ATOMIC AND CRYSTAL STRUCTURE OF MATERIALS II

By G M Munakaampe

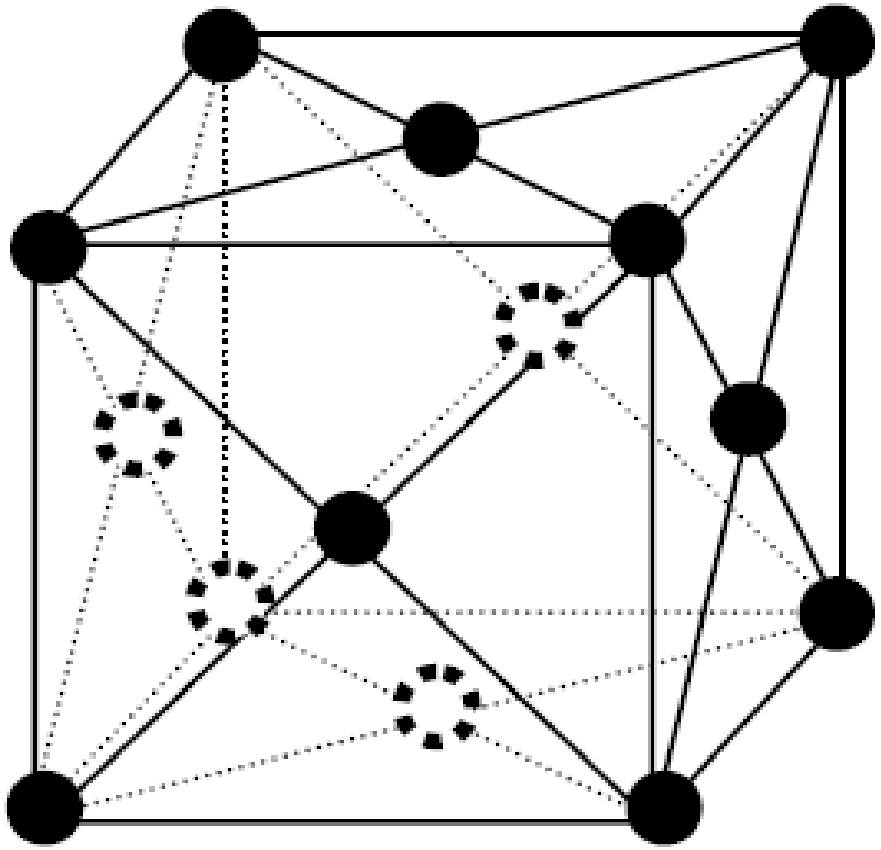
Common Crystal Lattices

Most metals crystallise in one of the three structures:

- face-centred cubic (fcc)
- body-centred cubic (bcc) and
- hexagonal close packed structure (hcp or cph), (a special example of the hexagonal lattice.
- Very few metals crystallise in the simple cubic (sc) or the simple hexagonal (sh or hs) lattices.

Face-centred cubic (fcc)system

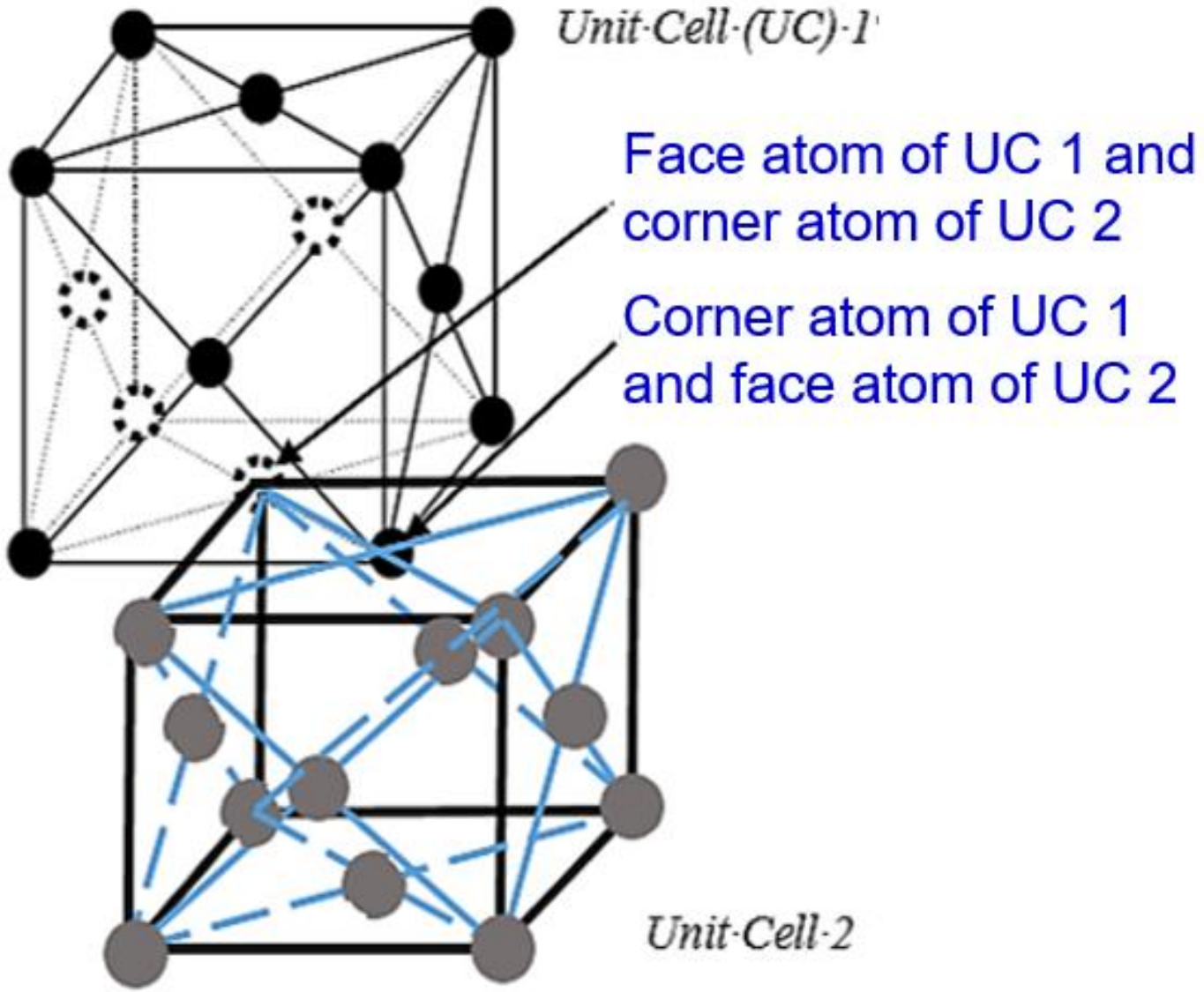
- Consider the unit cell given.
- Atom at corner and centre of each face.
- Now, let us make any one of the face atoms in this unit cell as a corner atom of a new unit cell.



Face-centred cubic unit cell. The circles represent the nuclei of atoms

Atomic Structure of Materials

- By making any one face atom as a corner atom, all face atoms become corner atoms
- The corner atoms become face atoms as shown.
- Therefore, all the atoms in the fcc are lattice points.



Atomic Structure of Materials

- Each corner atom shared by eight (8) unit cells &
- Each face atom is shared by two (2) unit cells.
- Therefore the number of atoms per unit cell is:

$$(8 \times {}^{1}/_{8}) + (6 \times ½) = 4$$

- Volume unit cell = a^3

- Therefore, the packing density, ***PD = 4/a³*** atoms per unit cell.
- The material density for fcc is:

$$\rho = \frac{mass}{volume} = \frac{No.of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

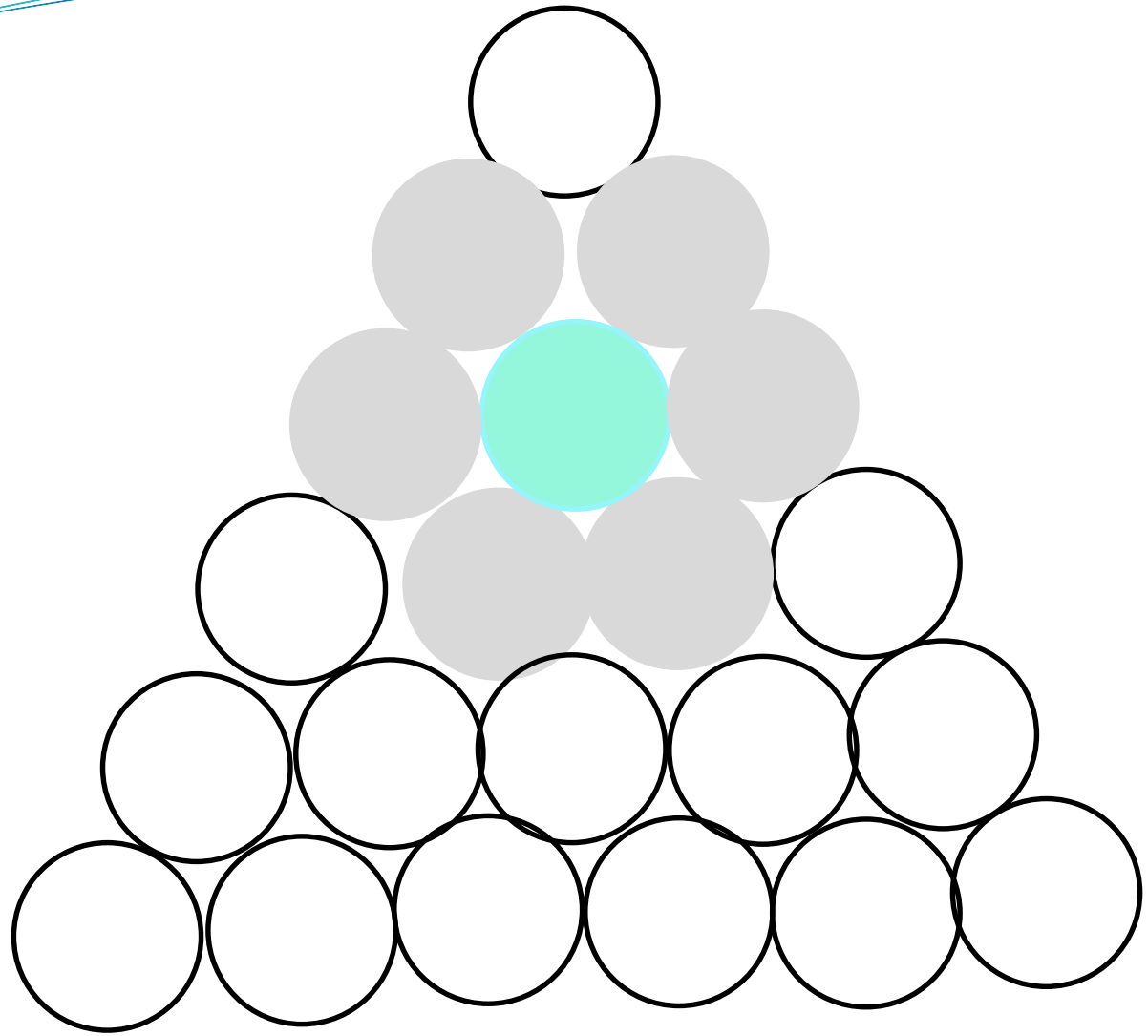
for fcc,

$$\boldsymbol{\rho = \frac{4\times \text{atomic mass}}{a^3}}\ [kg/m^3]$$

Atomic Structure of Materials

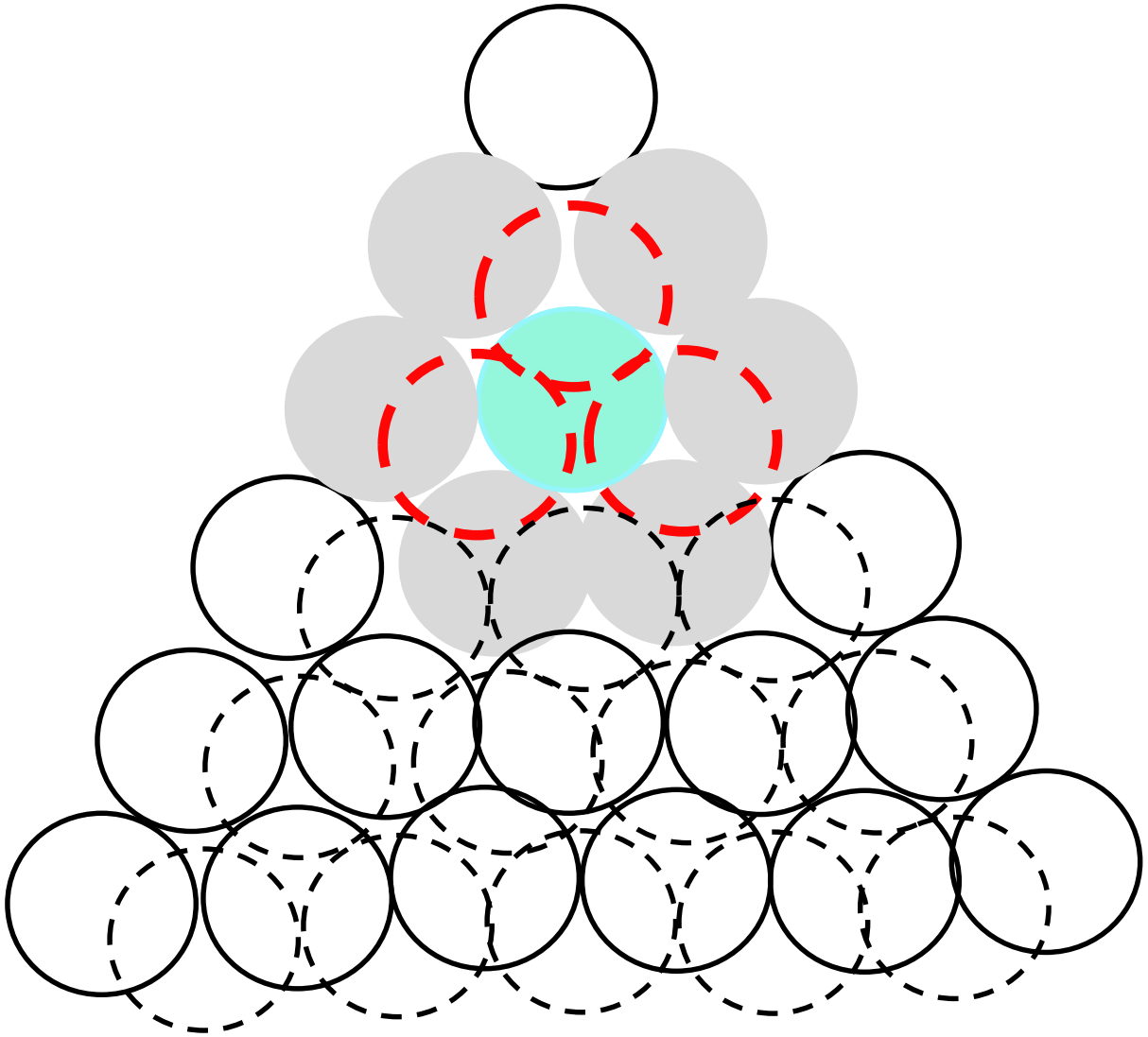
- Each atom has 12 near neighbours; $\Rightarrow$ the closest packing possible (Coordination No. = 12).
- Six of these in one plane form a hexagon around the centre atom,
- Three are in parallel planes on each side, this being (111) planes.
- All {111} planes are of closest packing.
- The spheres touch along the <111> directions, the directions of closest packing.

Atomic Structure of Materials



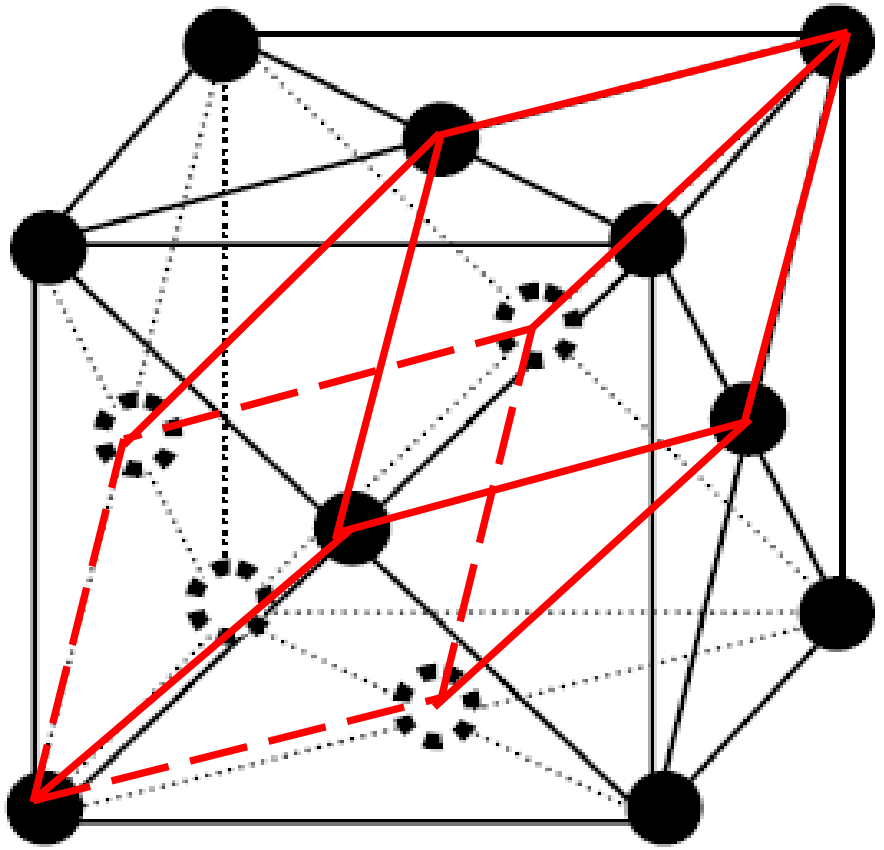
{111} Planes

{111} Planes



Fcc Primitive Cell

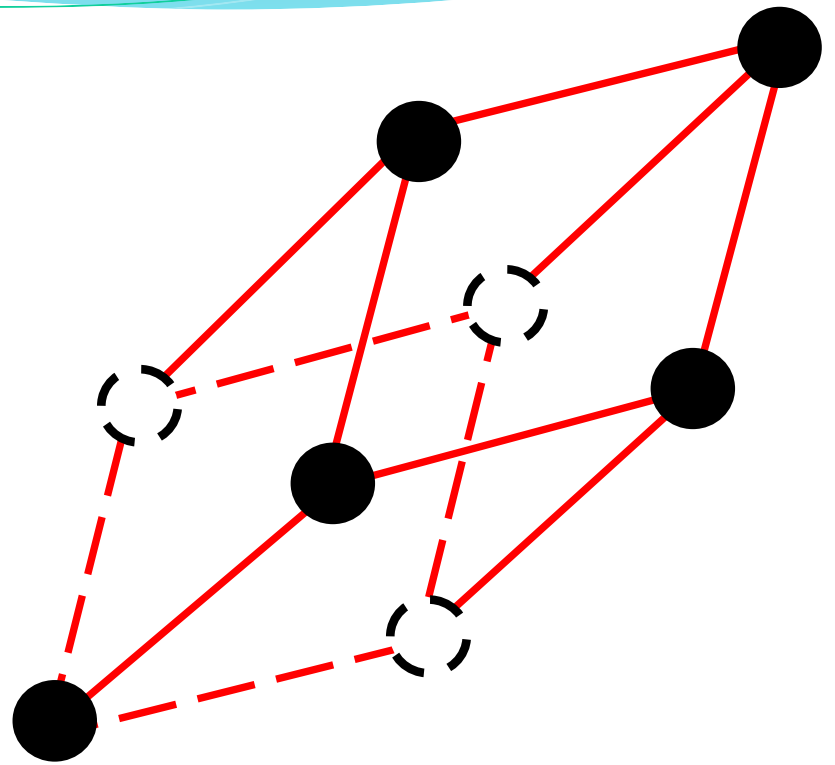
- Taking the two corner atoms across the major diagonal and the six face atoms, such that each corner atoms is joined to the face atoms of its three adjacent faces, as shown, a new, **smaller** unit cell can be formed.



- It is **different from** in shape and orientation and **smaller than** the actual unit cell of the fcc.

FCC Primitive Cell

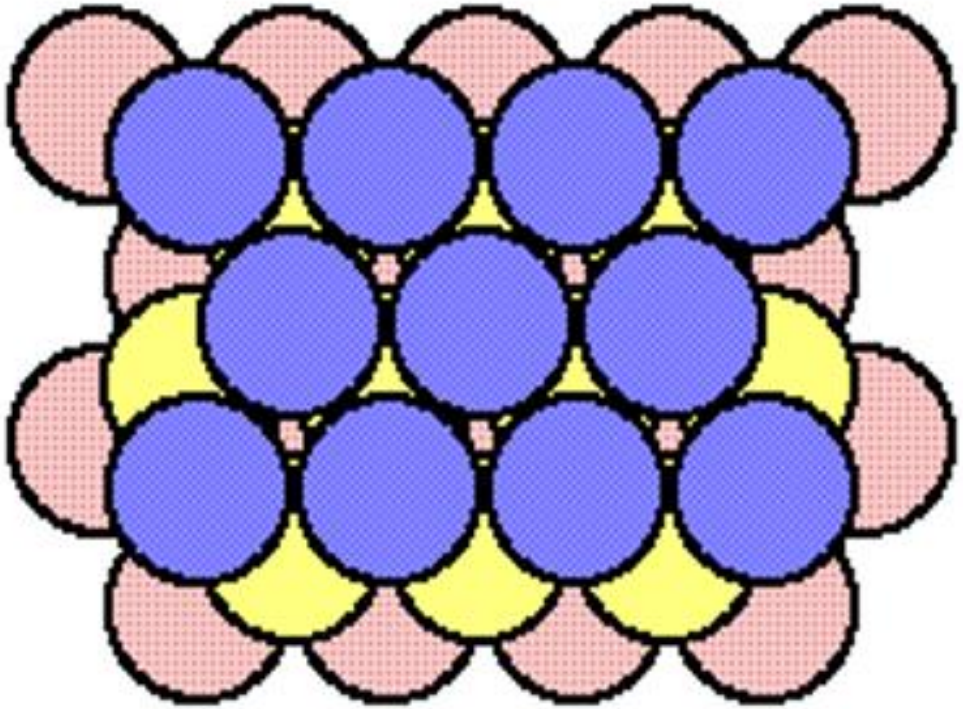
- Taking two corner atoms across the major diagonal and the six face atoms, a new, **smaller** unit cell can be formed
- It is different from actual unit cell of the fcc.
- It is called a ***primitive cell***, the ***smallest unit*** that the lattice can be divided into.

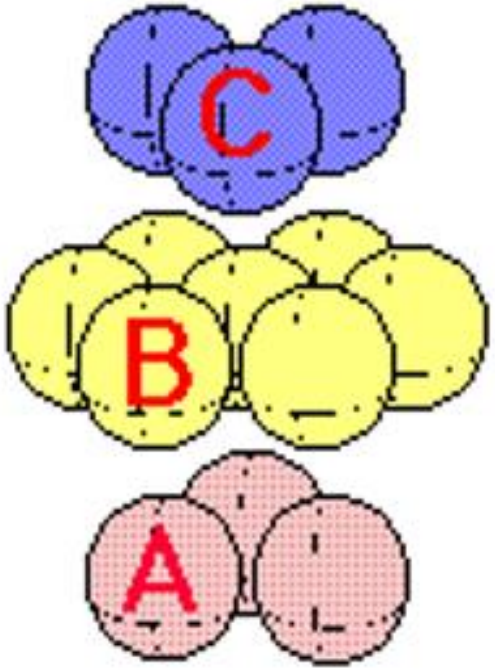


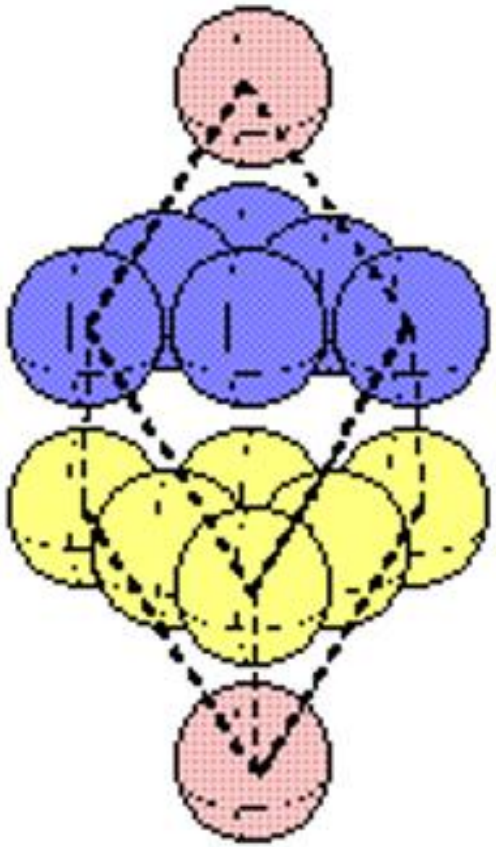
FCC Primitive Cell

- It runs along the major diagonal of the unit cell (so, it has four possible orientations since the cube has four major diagonals.

Cubic close packing (ABCABC…)







Atomic Structure of Materials

Metals that crystallise in fcc include:

Copper (Cu), Nickel (Ni), Aluminium (Al), Iron (Fe), Silver (Ag) and Gold (Au).

Properties:

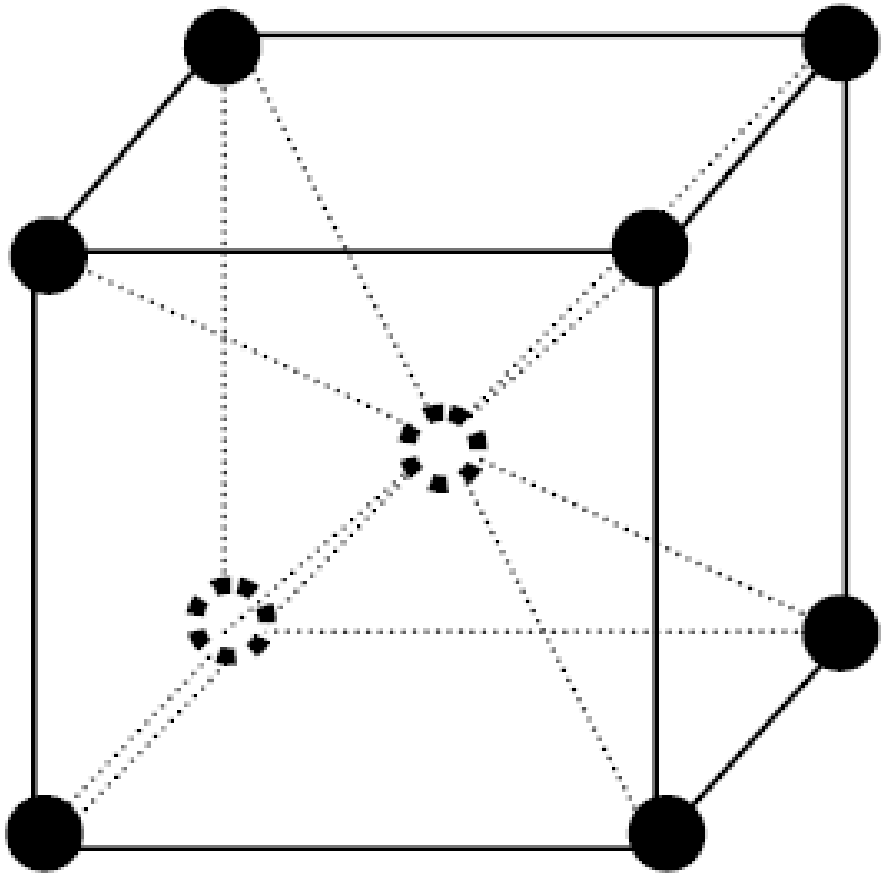
Generally soft, ductile and easy to form.

Body-centred cubic (bcc) unit cell.

- One atom at each corner and also
- One atom at the centre.
- The number of atoms per unit cell:

  $(8 \times {}^{1}/_{8}) + (1) = 2$

- The volume of the unit cell is a^3.



Body-centred cubic unit cell.

- As in fcc, each atomic site in bcc is a lattice point.

- Therefore, the packing density, ***PD = 2/a³*** atoms per unit cell.
- The material density for bcc is:

$$\rho = \frac{mass}{volume} = \frac{No.of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

for bcc,

$$\rho = \frac{\mathbf{2\times\ atomic\ mass}}{\mathbf{a^3}}\ [kg/m^3]$$

Atomic Structure of Materials

- Each atom has eight (8) near neighbours (Coordination No. = 8), so that this system is ***not*** one of closest packing.
- There is no close-packed plane in this system.
- In bcc, primitive cell is the same as the unit cell.

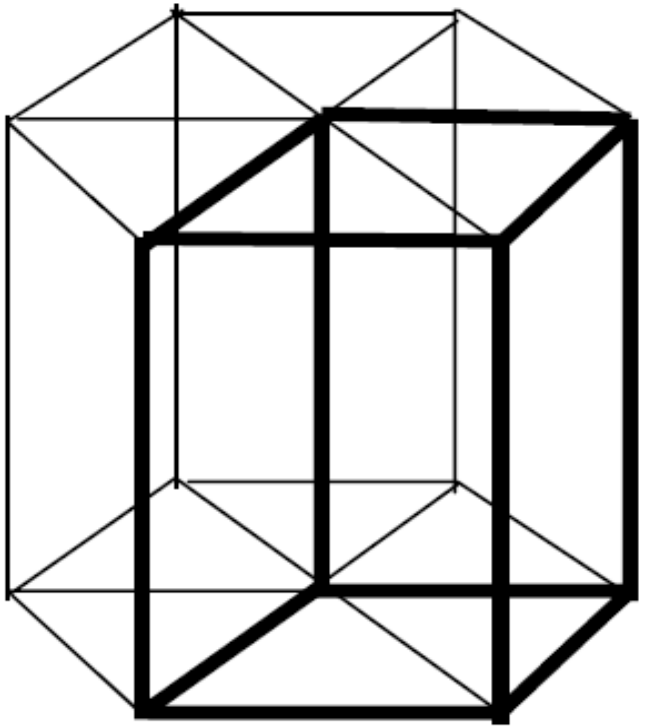
Metals that crystallise in bcc include:

Sodium (Na), Potassium (K), Iron (Fe), Chromium (Cr), Molybdenum (Mo), Wolfram or Tungsten (W).

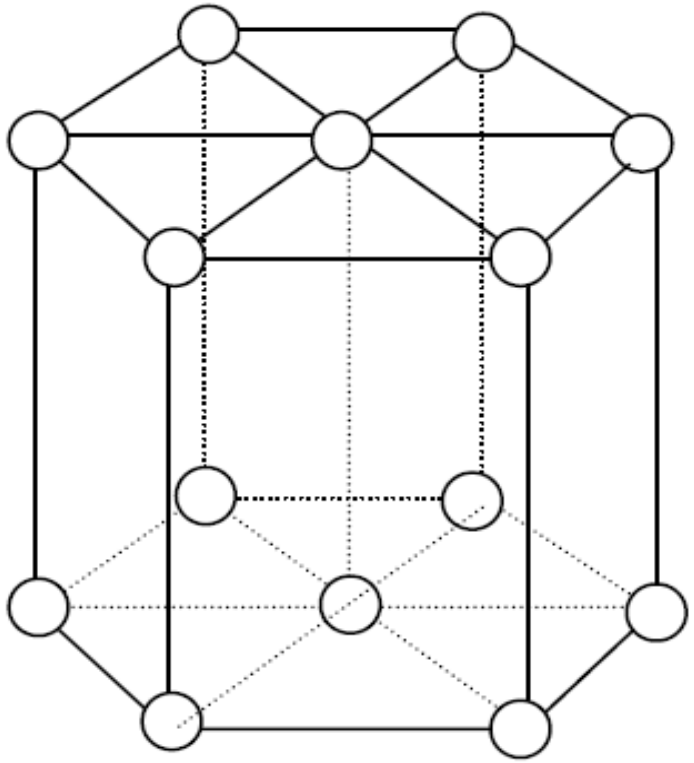
Properties:

Brittle and difficult to form.

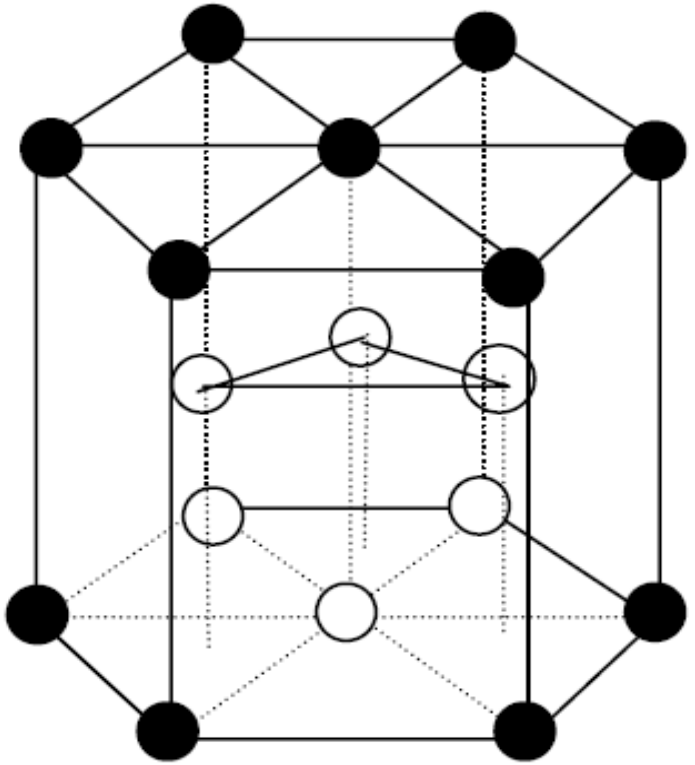
Close-packed hexagonal system



Relationship of unit cell to hexagon in the hexagonal close-packed structure



Lattice points of hexagonal system



Atom sites of hexagonal close-packed structure

Atomic Structure of Materials

- In hcp system, close-packed layers are packed on top of one another.
- Unit cell (which is a primitive cell) is related to the hexagonal structure as shown in the first figure.
- One corner atom is common to eight (8) unit cells,
- One body atom is unique to each unit cell.
- Thus number of atoms per unit cell:

  $(8 \times {}^{1}/_{8}) + (1) = 2$

- The volume of the unit cell is $\boldsymbol{a_1 \cdot a_2 \cdot c \cdot \sin 120^o = \frac{1}{2}\sqrt{3} \cdot a^2 c}$

- Therefore, the packing density,

$$PD = \frac{2}{\frac{1}{2}\sqrt{3}\cdot a^2 c} = \frac{4}{\sqrt{3}\cdot a^2 c}$$ atoms per unit cell.

- The material density for hcp is:

$$\rho = \frac{mass}{volume} = \frac{No.of\ atoms/unit\ cell\ \times mass\ of\ one\ atom}{Unit\ Cell\ Volume}$$

$$\rho = \frac{2\times \text{atomic mass}}{\left(\frac{1}{2}\sqrt{3}\cdot a^2 c\right)}$$ [kg/m^3]

Atomic Structure of Materials

- Each atom has twelve (12) near neighbours (Coordination No. = 12), so that this system **is** one of closest packing
- hcp has three primitive cells in each unit cell, at 120^{o} orientation with each other.
- Metals that crystallise in hcp include
- Cobalt (Co), Zinc (Zn), Titanium (Ti), Manganese (Mn) and Magnesium (Mg).
- Properties:
- Metals that crystallise in hcp structures are also brittle and difficult to form.

Crystal Defects

- Almost all crystals contain defects, i.e. the atoms are not perfectly arranged according to their crystal structures.

- Defects affect the properties of materials.

Crystal Defects

- Crystal defects can be classified into the following categories:
  - Point defects (vacancy, interstitial, etc.)
  - Line defects (dislocations)
  - Surface defects (grain boundaries)
  - Volume defects (voids)

The End