Crystal Structure

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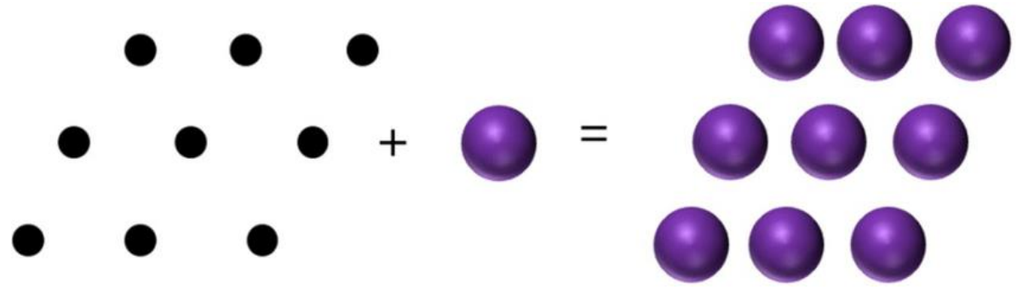
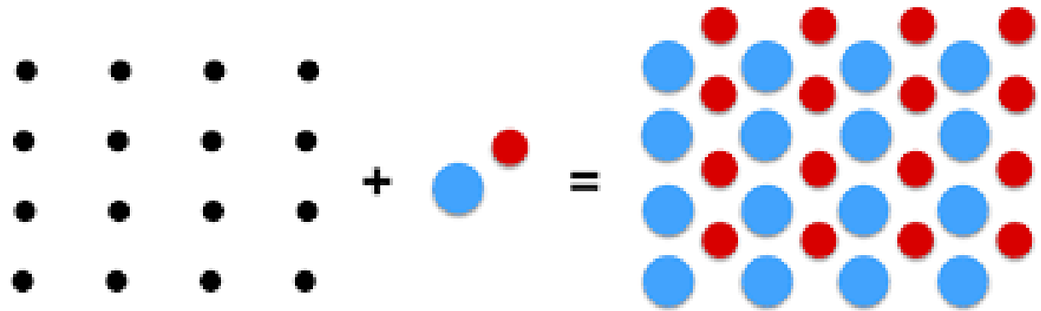
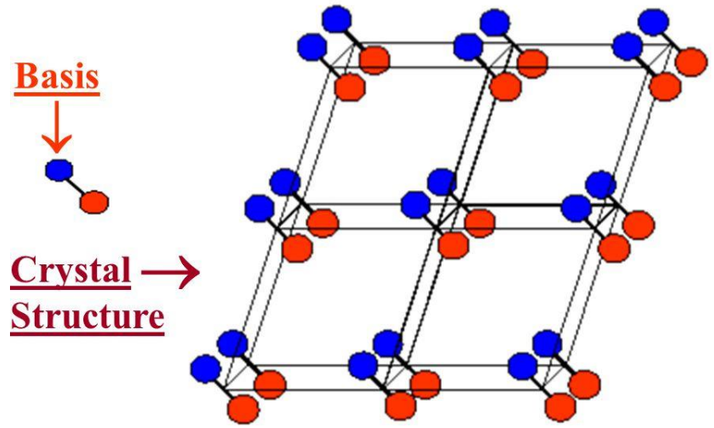
Basis or Motif

The atoms do not necessarily lie at lattice points !!





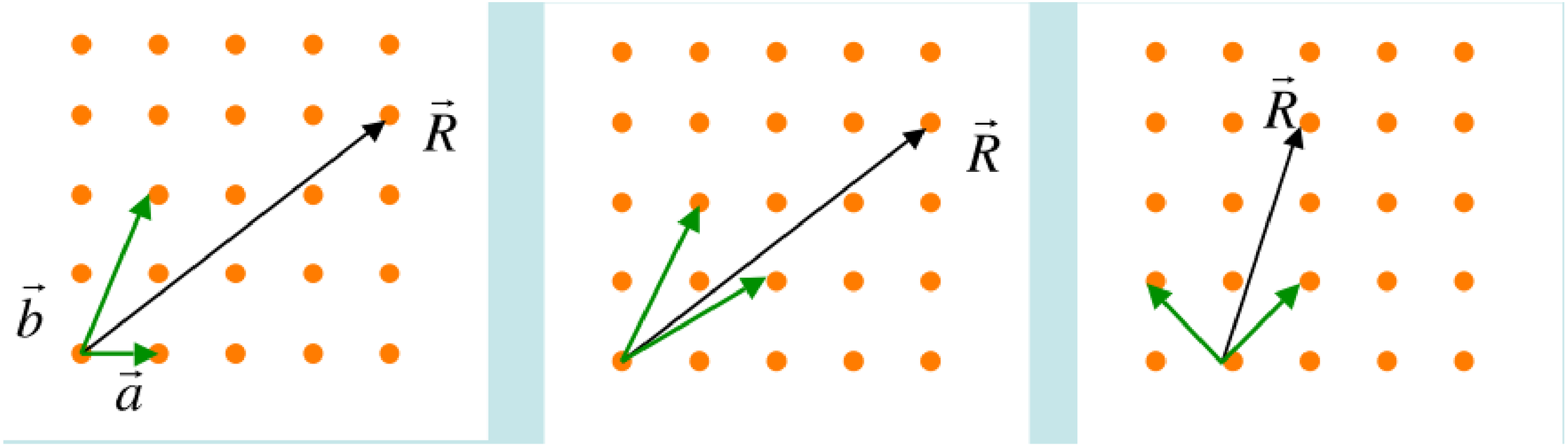


Lattice + Basis = Crystal Structure

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

Primitive vectors in 2-D

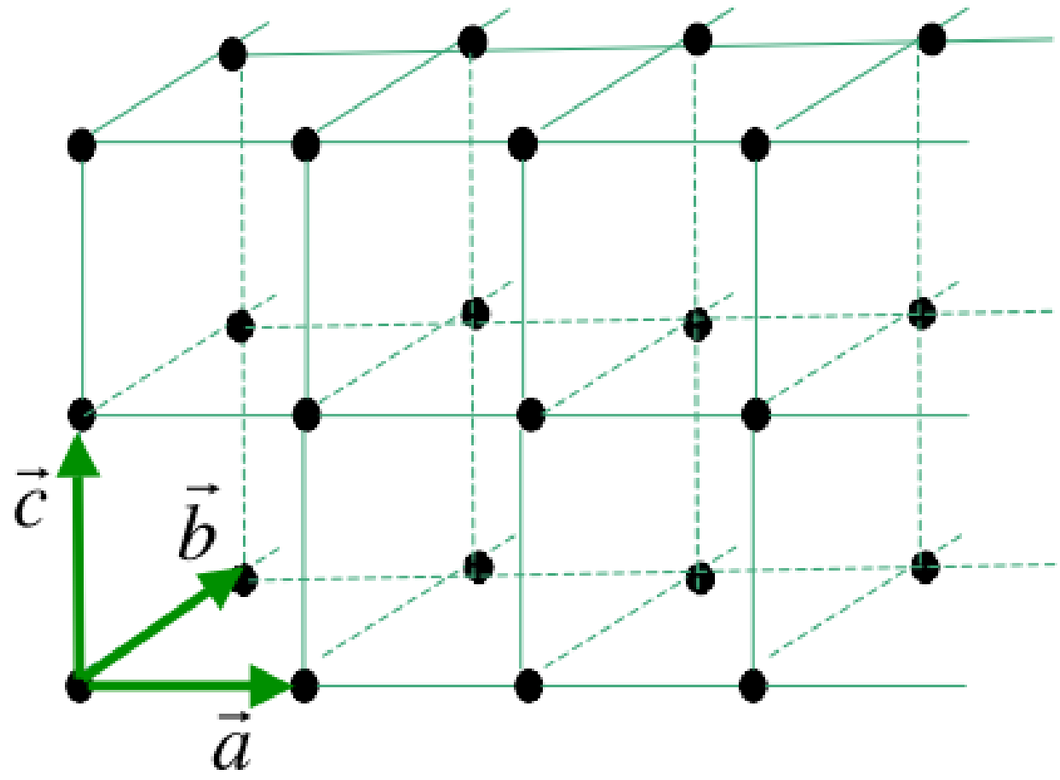
$\overrightarrow{R} = n_1 \overrightarrow{a} + n_2 \overrightarrow{b}$, "a" and "b" are the repeating distance in 2-D



The repetition of translation vector R gives the crystal structure in 2-D

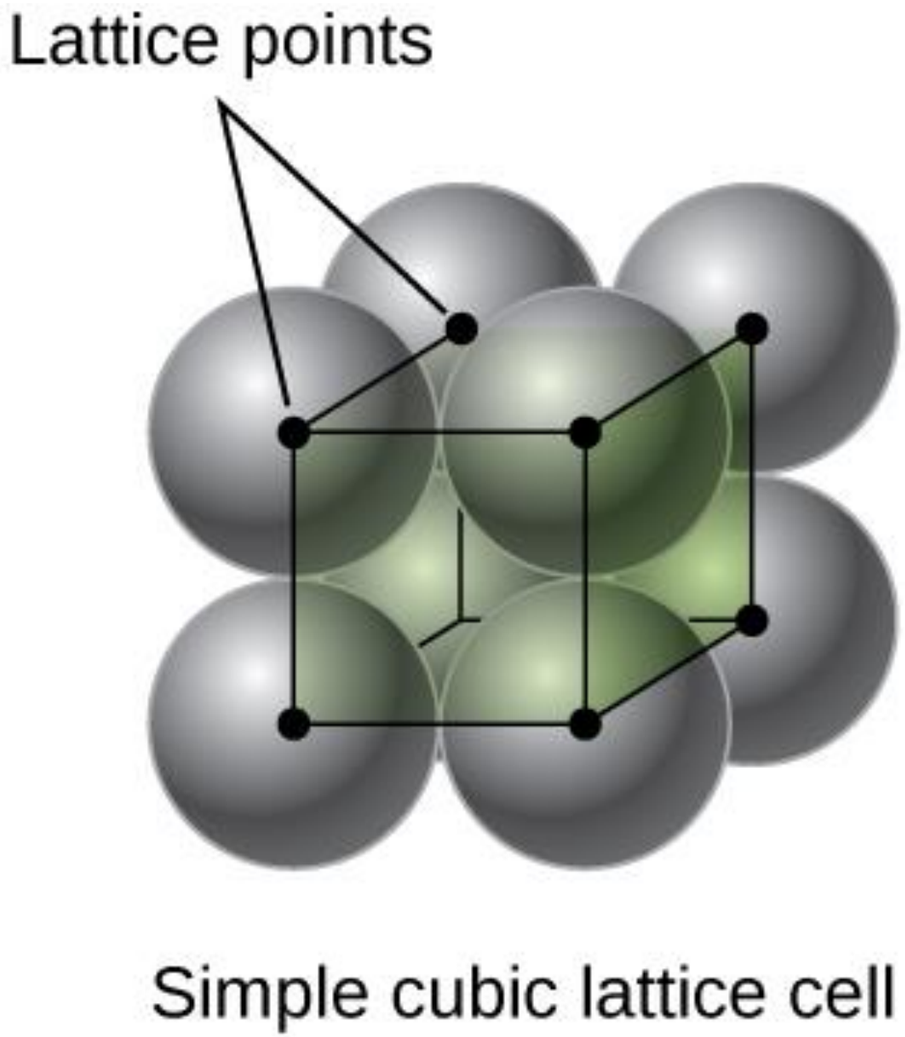
Primitive vectors in 3-D

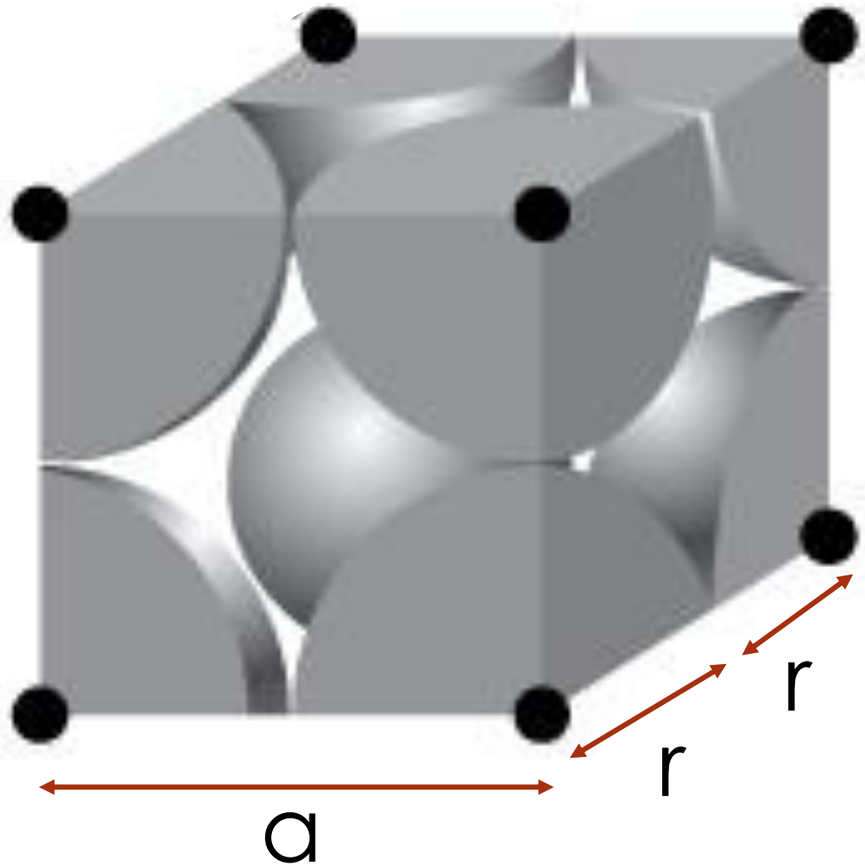
$\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$ "a" and "b" and "c" are the repeating distance in 2-D



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

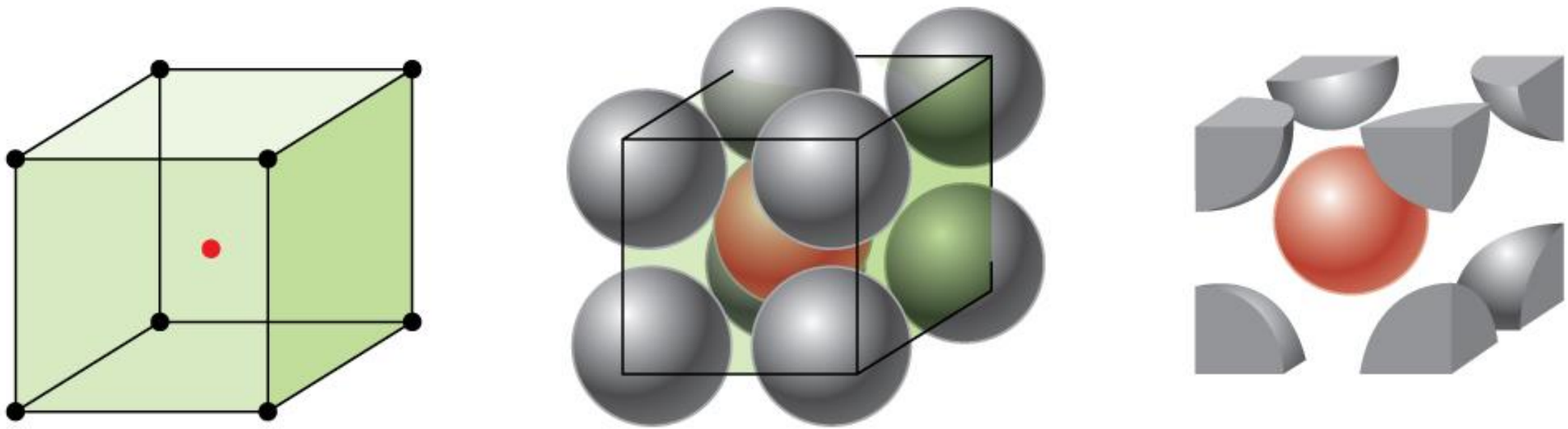
Simple Cubic (SC)





Lattice points in a unit cell : 1/8 * 8 = 1

Body centered cubic (BCC)

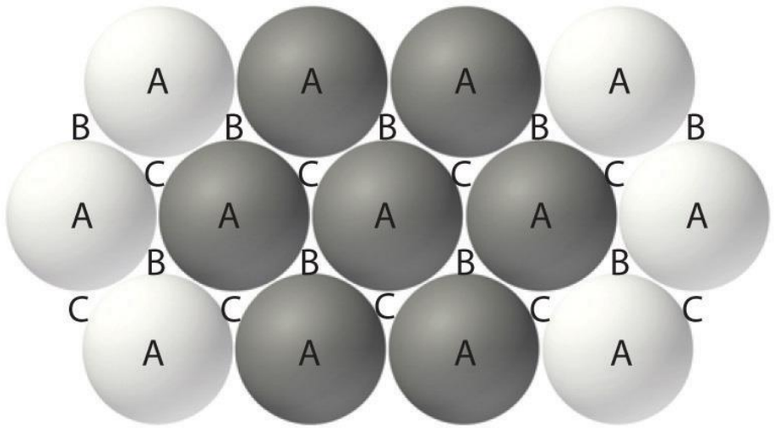


Body-centered cubic structure

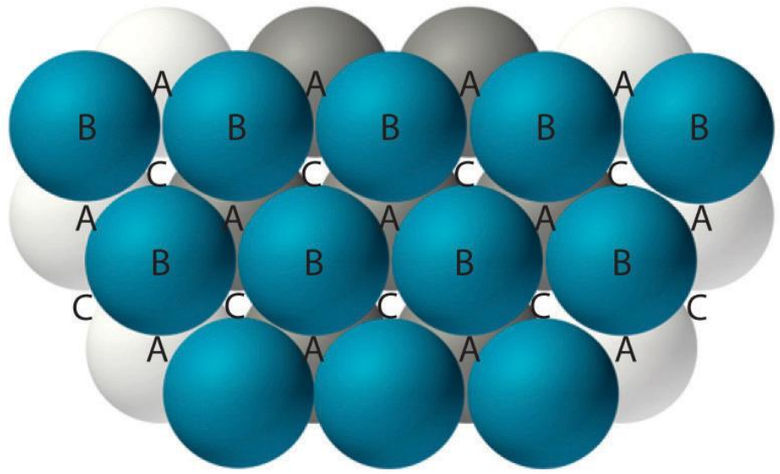
Lattice points in a unit cell : 1/8 * 8 + 1= 2

Closed packed structures

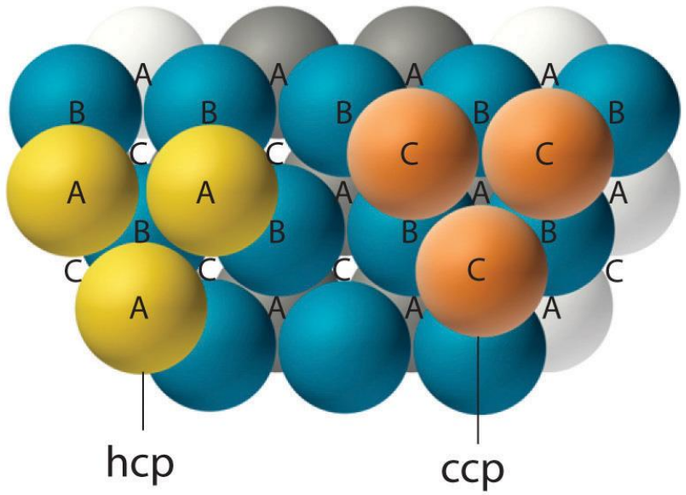
Closed packed structures have highest density in a unit cell



(a) Single layer



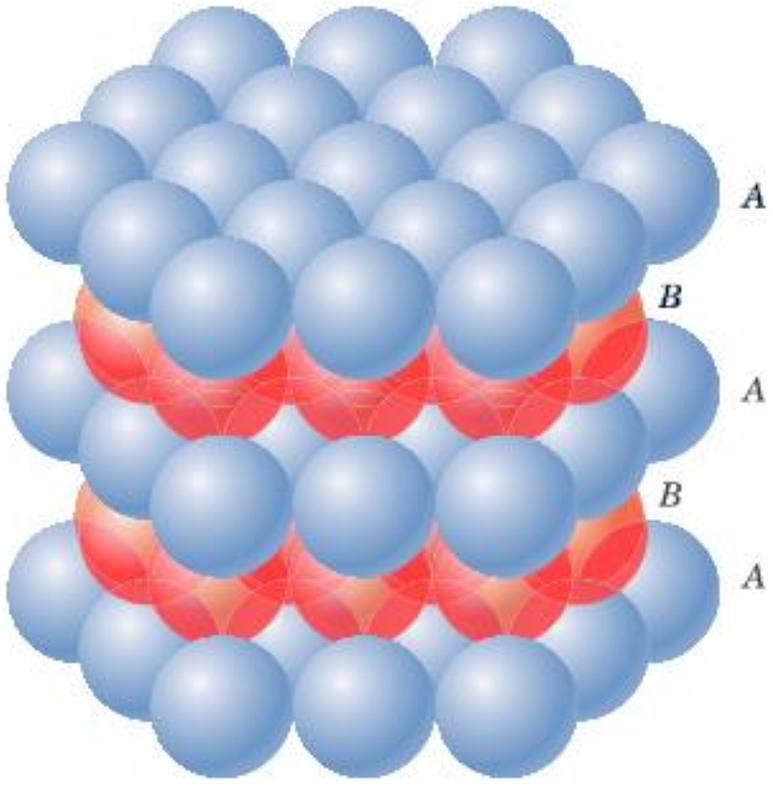
(b) Two layers

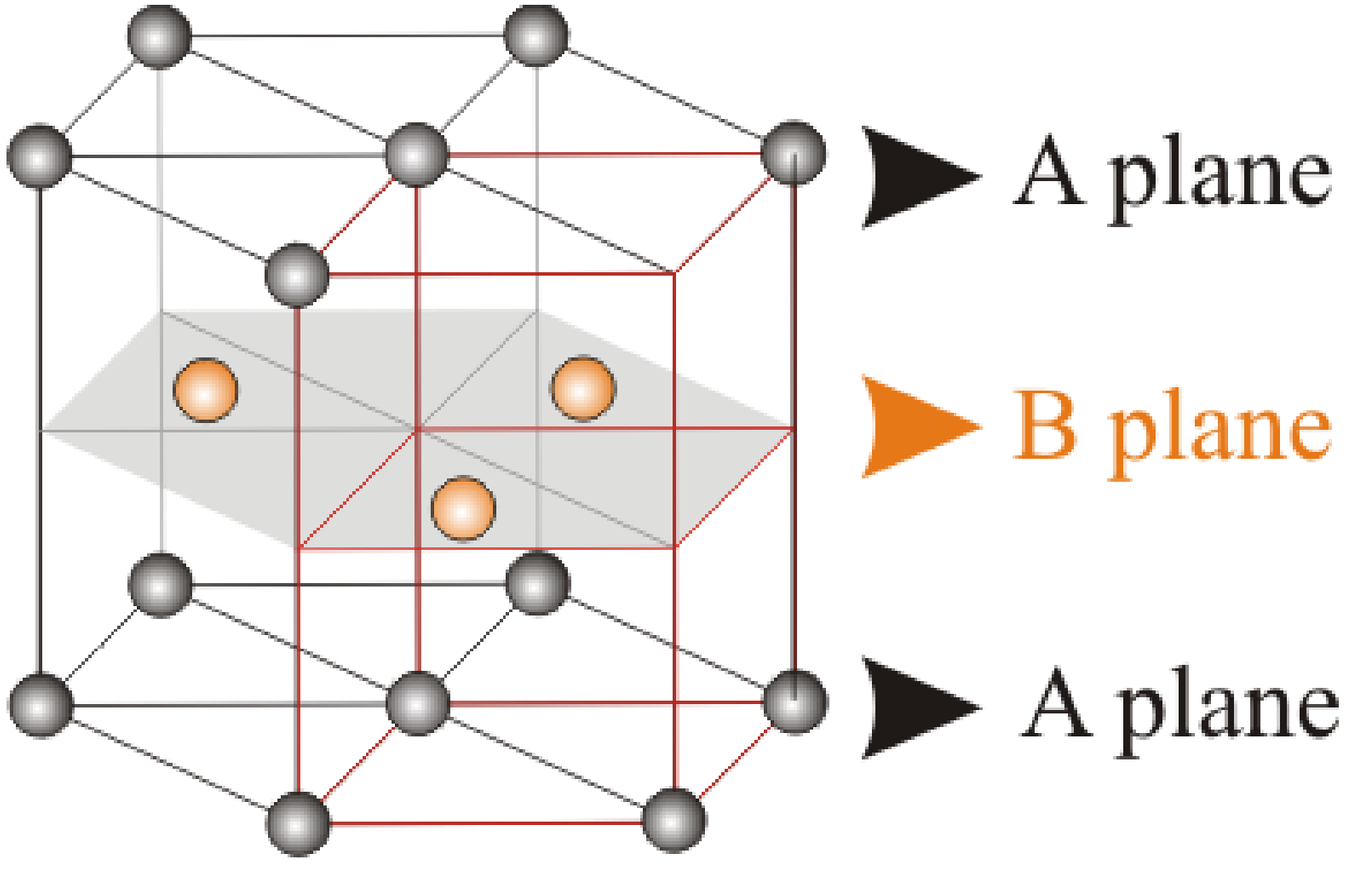


(c) Three layers

Hexagonal closed packed cubic (HCP)

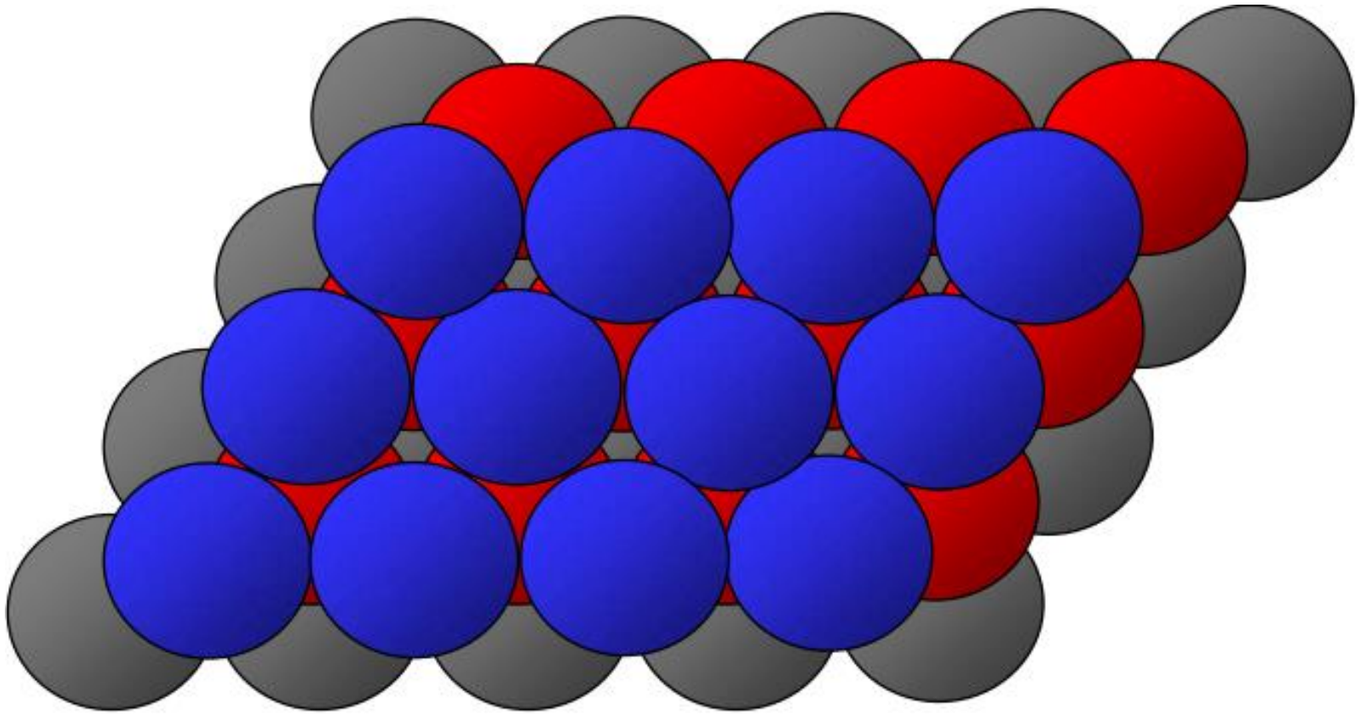
Both FCC and HCP are closed packed structures

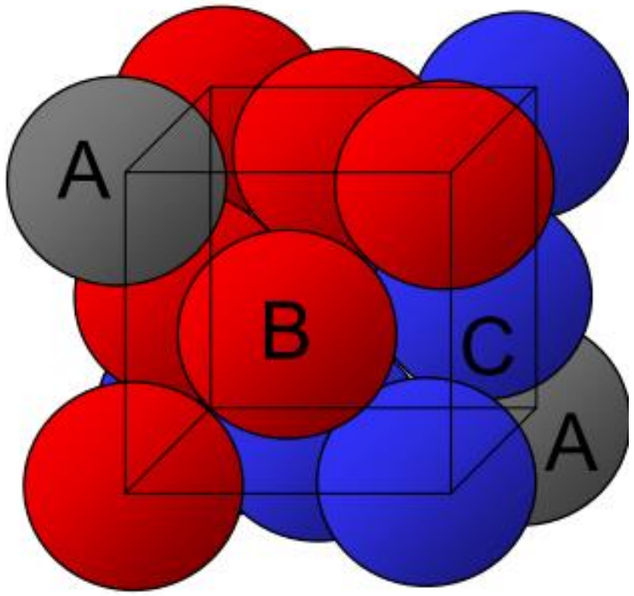




Showing 3 unit cells and the rhombic prism UC

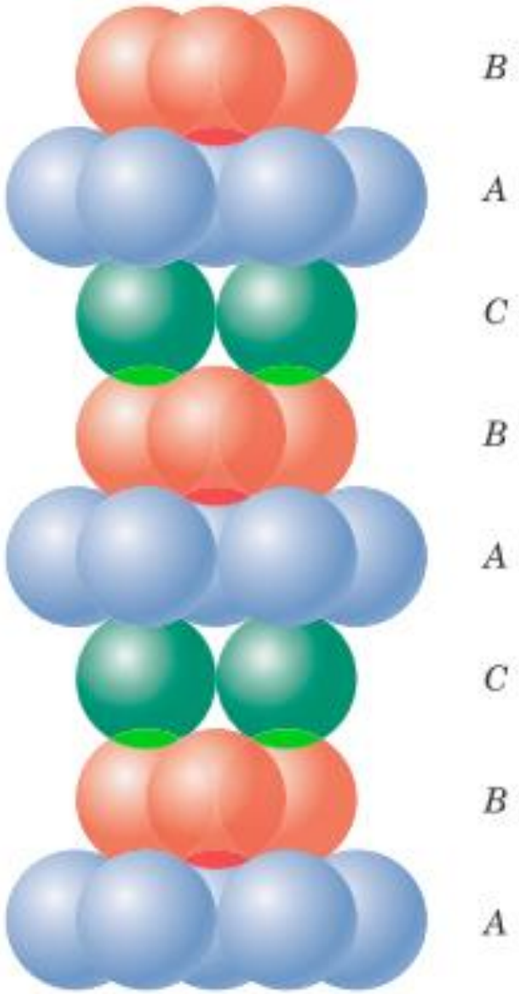
Face centered cubic (FCC)

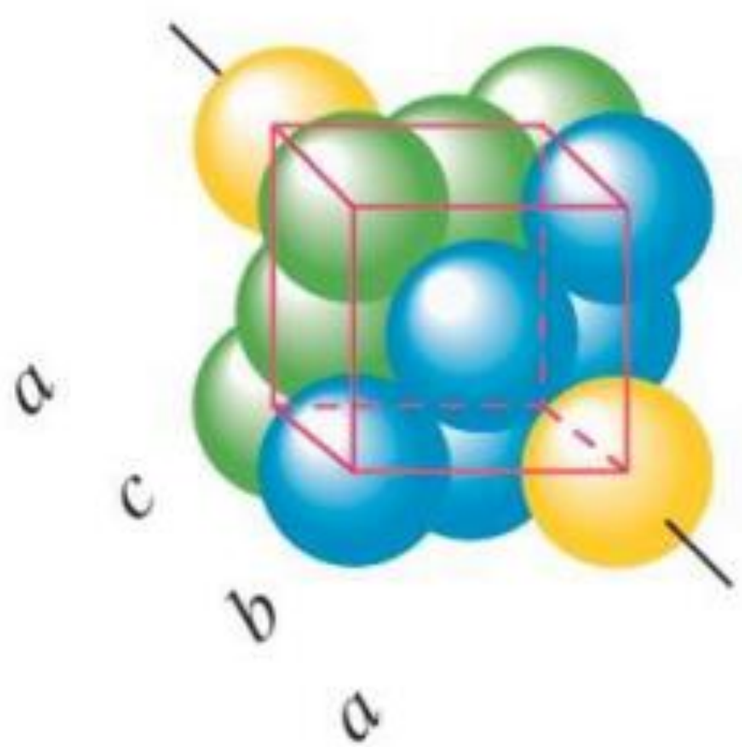


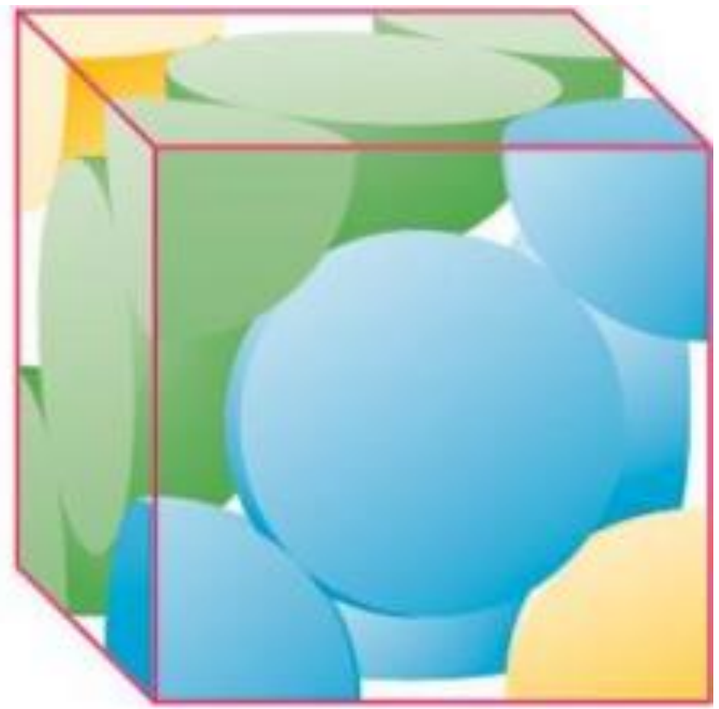


Face centered cubic (FCC)

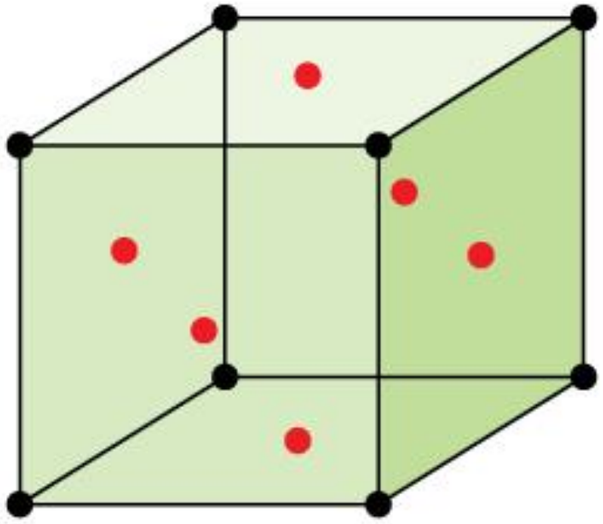
Both FCC and HCP are closed packed structures

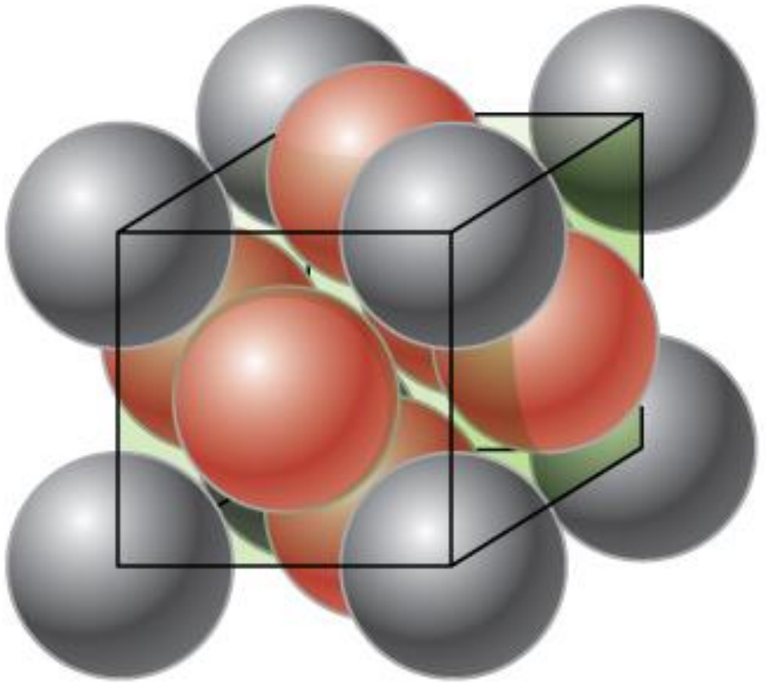


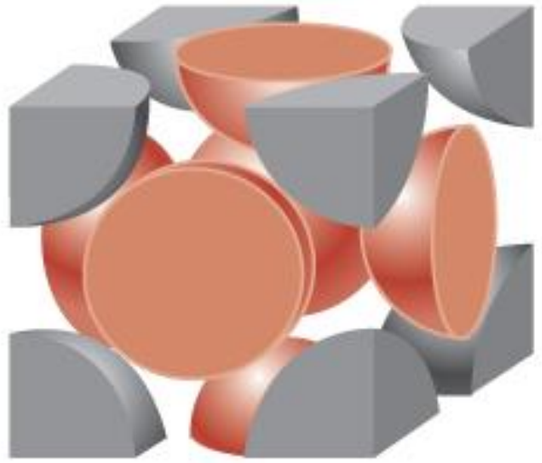




Face centered cubic (FCC)

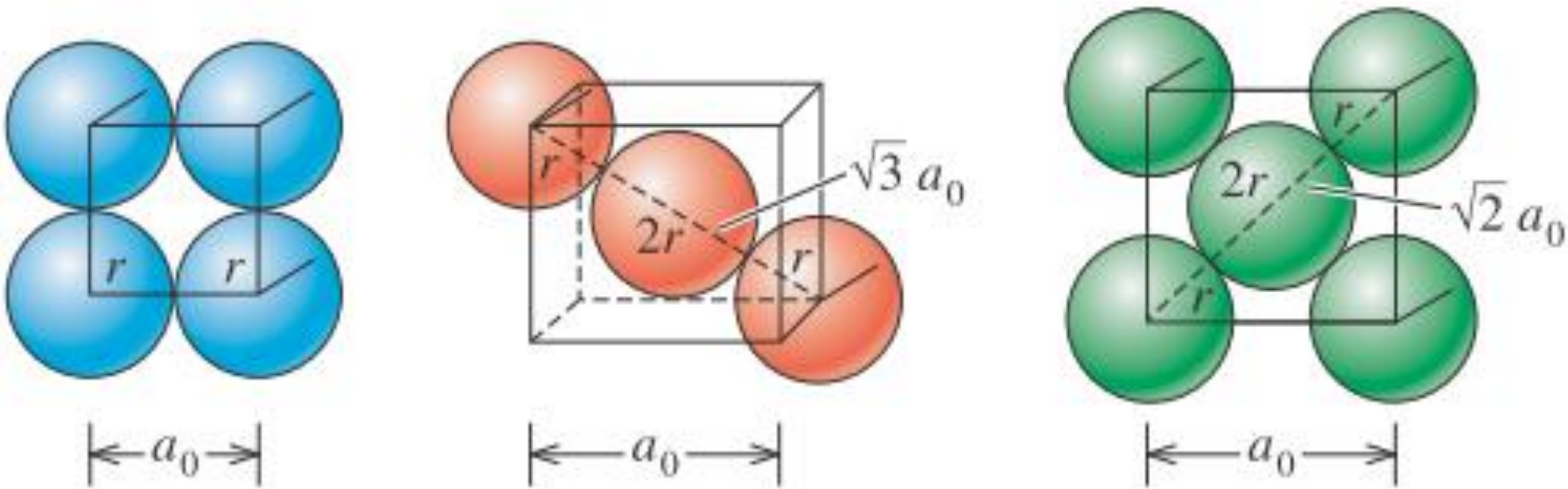






Lattice points in a unit cell : 1/8 * 8 + 1/2 * 6 = 4

Relation between r and a



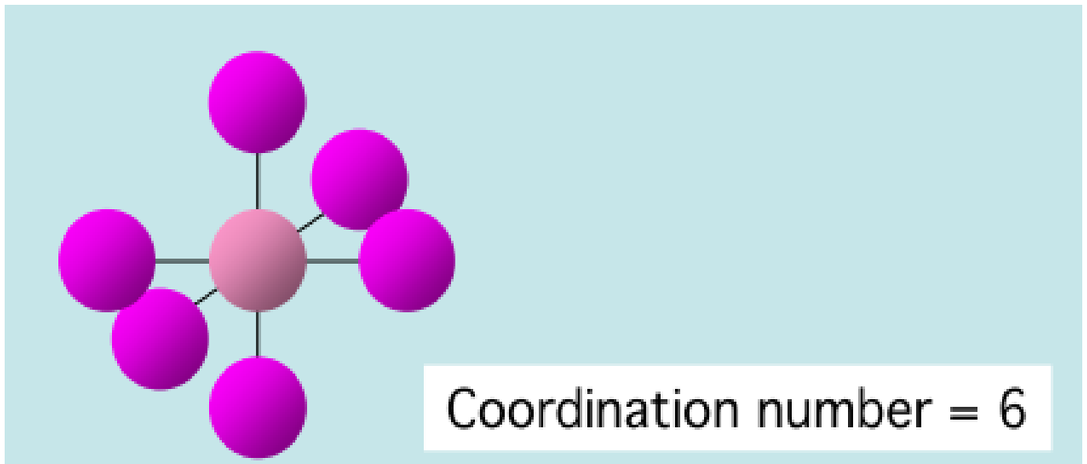
SC: $a = 2r$

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

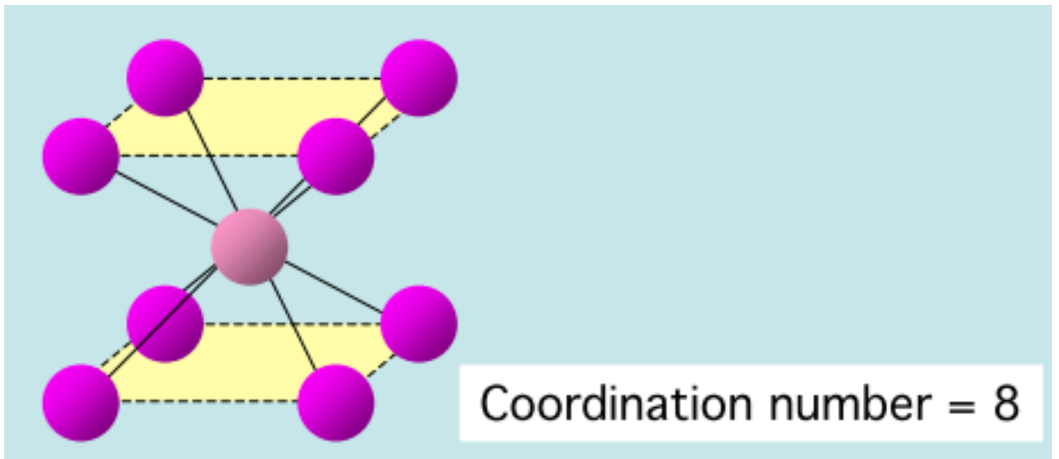
FCC: $a\sqrt{2} = 4r$ (face diagonal)

Co-ordination number(CN)

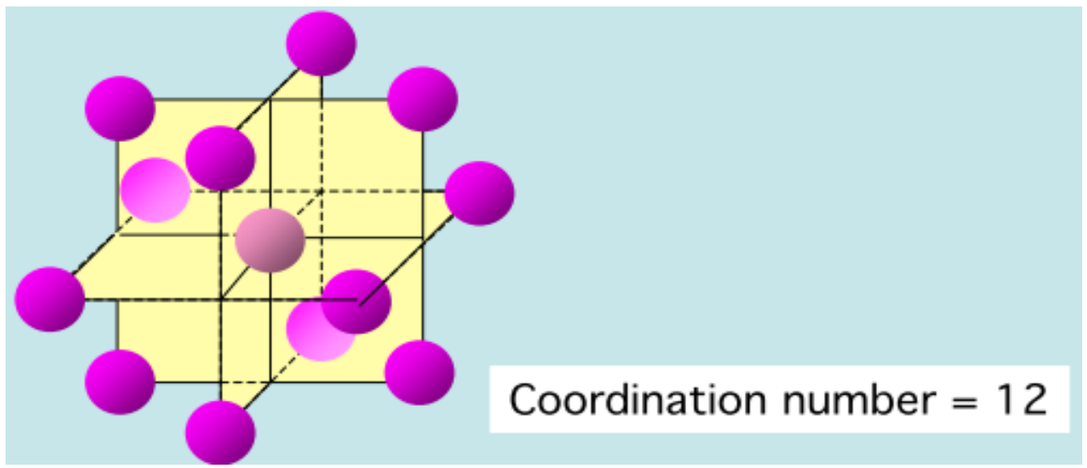
No. of nearest neighbors (No. of atoms touching)



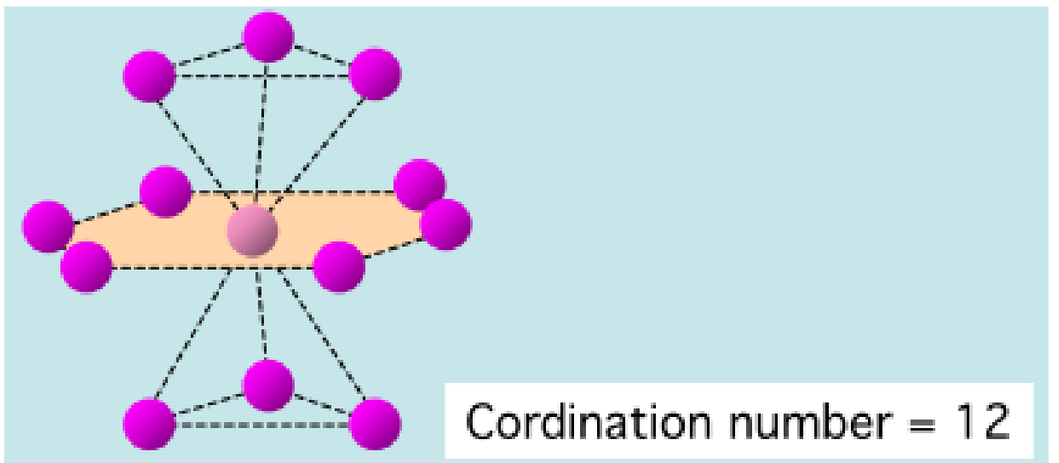
SC



BCC



FCC



HCP

Atomic Packing Fraction (APF)

Packing density of the monoatomic unit cell

Atom is assumed as a hard sphere

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

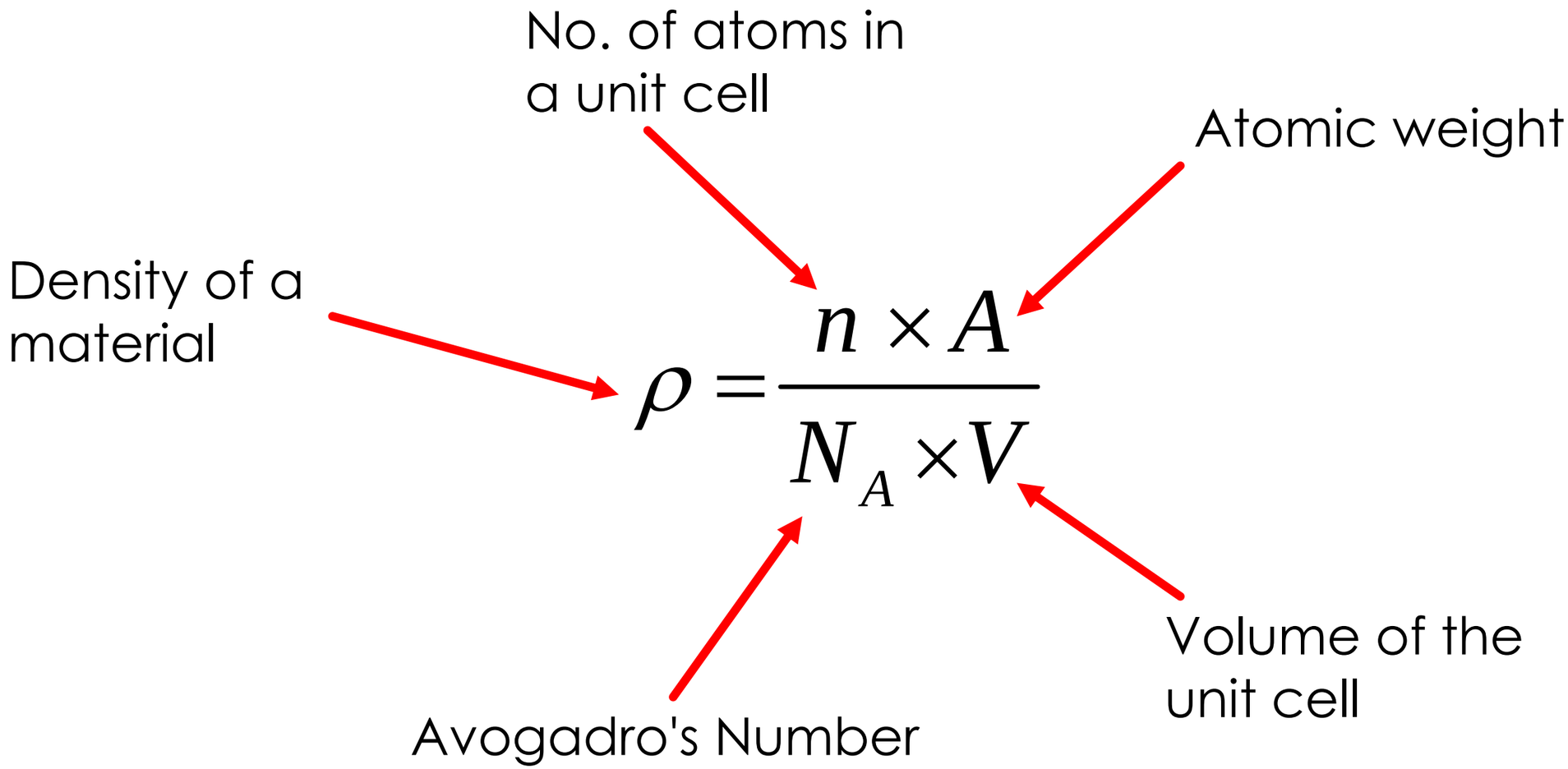
Unit cell is cubic

So a^3

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

Density of a Material

Density of a crystalline material can be calculated by



Summary

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.

Assignments

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_{BCC} = 3.32 Å, a_{HCP} = 2.956 Å, c = 4.683 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/m^3. Calculate the unit cell dimension and the atomic diameter.