Condensed Matter Physics

Common Crystal Structures & Atomic Packing factor

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What kinds of **forces hold the atoms together** in a solid?

Binding or Bonding

- Interatomic forces between the atoms
- Attractive or repulsive depending upon the interatomic distance.
- Attractive forces comes from electrostatically
- When the atoms come closure and combine to form molecules, a change in arrangement of electrons, takes place until a stable configuration is formed.
- The arrangements of electrons, results in the formation of different types Bonds.

Classification of bonds

Based on the bond strength

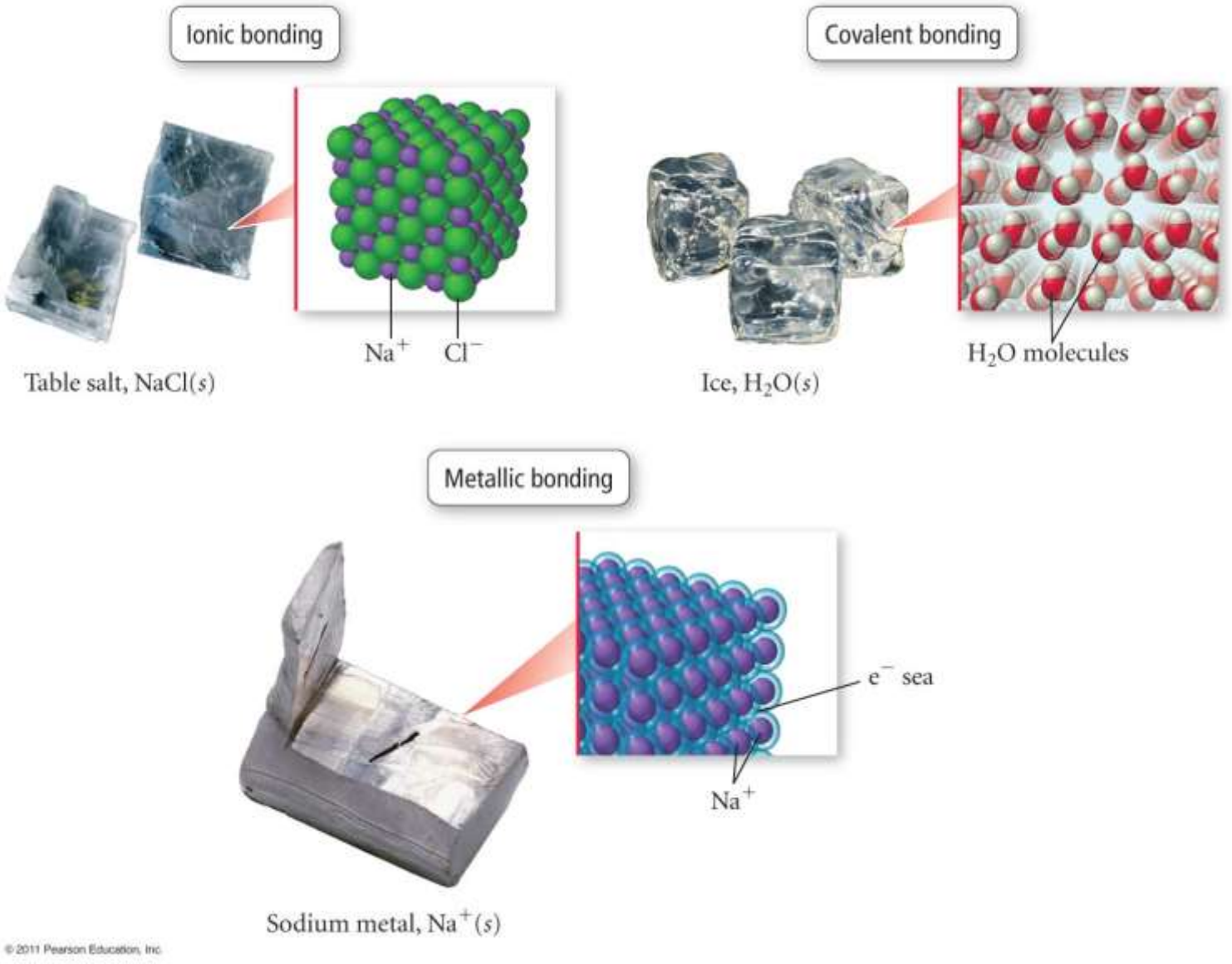
- Primary bonds – Ionic,
  (1-5 eV) Covalent and
  (1-2 Å) Metallic bond
- Secondary bonds (or) Molecular bonds
- (or) (Vander waals bonds)
- (0.02-0.5eV) & (2-5 Å)
  Dispersion bonds,
  dipole bonds and
  hydrogen bonds

Types of Bonds

We can classify bonds based on the kinds of atoms that are bonded together

Types of Atoms	Type of Bond	Bond Characteristic
metals to nonmetals	Ionic	electrons transferred
nonmetals to nonmetals	Covalent	electrons shared
metals to metals	Metallic	electrons pooled

Types of Bonding

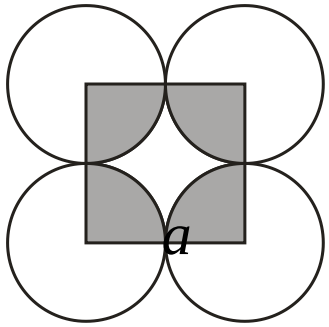


Some important crystal structure terms are defined below

- **Coordination number (N):** The coordination number is defined as the number of equidistant nearest neighbours that an atom has in the given structure. Greater is the coordination number, the more closely packed up will be the structure.

- **Nearest neighbour distance (a)** The distance between the centres of two nearest neighbouring atoms is called nearest neighbour distance. It will be where, is the radius of the atom.

- **Atomic radius(r):** Atomic radius is defined as half the distance between nearest neighbours in a crystal of pure element.

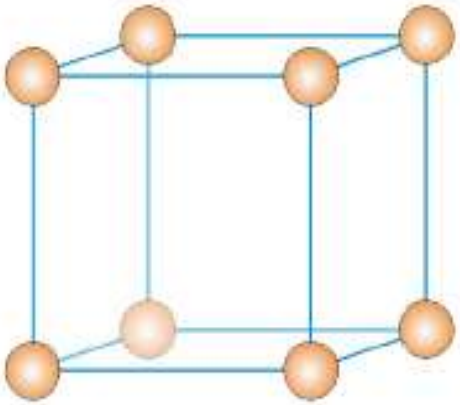


Some important crystal structure terms are defined below

- **Atomic packing factor:** The fraction of the space occupied by atoms in a unit cell is known as **atomic packing factor (APF)**; or simply packing factor; i.e., it is the ratio of the volume of the atoms occupying the unit cell to the volume of the unit cell relating to that structure.

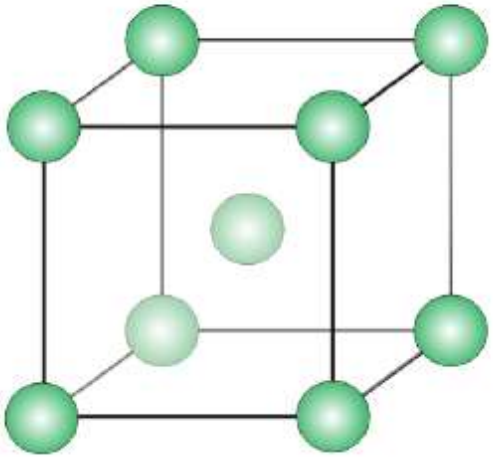
$$APF = PF = \frac{v}{V} = \frac{Volume\ of\ \ atoms\ in\ a\ unit\ cell}{Volume\ of\ \ primitive\ cell}$$

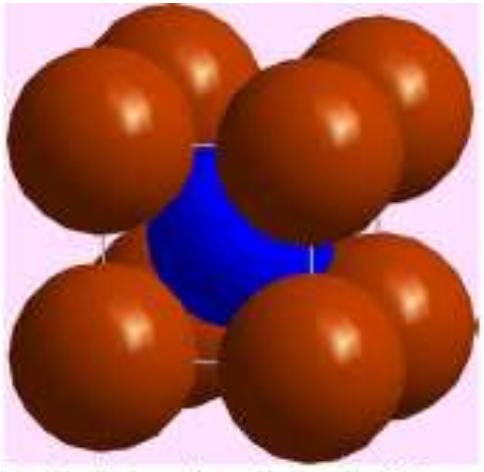
Basic Crystal Structures



Unit cell of the SC lattice

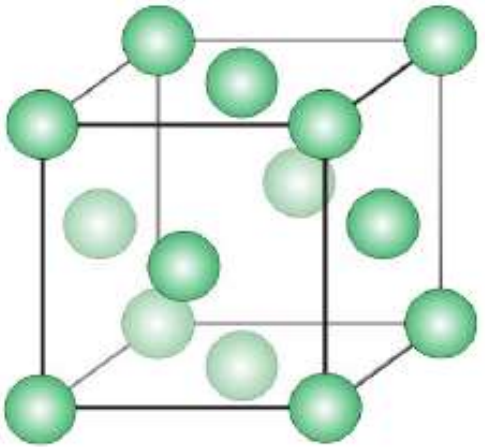
Body Centred Cubic Crystal

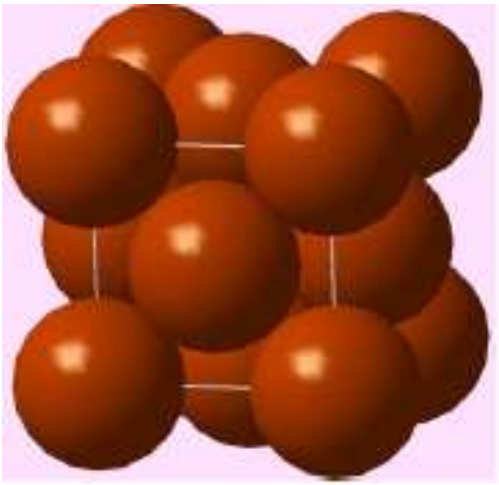




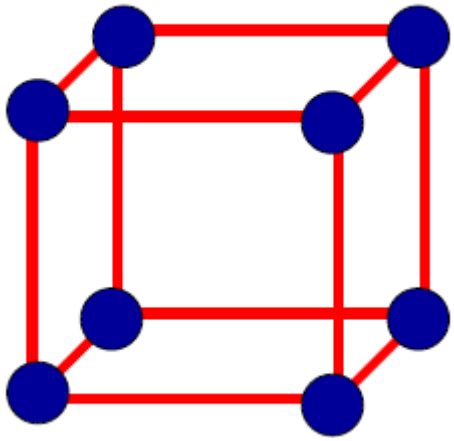
Cubic Close Packed Crystal

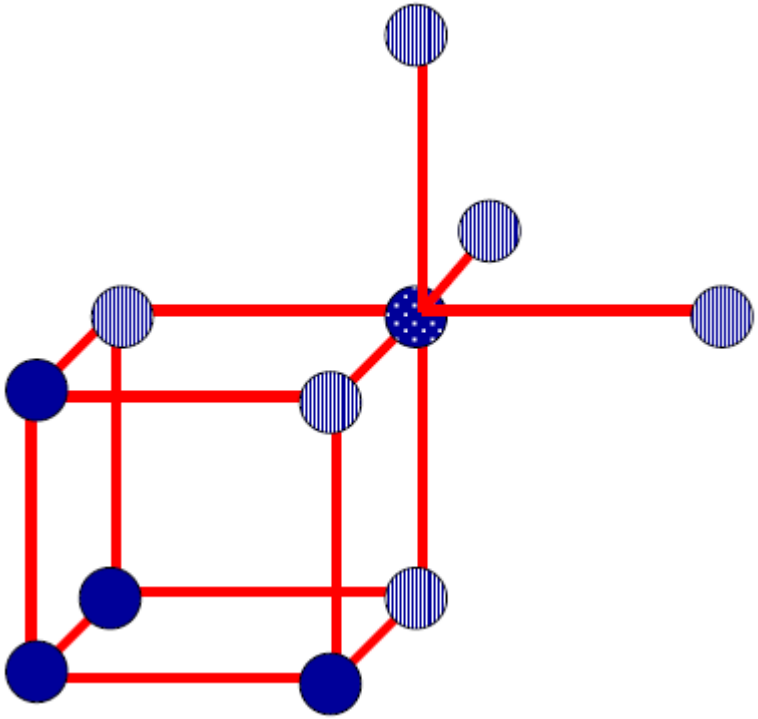
(Sometimes casually called the FCC crystal)

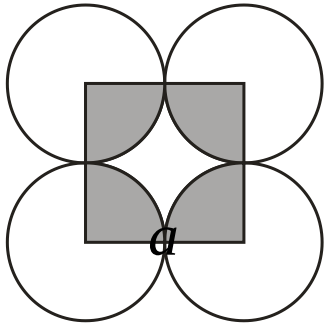




Packing Fraction – Simple cubic structure





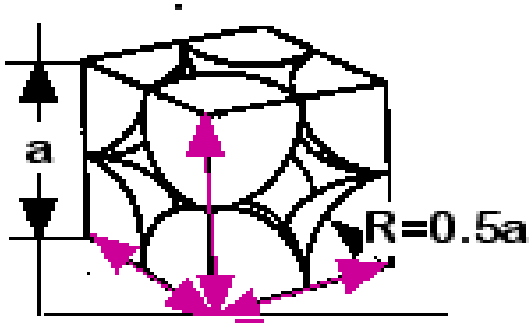


Atomic radius (r) = a/2

Number of atoms per unit cell	1/8 X 8 = 1
Coordination number	6
Atomic packing factor	0.52

Packing Fraction – Simple cubic structure

- Simple Cubic has one lattice point so its primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) belongs to that cell. The rest of the atom belongs to neighboring cells.
- Coordinatination number of simple cubic is 6.

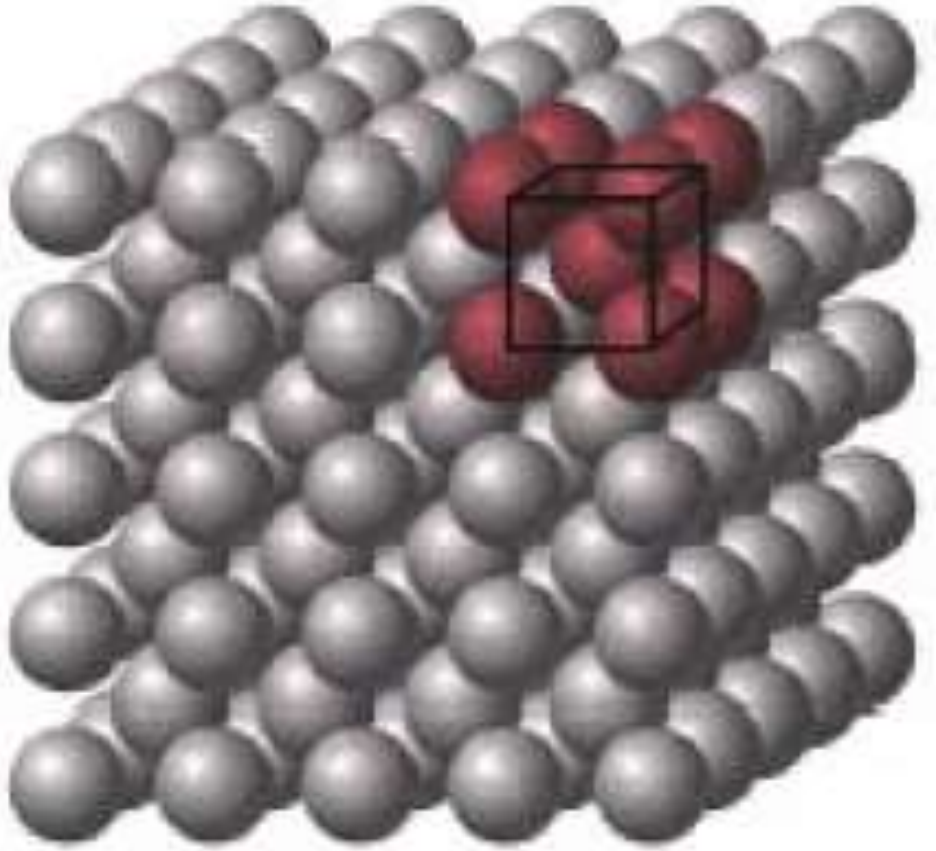


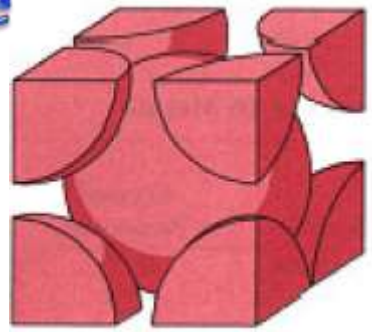
contains 8 x 1/8 =
1atom/unit cell

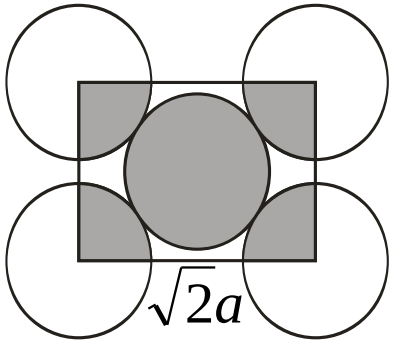
APF = 0.52 for simple cubic

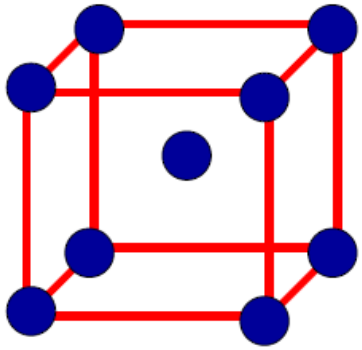
$$APF = \frac{\frac{\text{atom}}{\text{unit cell}} \times \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}} = \frac{1 \times \frac{4}{3}\pi (0.5a)^3}{a^3}$$

Packing Fraction – Body centered cubic structure





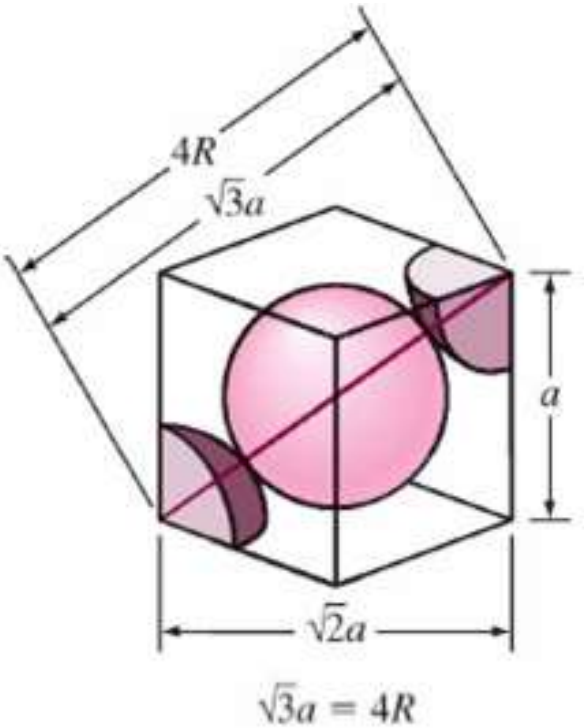




Number of atoms per unit cell	1/8 X 8 + 1 = 2
Coordination number	8
Atomic packing factor	0.68

Packing Fraction – Body centered cubic structure

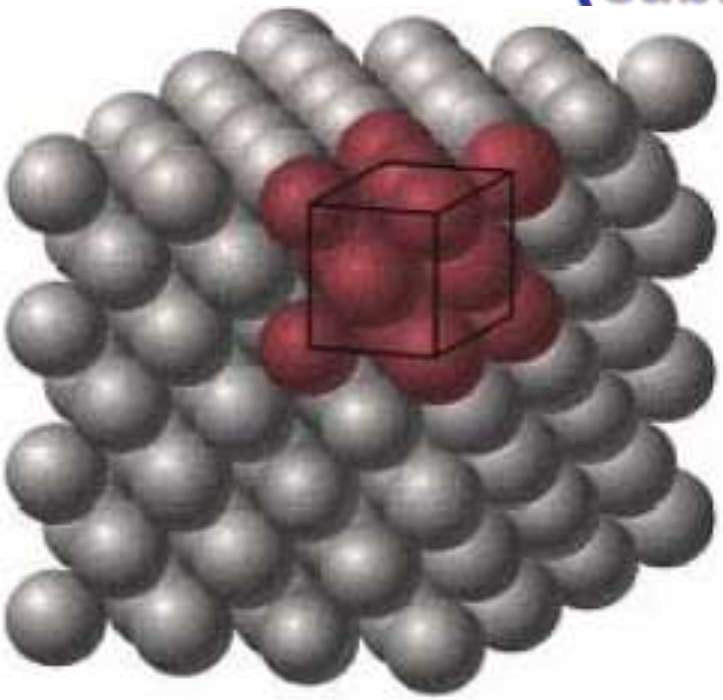
- BCC has two lattice points so BCC is a non-primitive cell.
- BCC has eight nearest neighbors. Each atom is in contact with its neighbors only along the body-diagonal directions.
- Many metals (Fe,Li,Na..etc), including the alkalis and several transition elements choose the BCC structure.

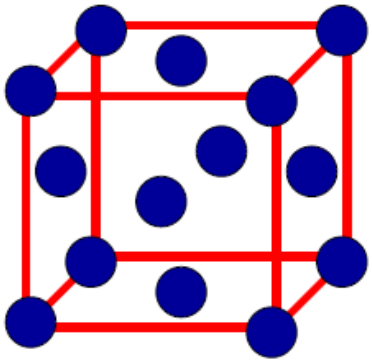


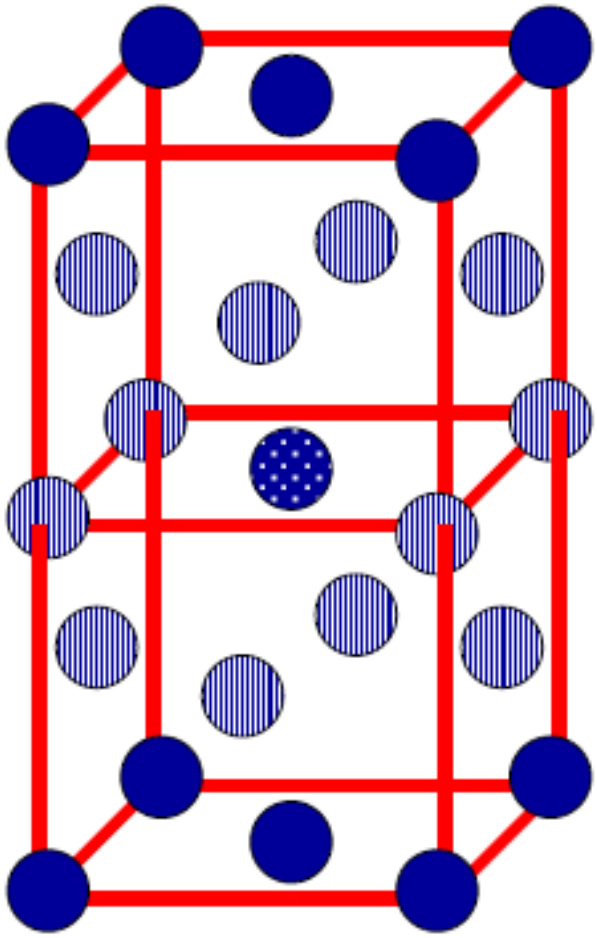
$$APF_{BCC} = \frac{V_{atoms}}{V_{unit\,cell}} = 0.68$$

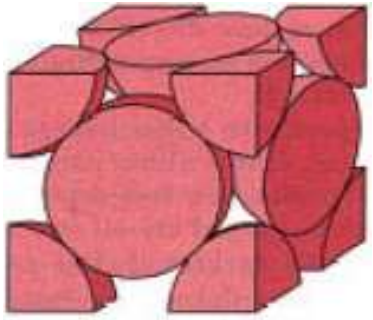
$$APF = \frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{2 \cdot \frac{4}{3}\pi (0{,}433a)^3}{a^3}$$

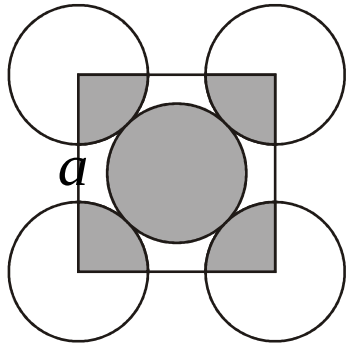
Packing Fraction – Face centered cubic structure (Cubic close packed structure)







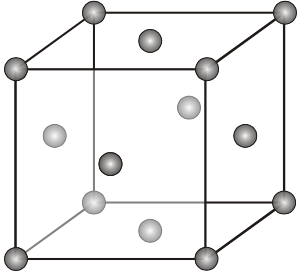


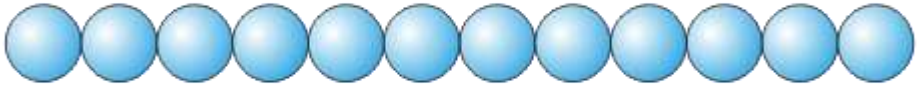


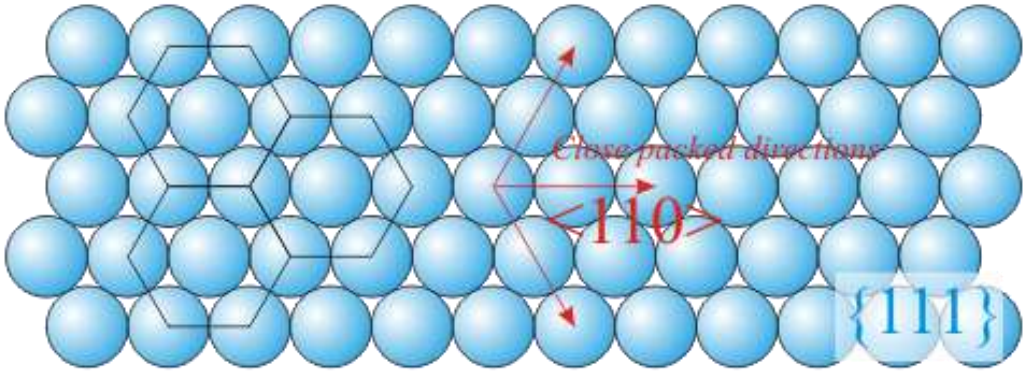
Number of atoms per unit cell	1/8 X 8 + 1/2 X 6 = 4
Coordination number	12
Atomic packing factor	0.74

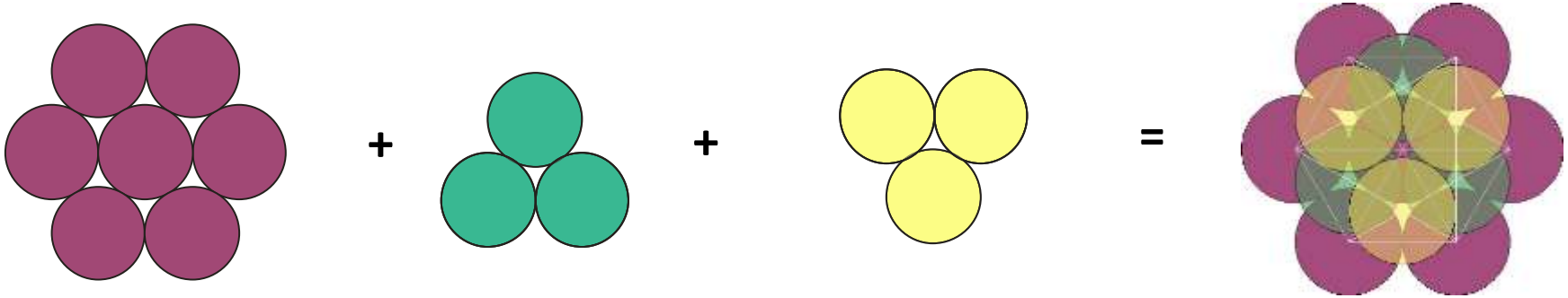
CLOSE PACKING

FCC







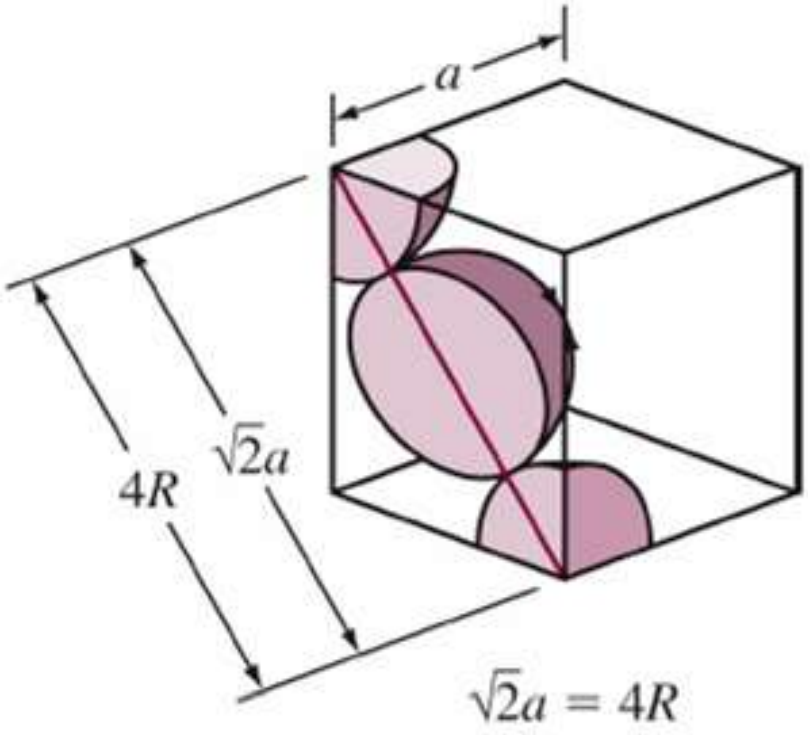


A B C **FCC**

Note: Atoms are coloured differently but are the same

Basic Crystal Structures

- There are atoms at the corners of the unit cell and at the center of each face.
- Face centered cubic has 4 atoms so its non primitive cell.
- Many of common metals (Cu,Ni,Pb..etc) crystallize in FCC structure.



$$APF_{FCC} = \frac{V_{atoms}}{V_{unit\,cell}} = 0{,}74$$

$$APF = \frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \cdot \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{4 \cdot \frac{4}{3}\pi(0{,}353a)^3}{a^3}$$