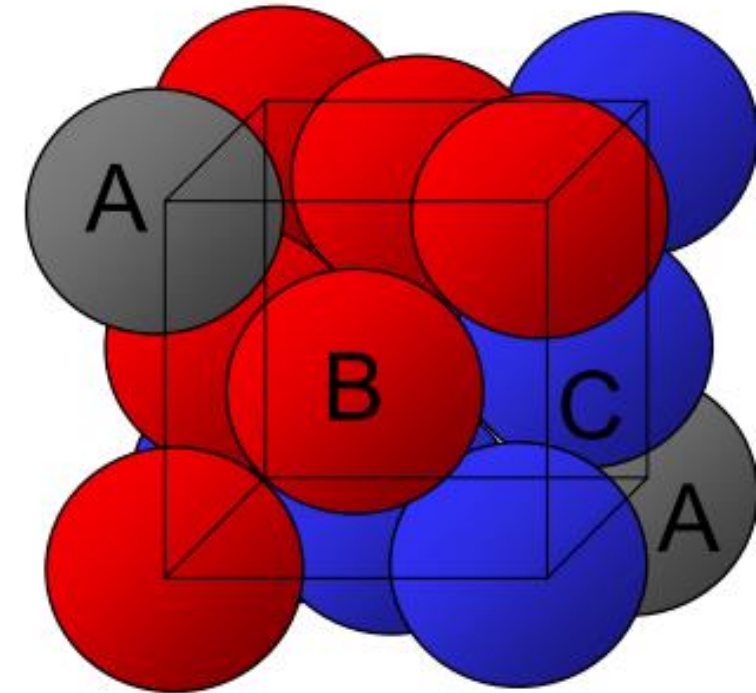
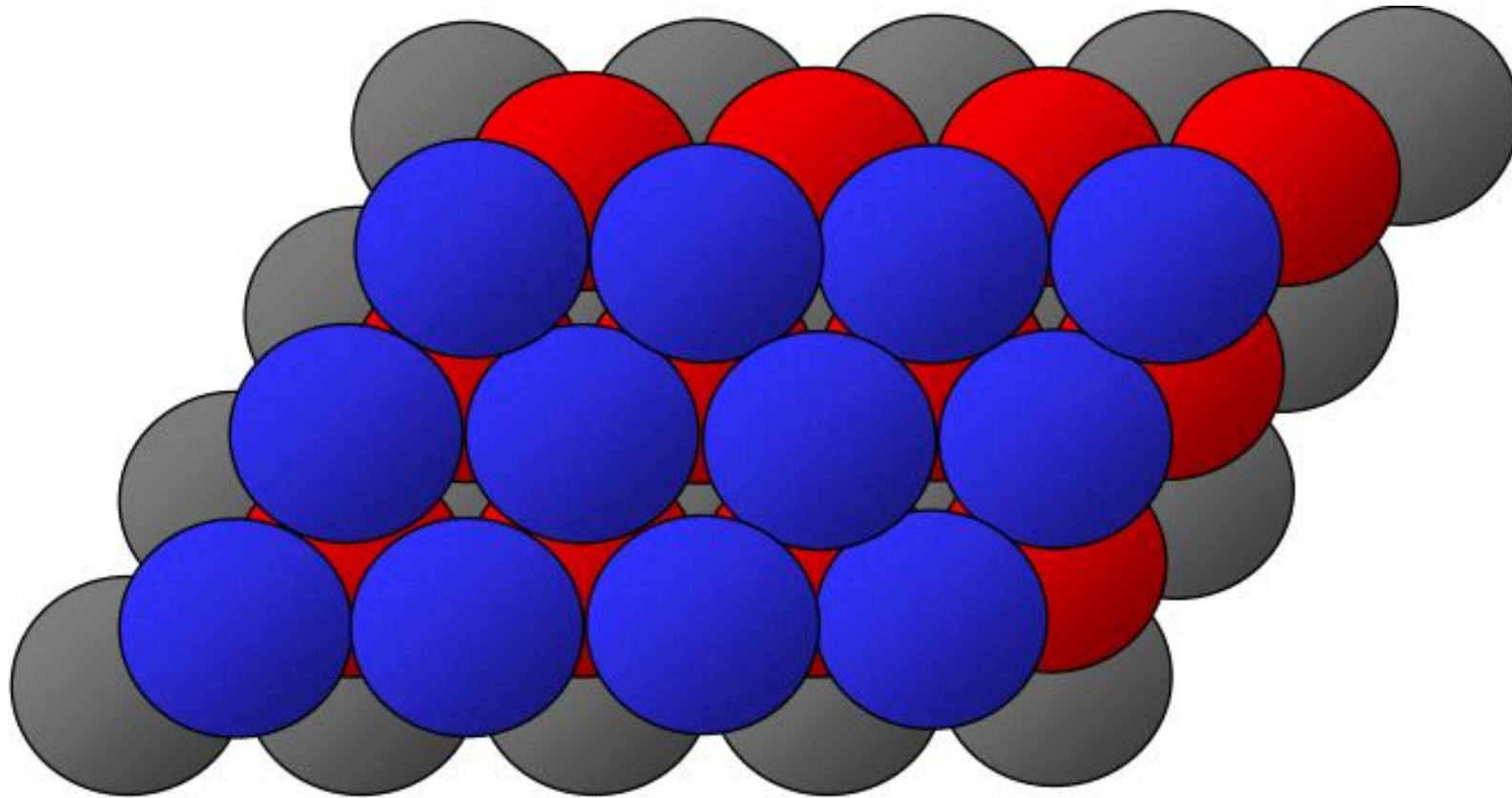
Hexagonal closed packed cubic (HCP)

Both FCC and HCP are closed packed structures



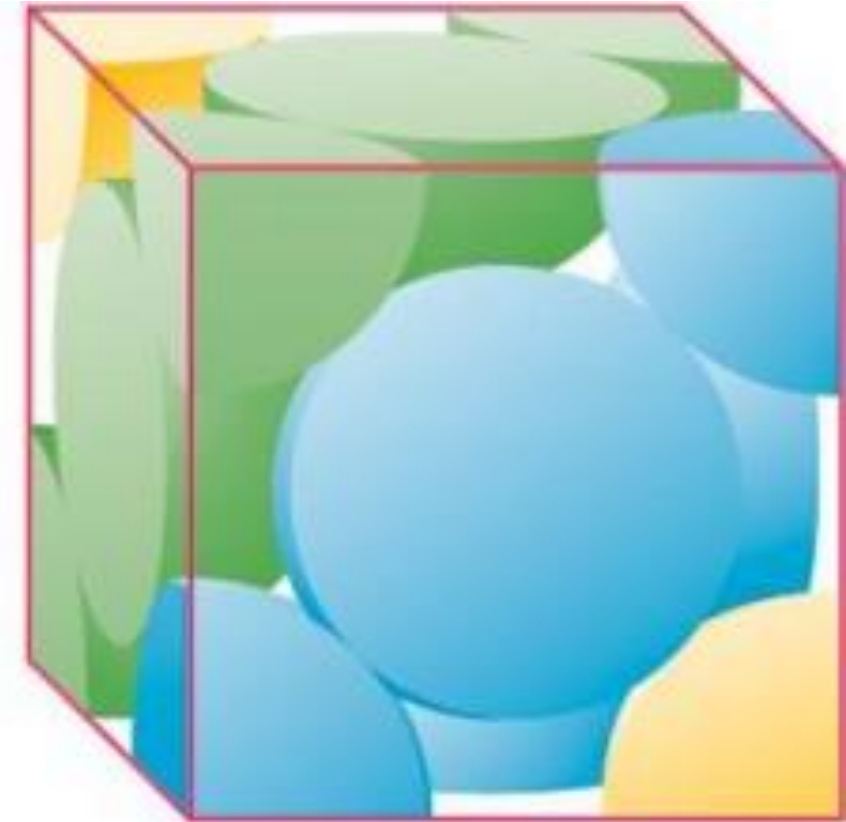
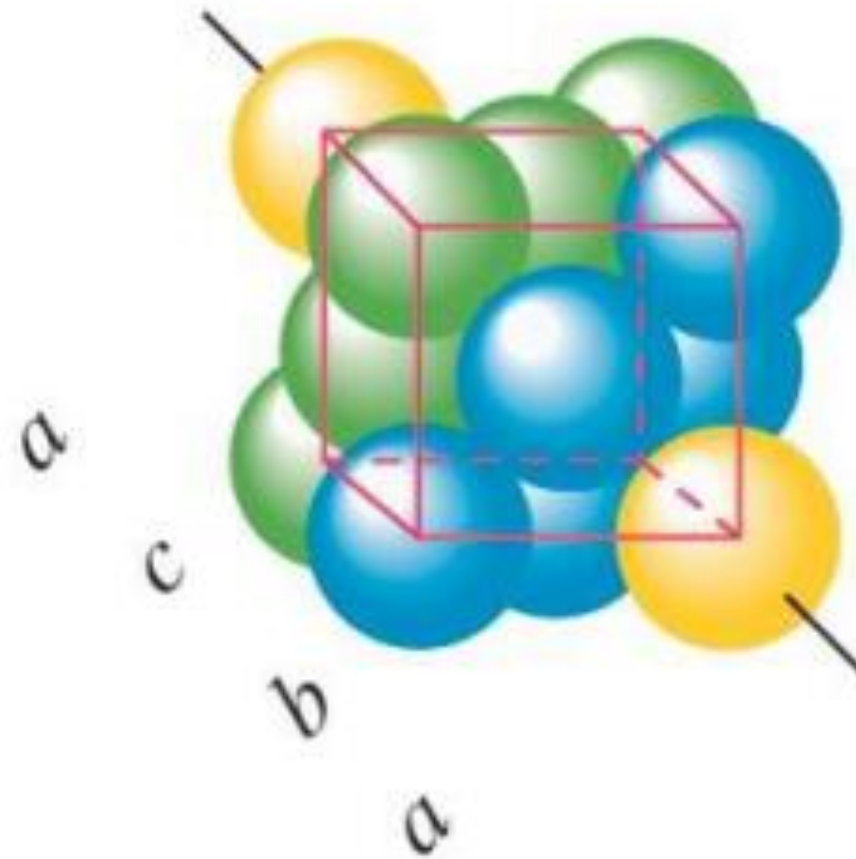
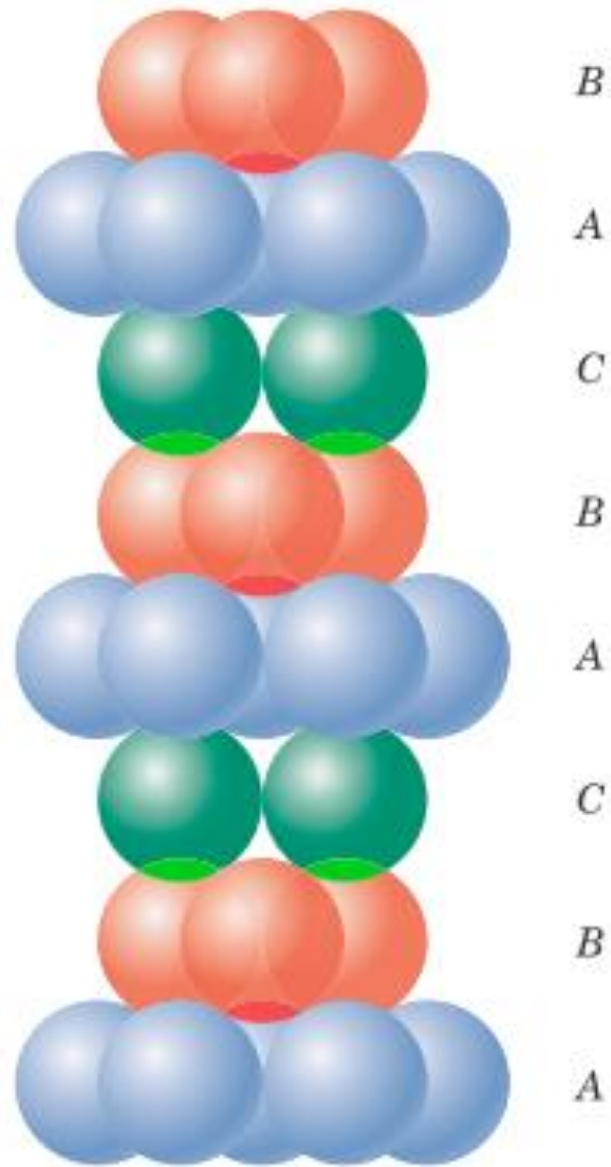
Showing 3 unit cells and the rhombic prism UC

Face centered cubic (FCC)

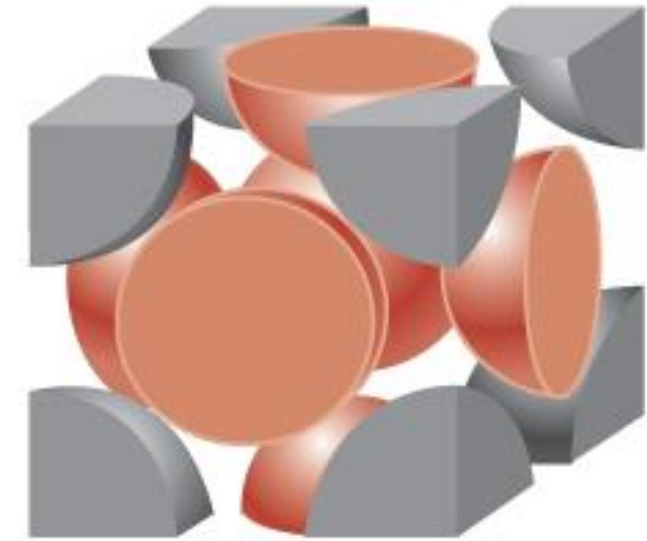
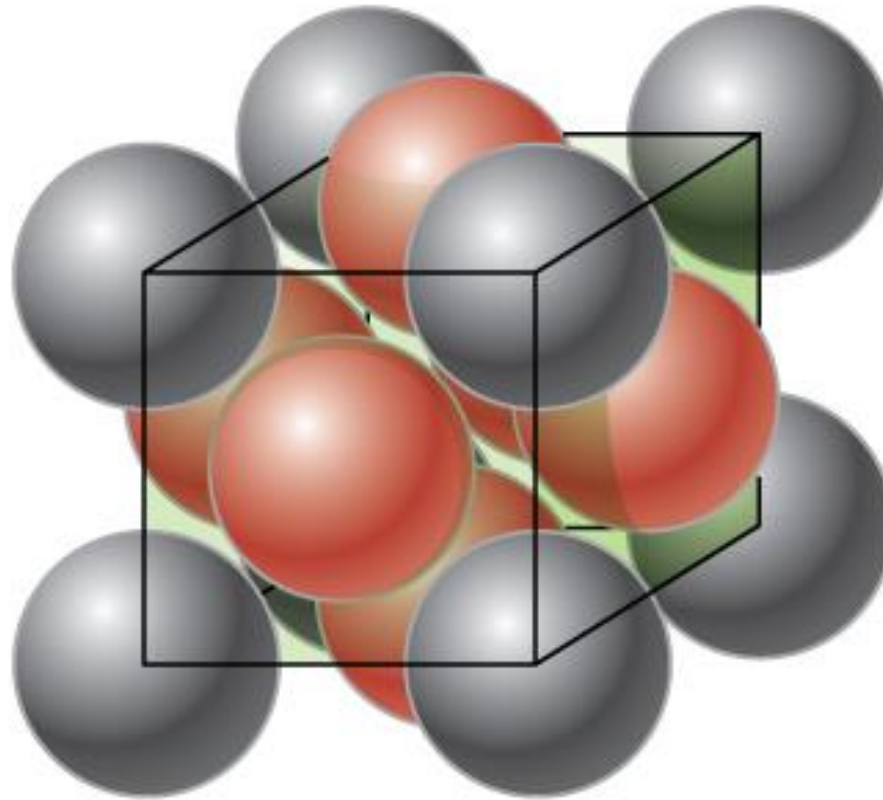
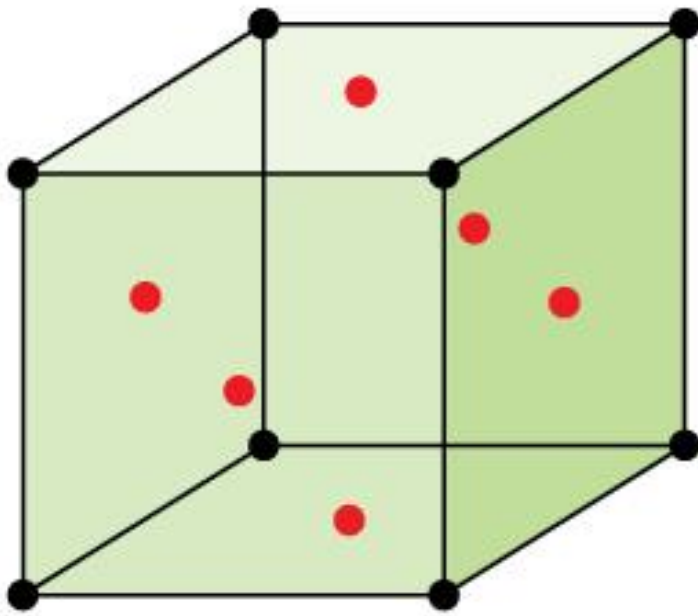


Face centered cubic (FCC)

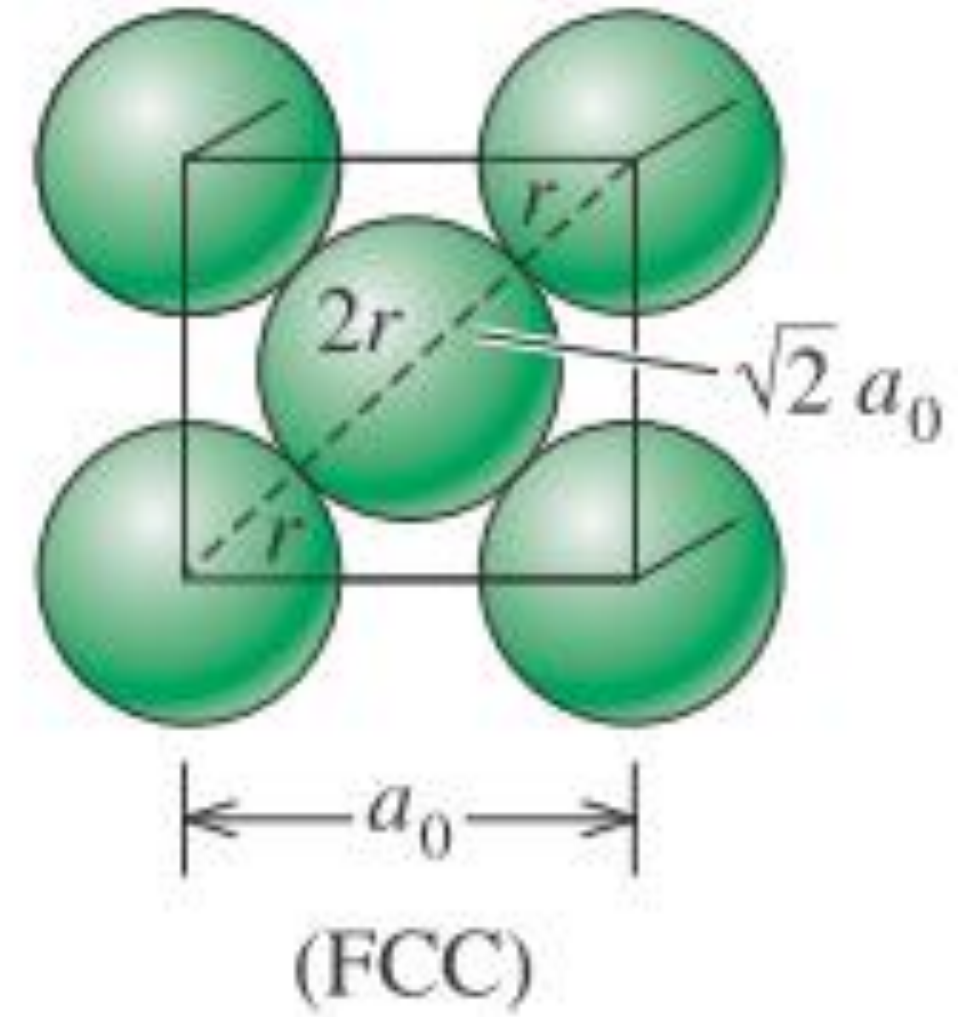
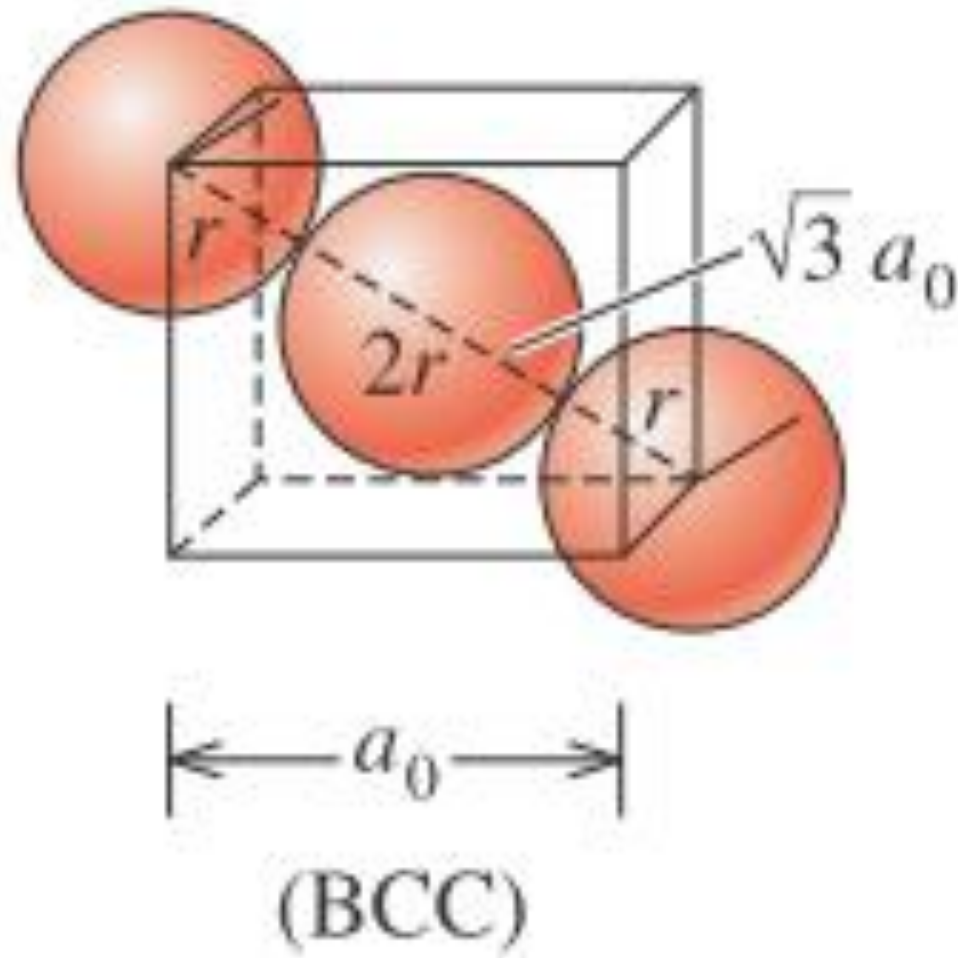
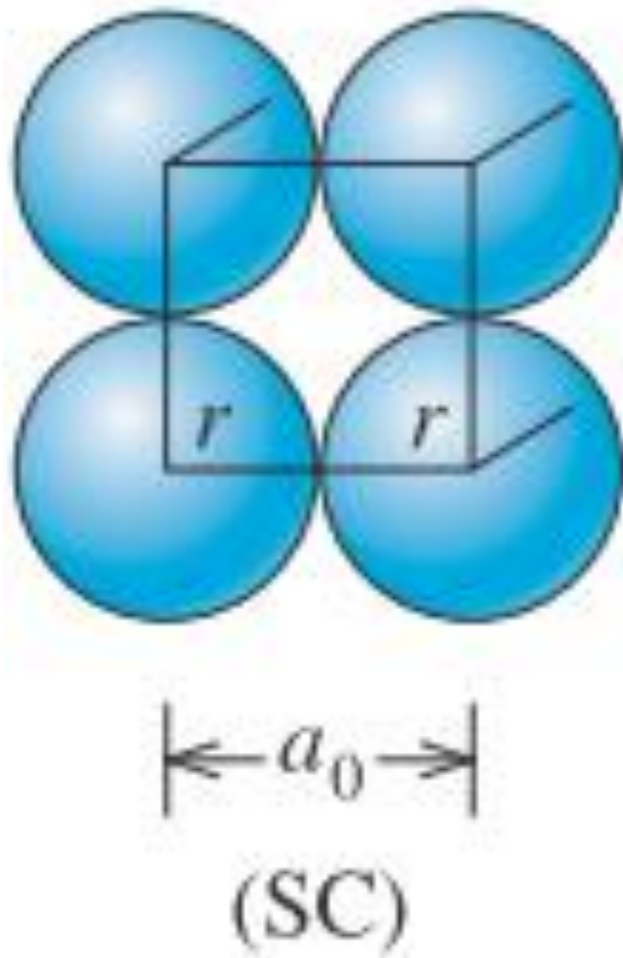
Both FCC and HCP are closed packed structures



Face centered cubic (FCC)



Lattice points in a unit cell : $\frac{1}{8} * 8 + \frac{1}{2} * 6 = 4$



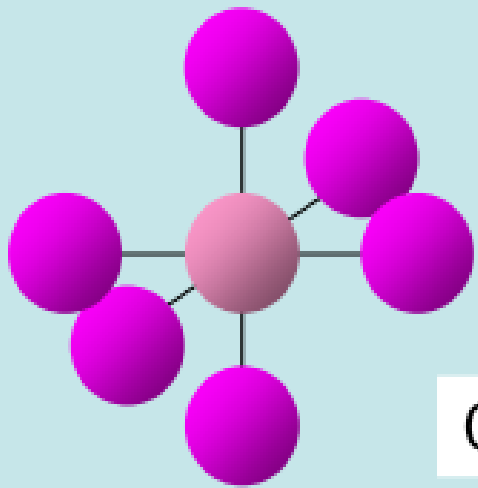
SC: $a = 2r$

BCC: $a\sqrt{3} = 4r$ (body diagonal)

FCC: $a\sqrt{2} = 4r$ (face diagonal)

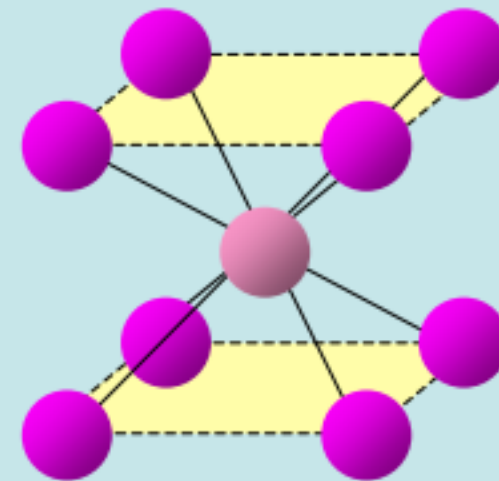
Co-ordination number(CN)

No. of nearest neighbors (No. of atoms touching)



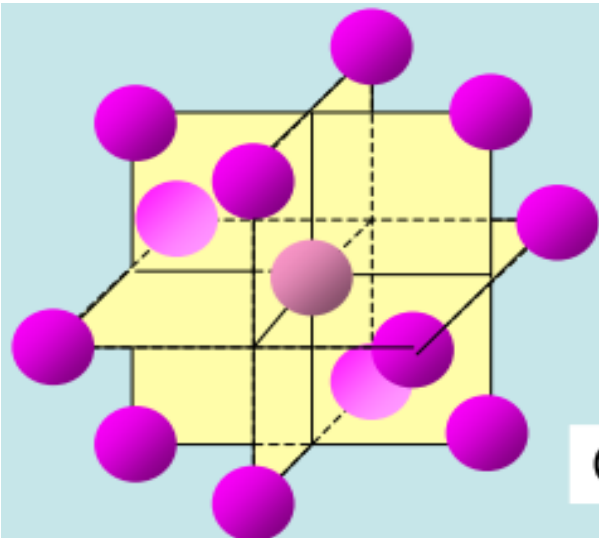
Coordination number = 6

SC



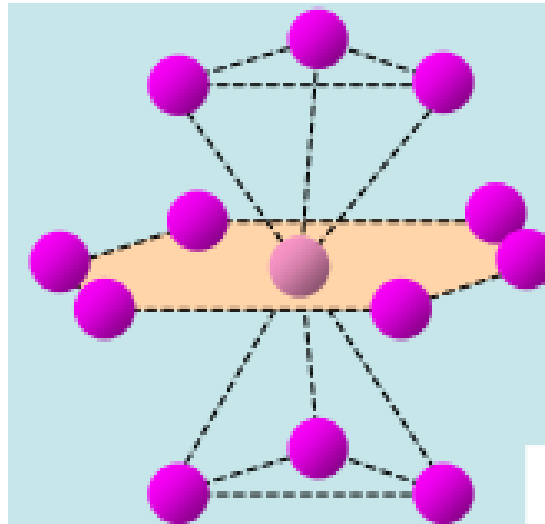
Coordination number = 8

BCC



Coordination number = 12

FCC



Coordination number = 12

HCP

Atomic Packing Fraction (APF)

14

Packing density of the monoatomic unit cell

Atom is assumed as a hard sphere

$$APF = \frac{\text{No of atoms in a unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}}$$

Unit cell is cubic
So a^3

Structure	No. of atoms	APF
SC	1	52%
BCC	2	68%
FCC	4	74%

Density of a crystalline material can be calculated by

The diagram illustrates the formula for the density of a crystalline material, $\rho = \frac{n \times A}{N_A \times V}$. Red arrows point from descriptive labels to the variables in the formula:

- Density of a material** points to ρ .
- No. of atoms in a unit cell** points to n .
- Atomic weight** points to A .
- Avogadro's Number** points to N_A .
- Volume of the unit cell** points to V .

$$\rho = \frac{n \times A}{N_A \times V}$$

1. Lattice + basis gives the crystal structure.
2. A lattice point can have more than one atom at its position.
3. Co-ordination number is the number of atoms touching to the particular atom.
4. CN of SC is 6, BCC is 8, and of FCC and HCP is 12.
5. Both FCC and HCP are closed packed structure.
6. In FCC, the atomic layer arrangement is like ABC ABC ABC.
7. In HCP, the atomic layer arrangement is like AB AB AB.
8. Monoatomic unit cell has equal number of atoms and lattice points.

1. What is mean by monoatomic cubic crystal?
2. Find the APF of SC, BCC and FCC unit cells.
3. Gold has atomic weight 197 and the density 19.3 gm/cc. What is the spacing between atoms in solid gold?
4. Cu has FCC structure and its atomic radius is 1.278 Å. Calculate the theoretical density of Cu. Atomic weight of Cu is 63.54 gm/mole.
5. Ti undergoes a phase change from BCC to HCP at 880°C on cooling. Calculate the percentage change in the volume. Given lattice parameter $a_{\text{BCC}} = 3.32 \text{ Å}$, $a_{\text{HCP}} = 2.956 \text{ Å}$, $c = 4.683 \text{ Å}$.
6. Iron (atomic weight 56.05 gm/mole) change from BCC to FCC at 910 °C. At this atomic radius of iron is 1.258 Å in BCC and 1.298 Å in FCC. What is the percentage of (a) volume change and (b) linear change in iron when heated through this temperature range?
7. Aluminum has FCC structure. Its density is 2700 Kg/m³. Calculate the unit cell dimension and the atomic diameter.