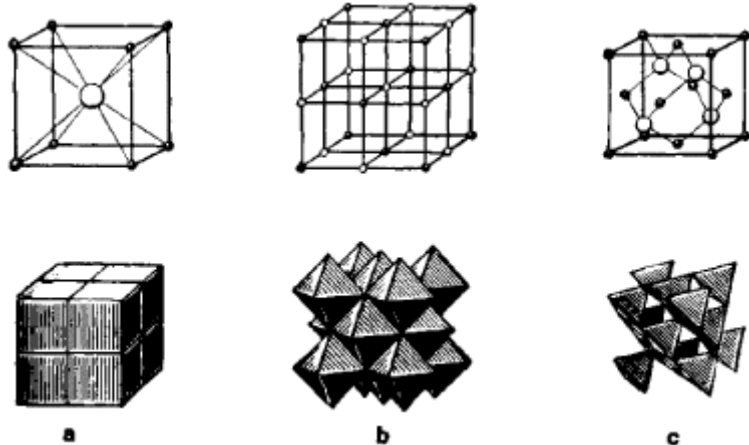


Crystal Structures

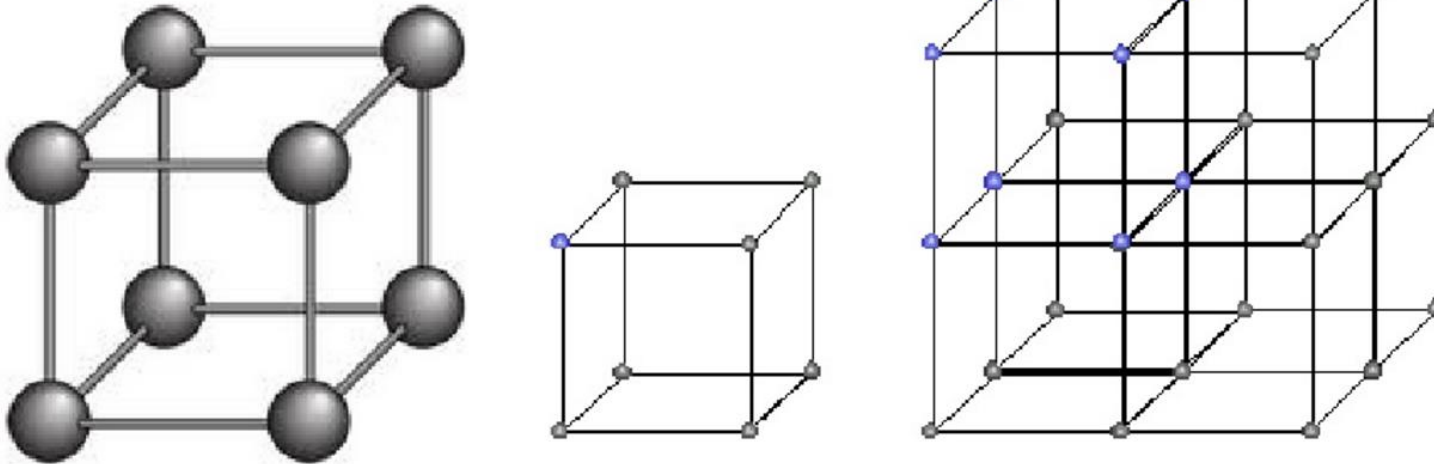
- Atoms form into a crystal lattice
- Structures that are not crystalline are called amorphous
- Metals are crystalline
- Polymers and ceramics can be crystalline and amorphous



Co-ordination Number

Co-ordination number is the number of nearest equidistant neighboring atoms surrounding an atom under consideration

1. Simple Cubic Structure:

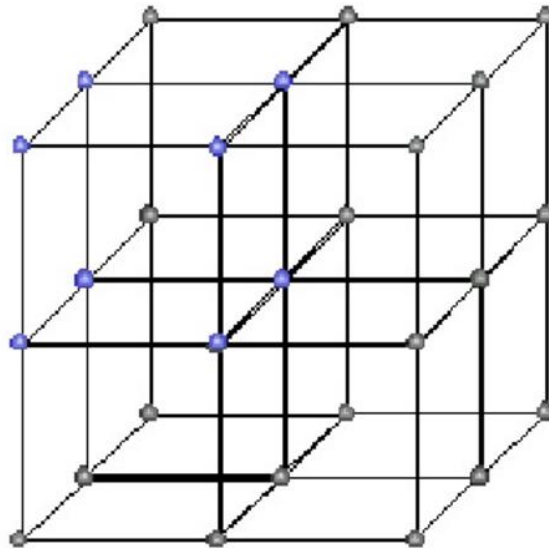
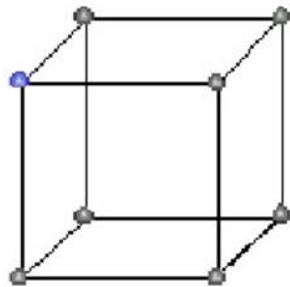
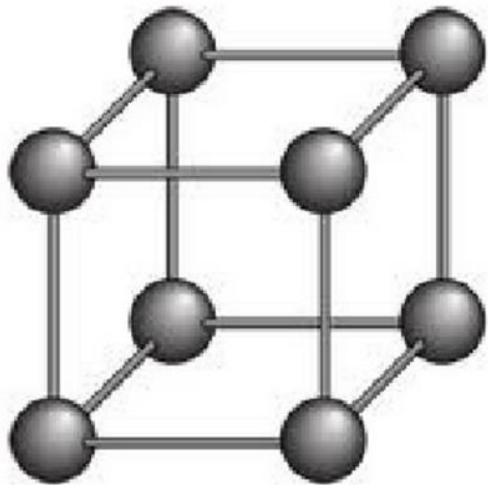


What is the coordination number of this cube?

Co-ordination Number

Co-ordination number is the number of nearest equidistant neighboring atoms surrounding an atom under consideration

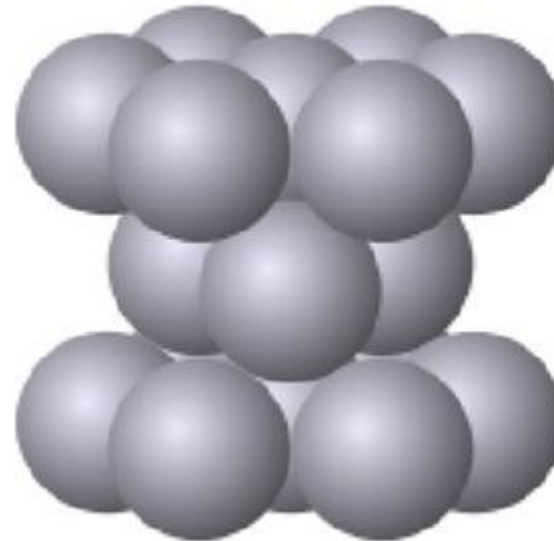
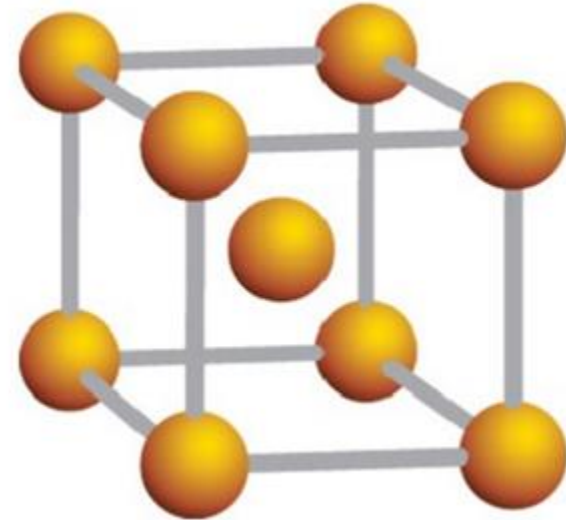
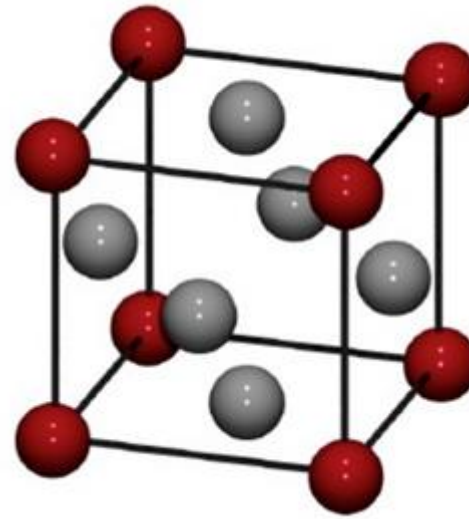
1. Simple Cubic Structure:



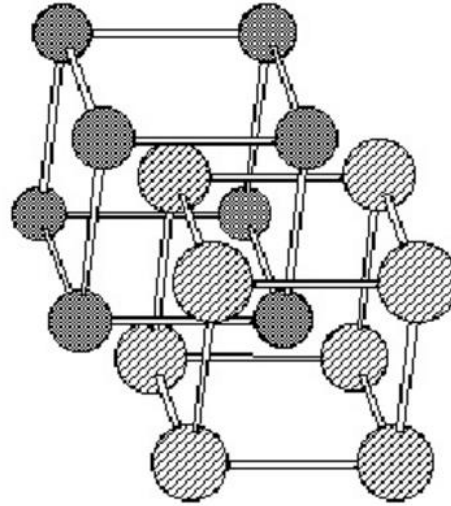
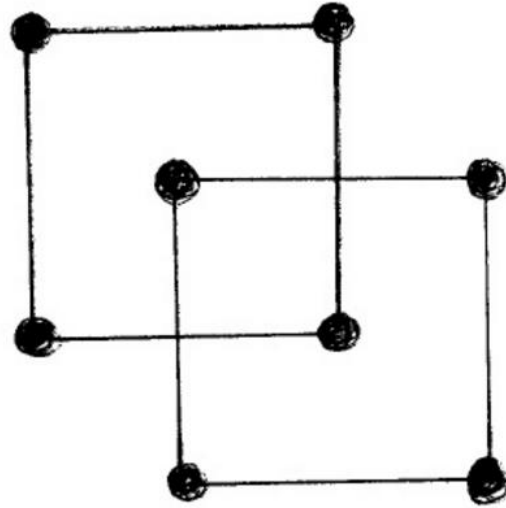
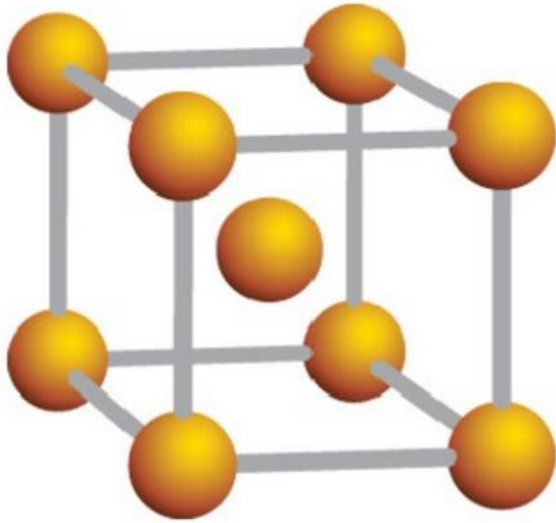
Simple cubic structure has a coordination number of **6**

Metals - Structure

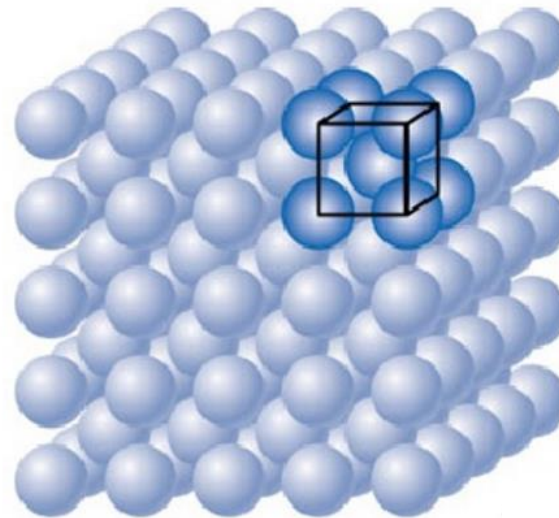
- The properties of some materials are related to their crystal structures.
- Body centred cubic structure BCC
- Face centred cubic structure FCC
- Hexagonal close-packed HCP



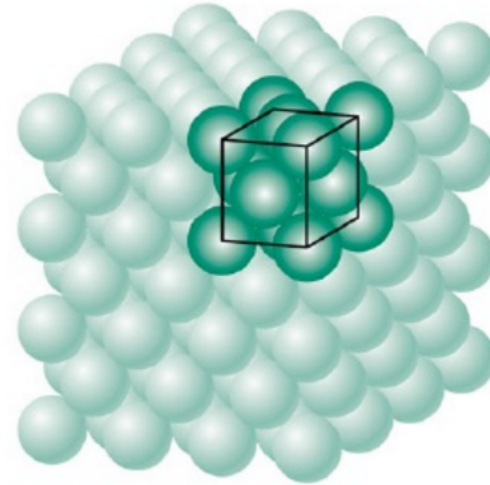
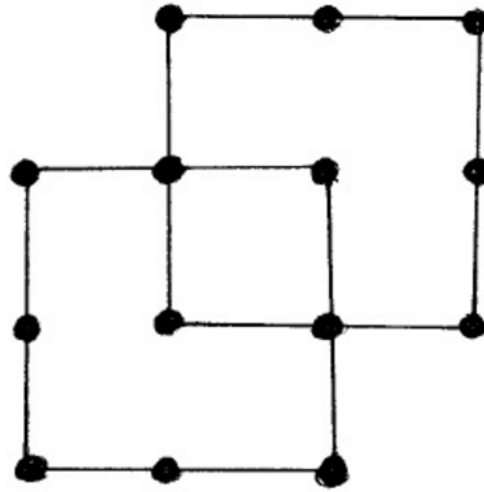
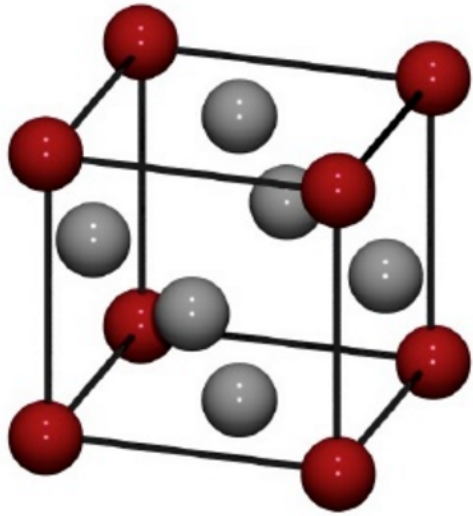
2. Body Centered Cubic Structure:



Body centered cubic structure
has a coordination number of **8**



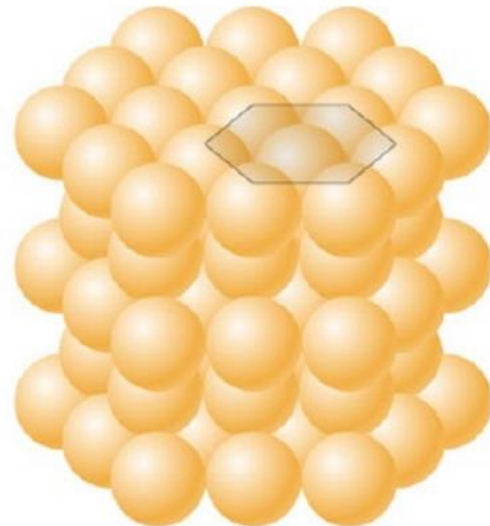
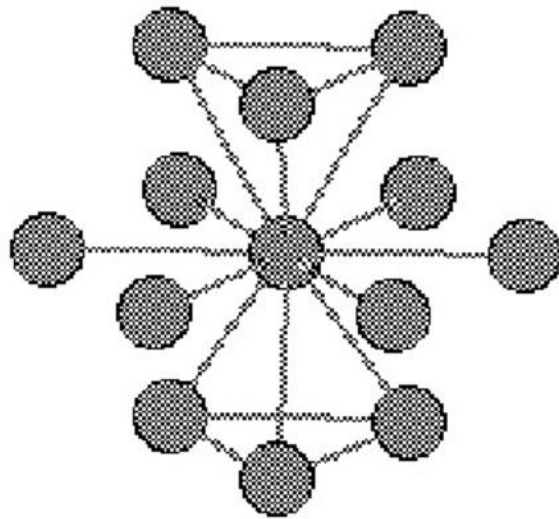
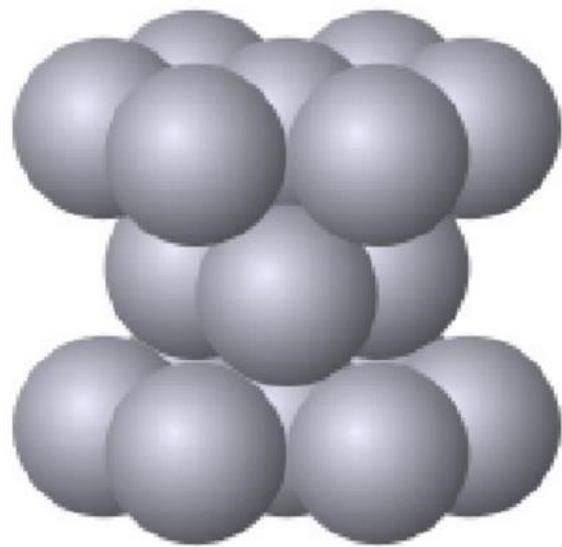
3. Face Centered Cubic Structure:



(c)

Face centered cubic structure has a coordination number of **12**

4. Hexagonal Close Packed Structure:



(b)

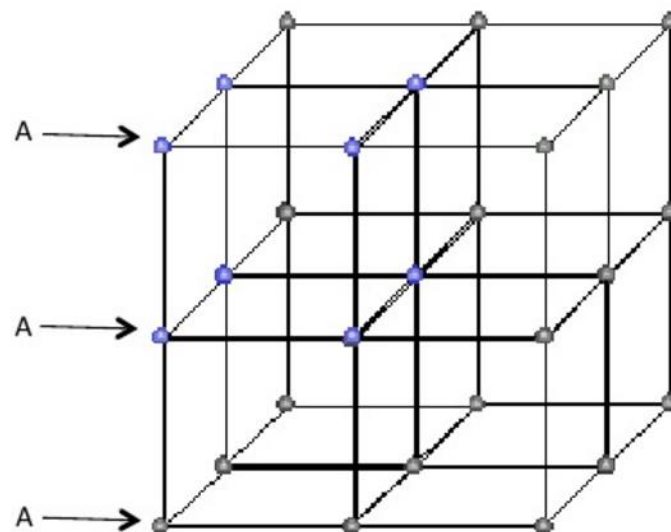
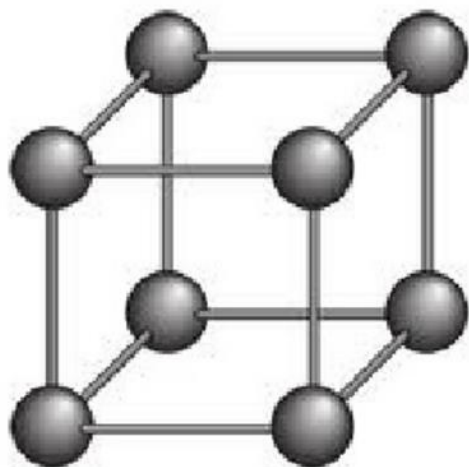
Hexagonal close packed structure has a coordination number of **12**

Stacking Sequence for SC, BCC, FCC and HCP

- Lattice structures are described by stacking of identical planes of atoms one over the other in a definite manner
- Different crystal structures exhibit different stacking sequences

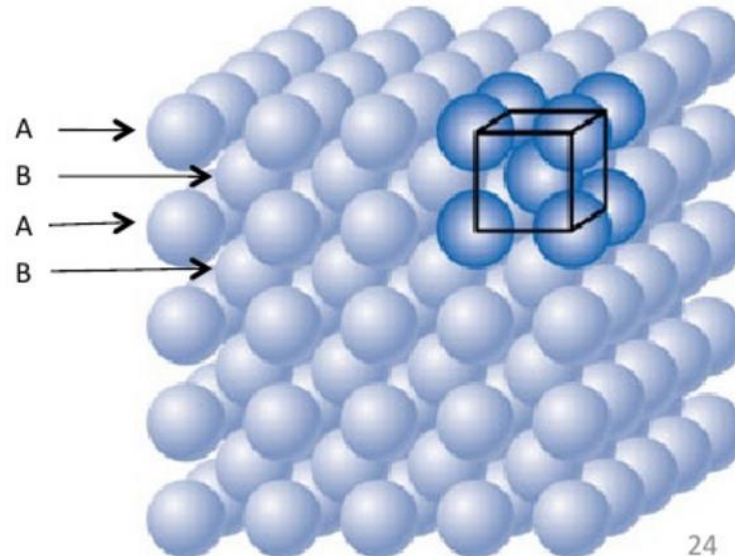
1. Stacking Sequence of Simple Cubic Structure:

Stacking sequence of simple cubic structure is AAAAAA....since the second as well as the other planes are stacked in a similar manner as the first i.e. all planes are stacked in the same manner.



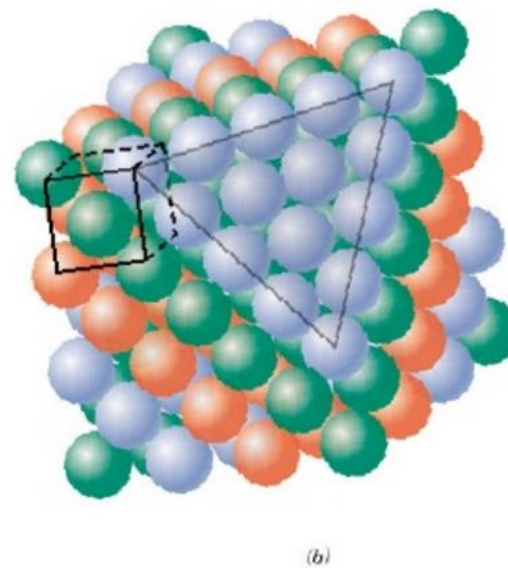
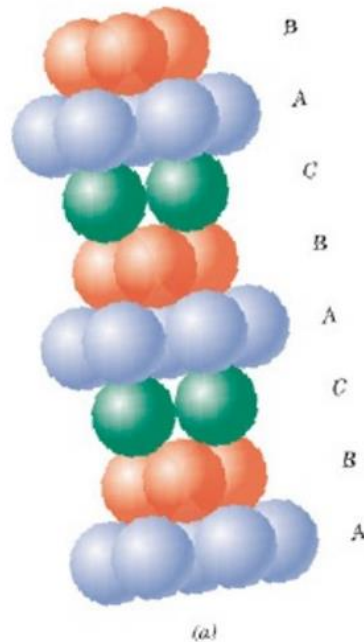
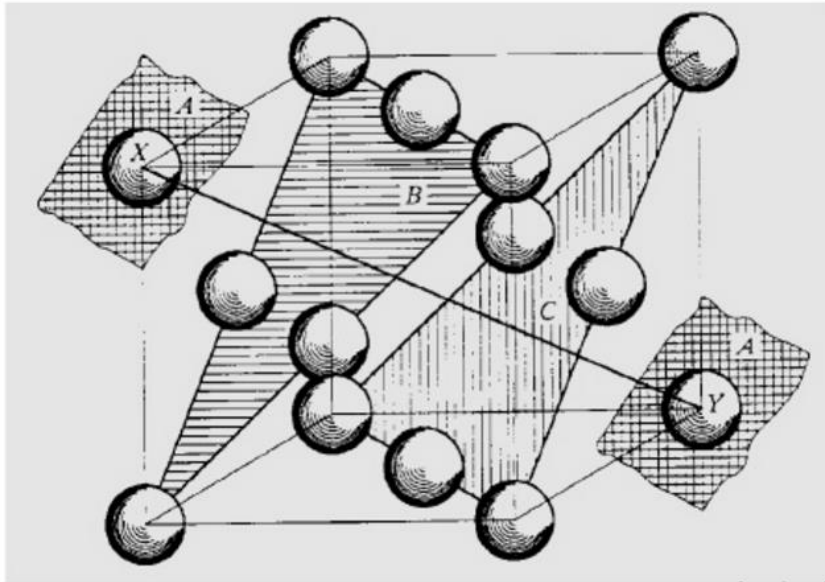
2. Stacking Sequence of Body Centered Cubic Structure:

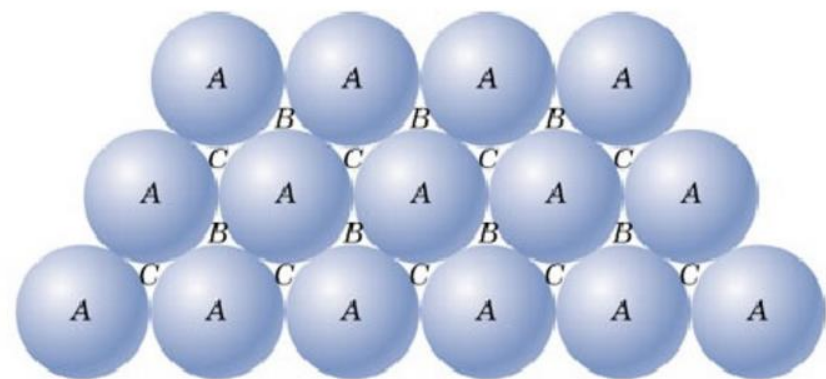
- Stacking sequence of body centered cubic structure is ABABAB....
- The stacking sequence ABABAB indicates that the second plane is stacked in a different manner to the first.
- Any one atom from the second plane occupies any one interstitial site of the first atom.
- Third plane is stacked in a manner identical to the first and fourth plane is stacked in an identical manner to the second and so on. This results in a bcc structure.



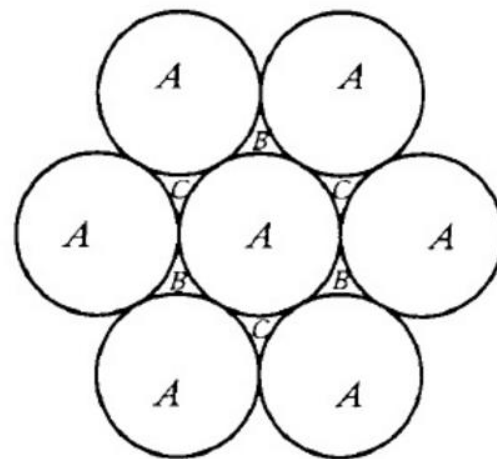
3. Stacking Sequence of Face Centered Cubic Structure:

- Stacking sequence of face centered cubic structure is ABCABC....
- The close packed planes are inclined at an angle to the cube faces and are known as octahedral planes
- The stacking sequence ABCABC... indicates that the second plane is stacked in a different manner to the first and so is the third from the second and the first. The fourth plane is stacked in a similar fashion to the first

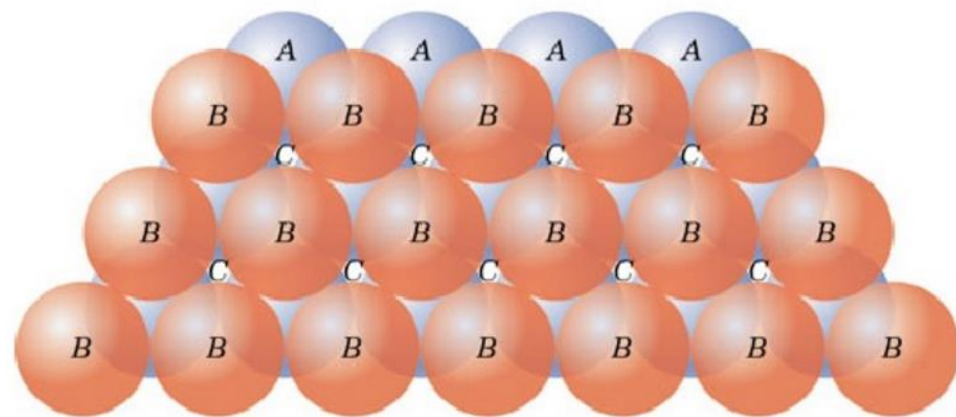




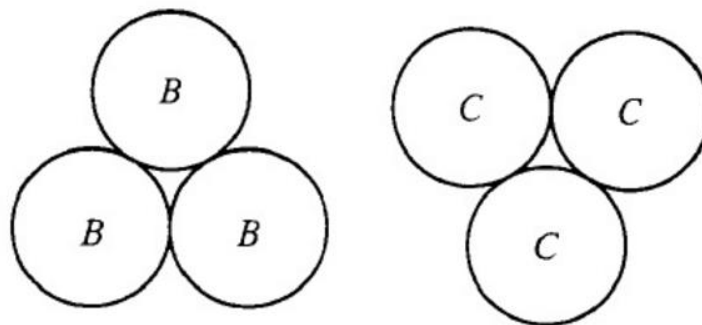
(a)



a

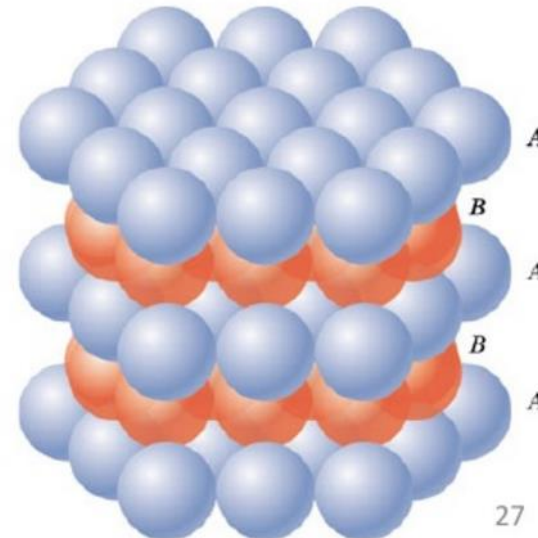
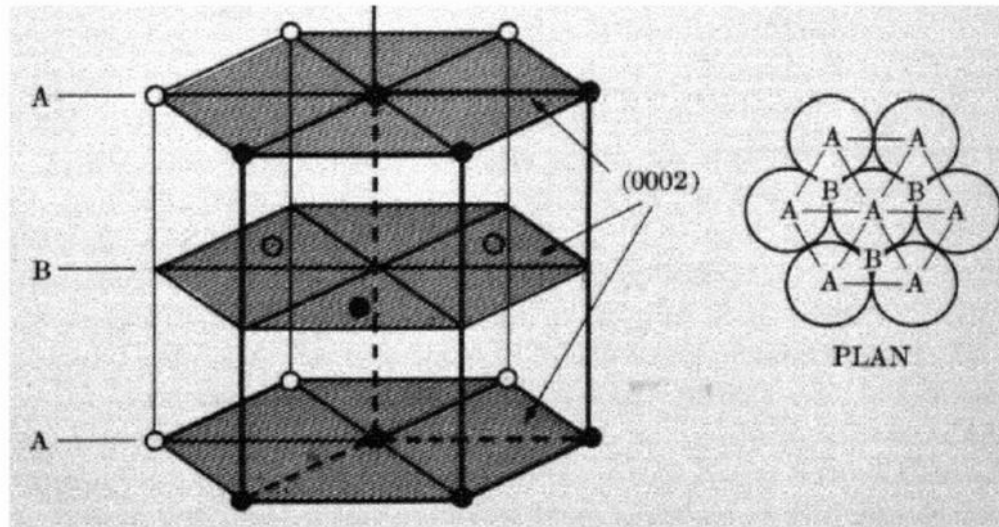


(b)



4. Stacking Sequence of Hexagonal Close Packed Structure:

- Stacking sequence of HCP structure is ABABAB.....
- HCP structure is produced by stacking sequence of the type ABABAB.....in which any one atom from the second plane occupies any one interstitial site of the first plane.
- Third plane is stacked similar to first and fourth similar to second and so on.

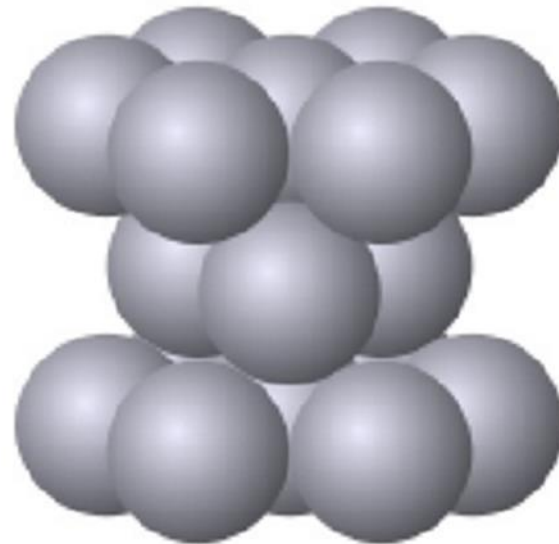
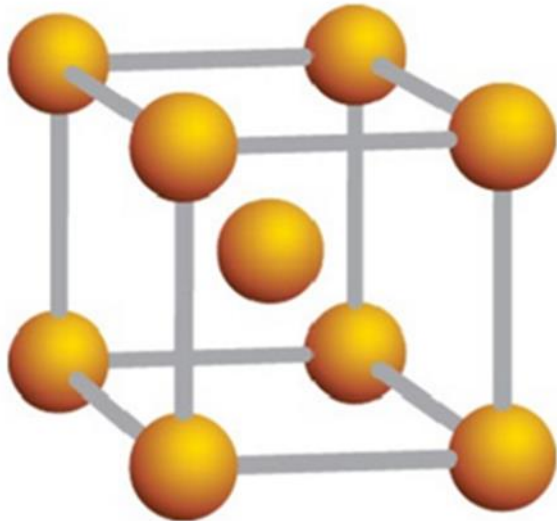
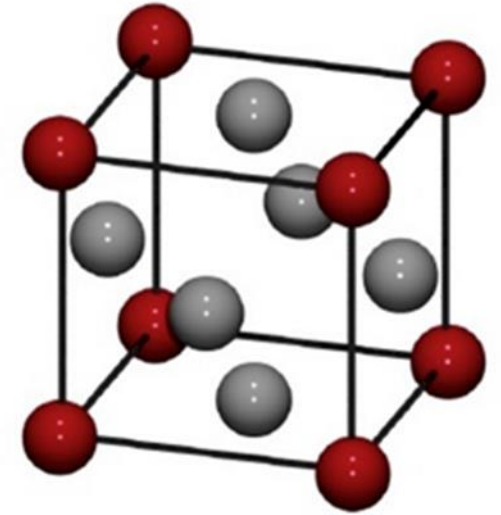


Of the three close-packed cell formations,
which is most efficient?

- FCC or BCC or HCP?

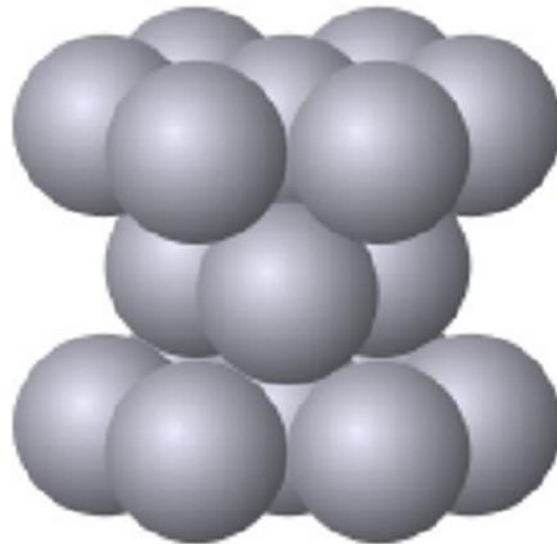
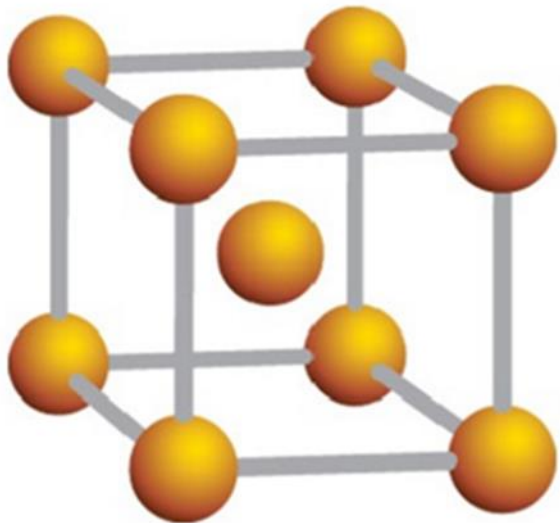
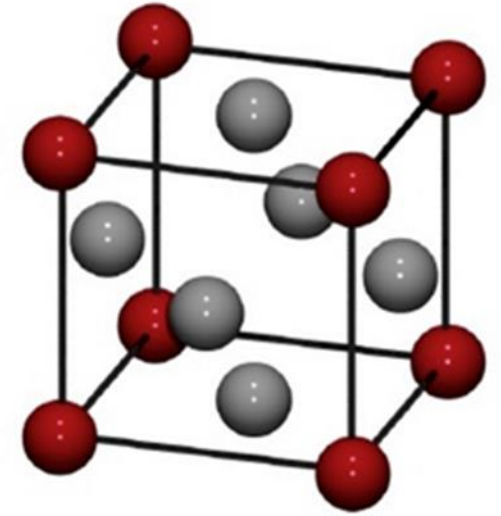
Of the three close-packed cell forms which is most efficient?

- FCC or BCC or HCP?
- How can we work out a measure of how much space compared to how much space is taken up with atoms



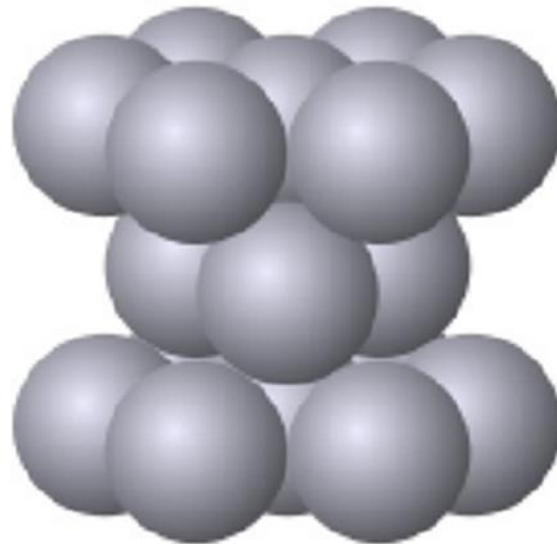
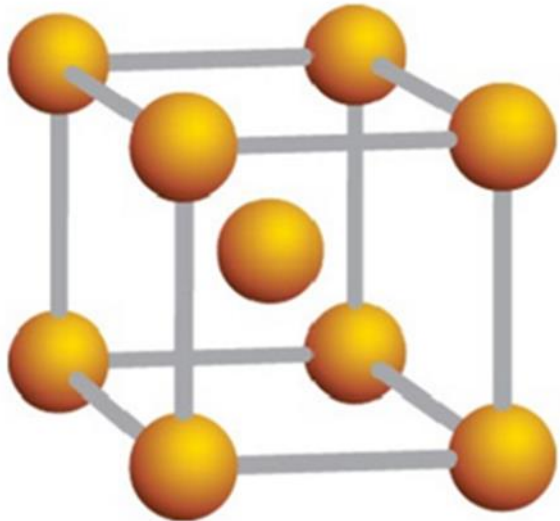
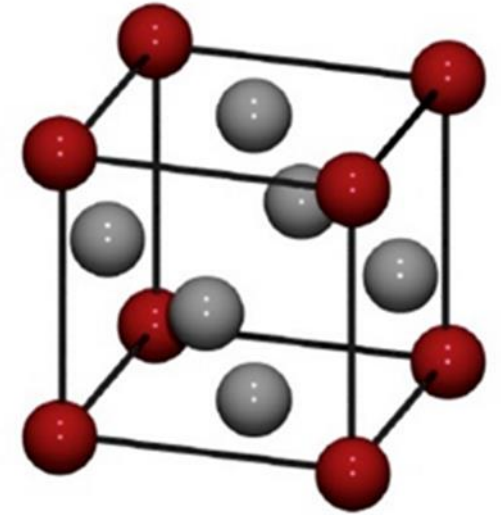
Of the three close-packed cell form which is most efficient?

- FCC or BCC or HCP?
- How can we work out a measure of how much space compared to how much space is taken up with atoms
- What do we need to know?



Of the three close-packed cell forms which is most efficient?

- FCC or BCC or HCP?
- How can we work out a measure of how much space compared to how much space is taken up with atoms
- What do we need to know? How big is the unit cell? How many atoms are inside the unit cell?

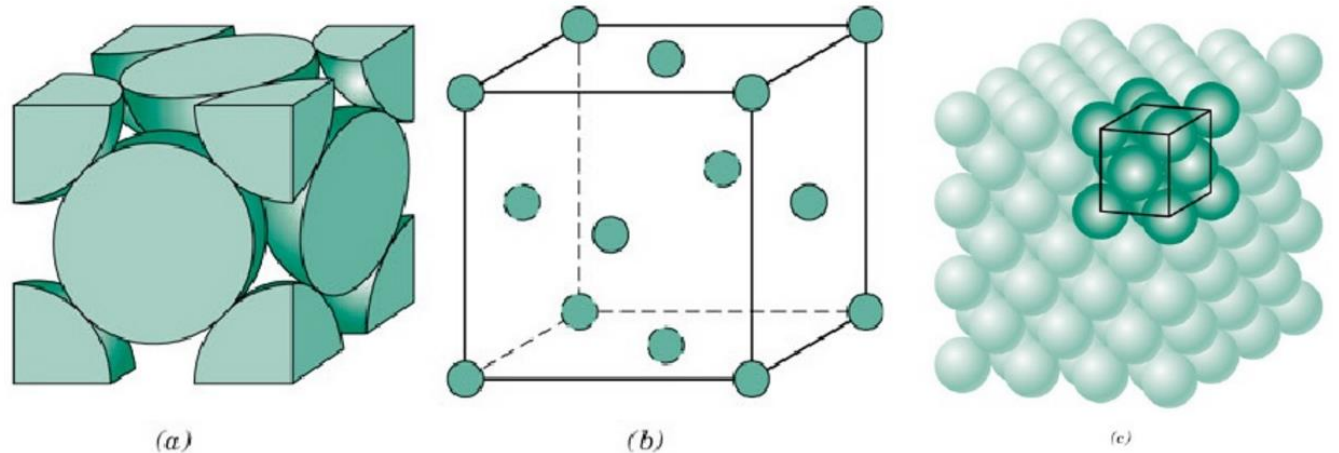


Atomic Packing Factor and Coordination Number

- Atomic Packing Factor– measure of packing efficiency or packing fraction of the volume in the structure occupied by particles.
- $APF = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$
- Coordination number- the number of nearest neighbour or touching atoms

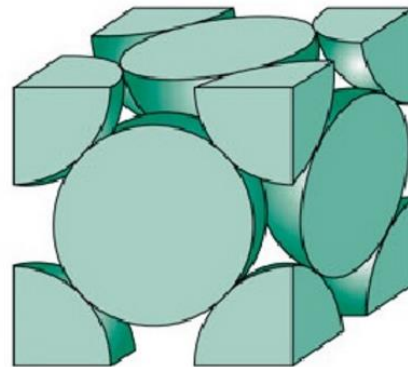
Question

- 1) Build a FCC unit cell
- 2) Calculate the volume of an FCC unit cell in terms of the radius R
- 3) What is the coordination number of an FCC unit cell
- 4) Determine the atomic packing factor for the FCC crystal structure



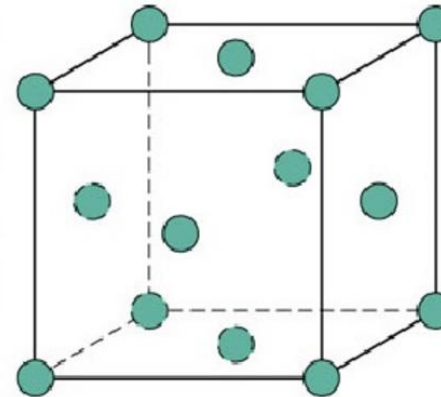
Face Centred Cubic Crystal Structure FCC

- ▶ Closely packed, stacking sequence ABCABC
- ▶ 6 half atoms, one per face
- ▶ 6 faces $(6 \times \frac{1}{2})=3$
- ▶ 8 corners $(8 \times \frac{1}{8})=1$
- ▶ 4 atoms per unit cell
- ▶ Coordination number 12
- ▶ Eg. copper, aluminium, silver, gold



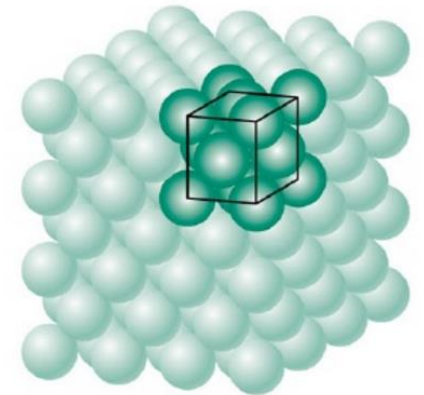
(a)

A unit cell



(b)

A reduced sphere unit cell



(c)

Face Centred Cubic Crystal Structure FCC

- ▶ Closely packed, stacking sequence ABCABC

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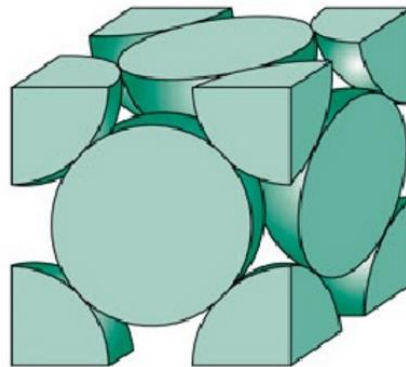
- ▶ 4 atoms per unit cell

- ▶ If length of unit cell is a and R is

the radius of an atom, then $a = 2R\sqrt{2}$

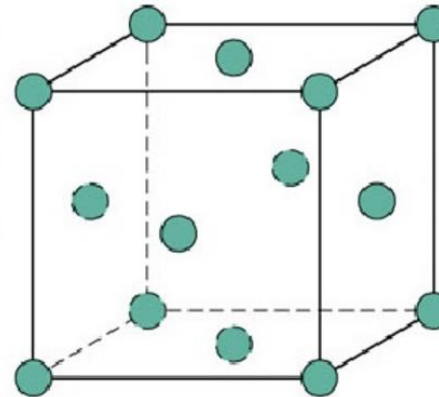
- ▶ Coordination number 12

- ▶ Eg. copper, aluminium, silver, gold



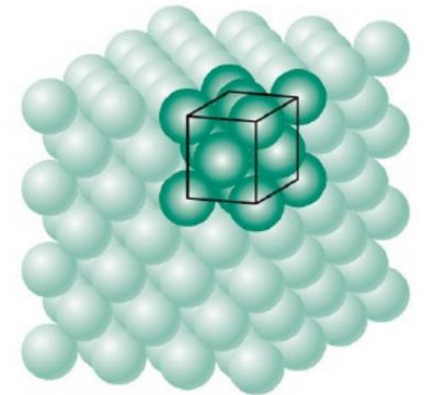
(a)

A unit cell



(b)

A reduced sphere unit cell



(c)

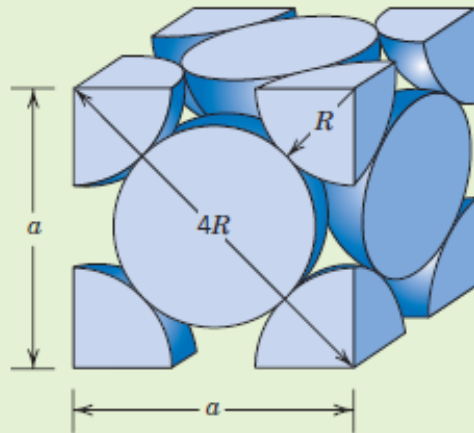
Problem 3.1

Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R .

Solution

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is $4R$. Since the unit cell is a cube, its volume is a^3 , where a is the cell edge length. From the right triangle on the face,

$$a^2 + a^2 = (4R)^2$$

or, solving for a ,

$$a = 2R\sqrt{2} \quad (3.1)$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \quad (3.4)$$

Callister,
Materials Science and
Engineering

Computation of the Atomic Packing Factor for FCC

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R . The volume for a sphere is $\frac{4}{3}\pi R^3$, and since there are four

Computation of the Atomic Packing Factor for FCC

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Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R . The volume for a sphere is $\frac{4}{3}\pi R^3$, and since there are four

atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

Face Centred Cubic Crystal Structure FCC

- ▶ Closely packed, stacking sequence ABCABC

- ▶ 6 half atoms, one per face

- ▶ 6 faces $(6 \times \frac{1}{2})=3$

- ▶ 8 corners $(8 \times \frac{1}{8})=1$

- ▶ 4 atoms per unit cell

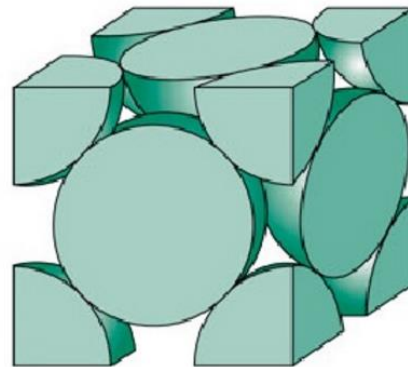
- ▶ If length of unit cell is a and R is

the radius of an atom, then $a = 2R\sqrt{2}$

- ▶ Atomic Packing Factor 0.74

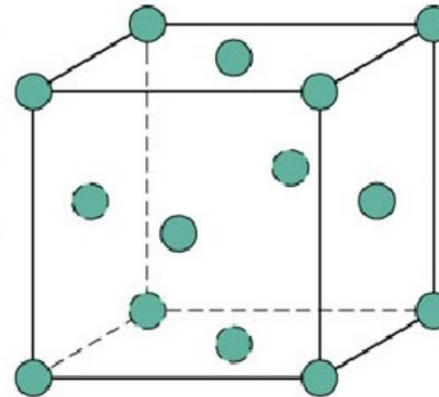
- ▶ Coordination number 12

- ▶ Eg. copper, aluminium, silver, gold



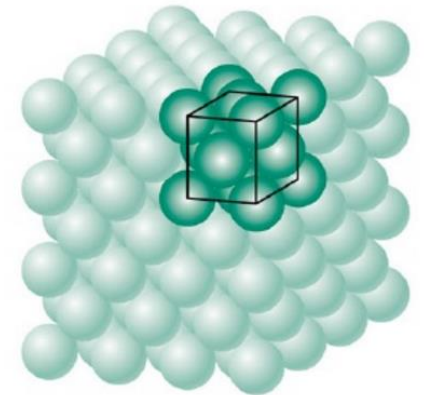
(a)

A unit cell



(b)

A reduced sphere unit cell



(c)

Question

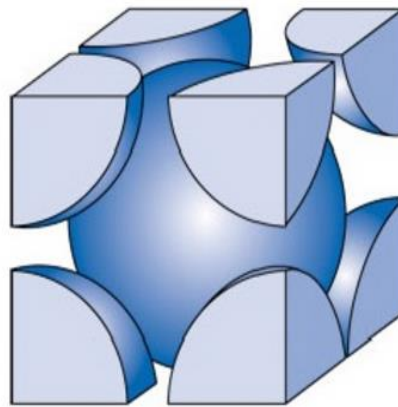
- An element crystallizes in a face centred cubic lattice and has a density of 1.45 g cm^{-3} . The edge of its unit cell is $4.52 \times 10^{-8} \text{ cm}$.
- a) How many atoms are in each unit cell?
- b) What is the volume of a unit cell?
- c) What is the mass of a unit cell?
- d) Calculate the approximate atomic mass of the element

Question - Answer

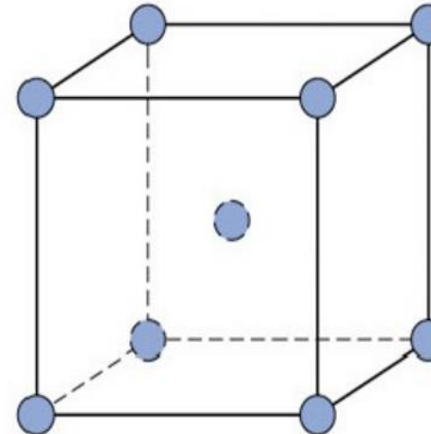
- An element crystallizes in a face centred cubic lattice and has a density of 1.45 g cm^{-3} . The edge of its unit cell is $4.52 \times 10^{-8} \text{ cm}$.
-
- a) How many atoms are in each unit cell? 4
-
- b) What is the volume of a unit cell? $(4.52 \times 10^{-8} \text{ cm})^3 = 9.23 \times 10^{-23}$
-
- c) What is the mass of a unit cell? $\text{Mass} = d \times v = 1.45 \text{ g cm}^{-3} \times 9.23 \times 10^{-23} = 1.338 \times 10^{-22} \text{ g}$
-
- d) Calculate the approximate atomic mass of the element. $1.338 \times 10^{-22} \text{ g} / 4 = 3.346 \times 10^{-23} \text{ g}$

Question

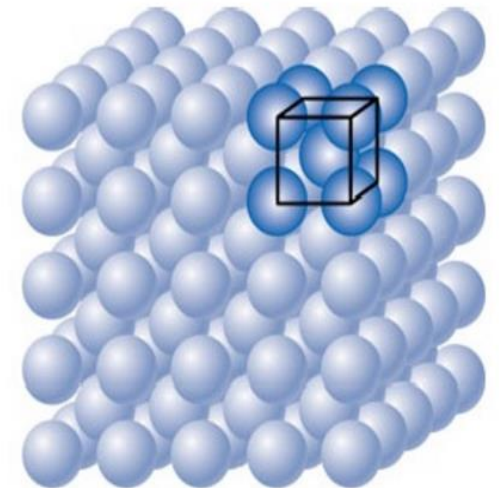
- 1) Build a BCC unit cell
- 2) Calculate the volume of an BCC unit cell in terms of the radius R
- 3) What is the coordination number of an BCC unit cell
- 4) Determine the atomic packing factor for the BCC crystal structure



(a)



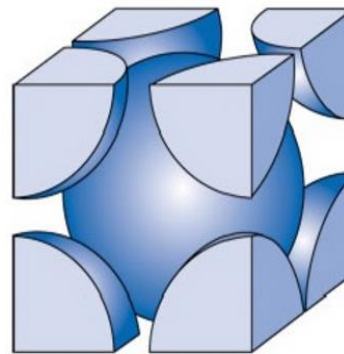
(b)



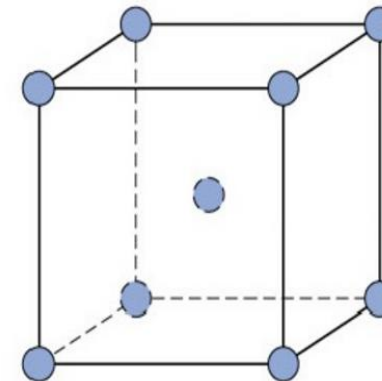
(c)

Question

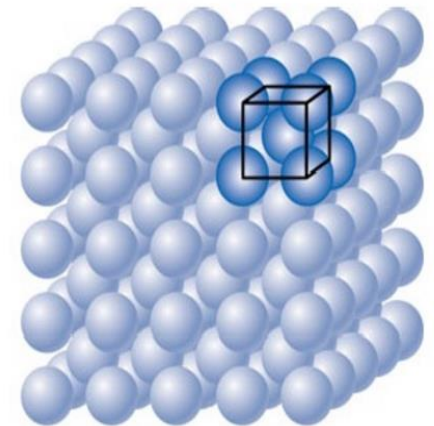
- 1) Build a BCC unit cell
- 2) Calculate the volume of an BCC unit cell in terms of the radius R
- $a = 4R/\sqrt{3}$ and $\text{vol} = (4R/\sqrt{3})^3 = 64R^3/3\sqrt{3}$
- $V_s = 8/3 \pi R^3$
- 3) What is the coordination number of an BCC unit cell
- 4) Determine the atomic packing crystal structure



(a)



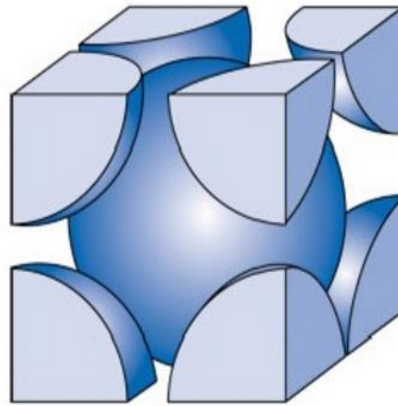
(b)



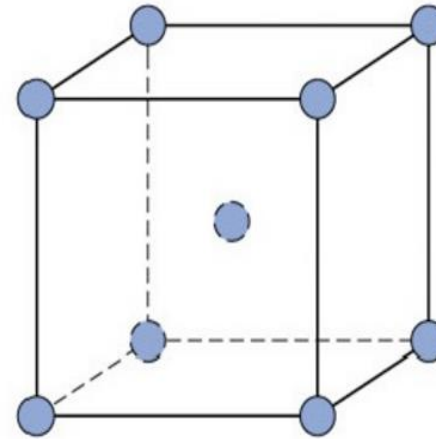
(c)

Body Centred Cubic Crystal Structure BCC

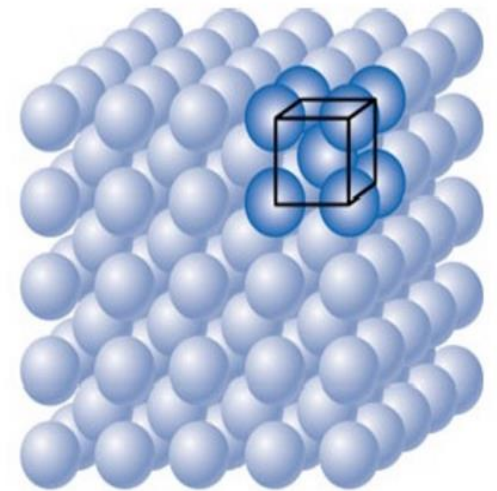
- Stacking sequence ABABAB
- 8 corners($8 \times \frac{1}{8}$)=1
- 1 central =1
- 2 atoms per unit cell
- Atomic Packing Factor (APF) = 0.68
- Coordination number 8
- Eg chromium, iron, tungsten



(a)



(b)



(c)