University of Anbar/ Faculty of Engineering

Department of Mechanical Engineering

2nd Semester (2018/2019)

Subject: Engineering of Metallurgy

Course Code: ME2304

Stage: 2nd Year

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Lecture # 5

CHAPTER THREE/ THE STRUCTURE OF CRYSTALLINE SOLIDS

Introduction

Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. A ***crystalline material*** is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms. All metals, many ceramic materials, and certain polymers form crystalline structures under normal solidification conditions. For those that do not crystallize, this long-range atomic order is absent; these ***noncrystalline or amorphous materials*** like glasses.

CRYSTAL STRUCTURE

Fundamental Concepts

Solids either Crystalline or Noncrystalline;

- ***Crystalline material***: Atoms in a crystalline solid are arranged in a repeating or periodic three dimensional pattern Long Range Order, like all metals.
- ***Noncrystalline or Amorphous material:*** Atoms in an amorphous solid are arranged randomly- No Order, like glasses.

- A ***crystal*** is a solid material that contains atoms or groups of atoms arranged in a highly ordered structure. This structural arrangement is three-dimensional.
- ***Crystalline lattice:*** is a regular repeating pattern (3D array) that describes the arrangement of atoms. (***Figure 1***)
- ***Unit Cell:*** is the basic structural unit of crystal structure describes the arrangement of atoms or molecules.
- ***Polycrystalline:*** a material consists of many crystals (grains) **and** each crystal (grain) is itself a ***single crystal***.
- ***Single Crystals***: Crystals can be single crystals where the whole solid is one crystal. Then it has a regular geometric structure with flat faces.
- ***Grain:*** small crystal in microstructure.

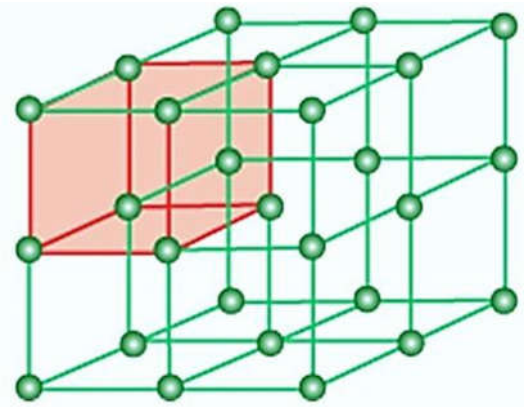
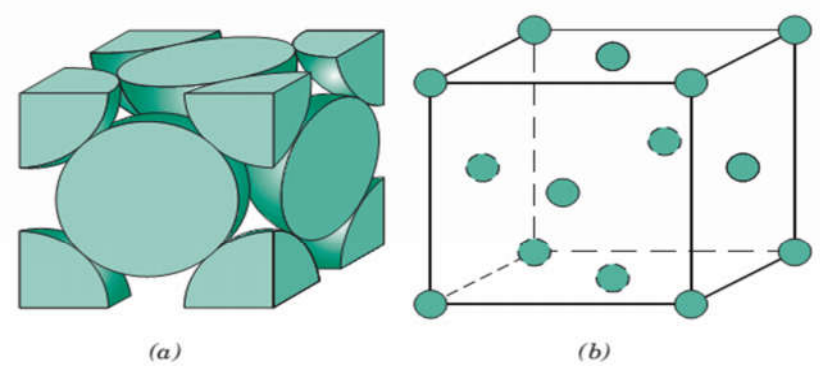


Figure 1. A regular repeating pattern (3D array) (Crystalline lattice).

For the face centered cubic crystal structure shown in ***Figure 2***, (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms.



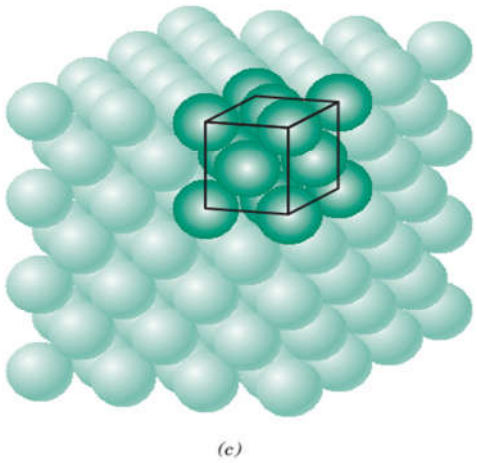


Figure 2. face centered cubic crystal structure.

H.W.(1). *What is the difference between atomic structure and crystal structure?*

Definition of Crystal systems

Crystal contains millions of atoms. The geometrical characteristics of the whole crystal can be expressed in terms of the size, shape and atomic arrangement of the unit cell.

- ***Lattice parameters:*** parameters that describe the size and shape of the unit cell, these parameters include unit cell length and angle. The geometry of unit cell is defined by six parameters are indicated in **Figure 3**:
  1) The three edge lengths **a, b, and c.**
  2) The three interaxial angles **α, β, and γ**

On this basis there are seven different possible combinations of *a*, *b*, and *c*, and α, β, and γ, each of which represents a distinct **crystal system.** These seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedra, monoclinic, and triclinic, **Table 1.**

- Most metals form cubic structures BCC, FCC, or Hexagonal Close Packed (HCP) structures.

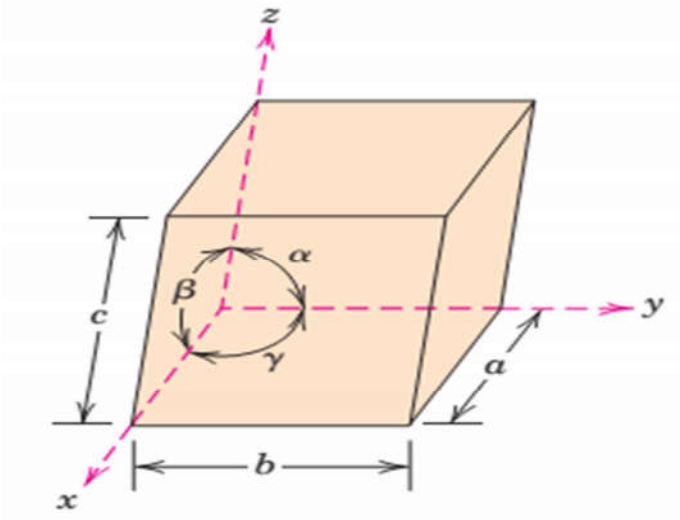


Figure 3. A unit cell with x, y, and z coordinate axes, showing axial lengths (a, b, and c) and interaxial angles (α, β, and γ).

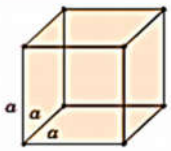
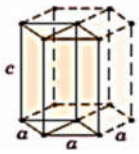
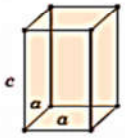
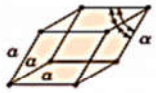
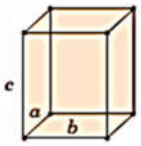
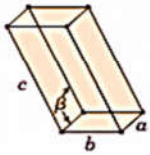
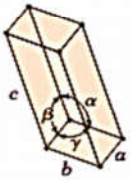
Parameters in Studying Crystal Structures

- ***Number and Position of Atoms in unit cell*** . For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, **1/m**.
- ***Coordination No.***: No. of touching-neighbor atoms **or** is the number of closest neighbors to which an atom is bonded.
- ***Cube edge (length)*** Cell dimensions (Lattice spacing a, b and c) in terms of R and Angle between the axis α, β, γ.
- ***Atomic Packing Factor (APF)***: Fraction of volume occupied by atoms.

Fraction of empty space = 1 – APF

APF = (Total volume of atoms in the unit cell / Volume of the unit cell)

Table 1. Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

METALLIC CRYSTAL STRUCTURES

Cubic System Structures

- **N:** *is the total number of lattice points (atoms) for cubic unit cell is:*

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Ni: *is the number of lattice points (atoms)at interior of the unit cell.*
Nf: *is the number of lattice points (atoms)on the face of the unit cell.*
Nc: *is the number of lattice points (atoms)at the corner of the unit cell.*

- ***CN (Coordination No.)***: No. of touching-neighbor atoms.
- ***Cube edge (length)*** Cell dimensions (Lattice spacing a, b and c) in terms of R and Angle between the axis α, β, γ.
- ***Atomic Packing Factor (APF)***: Fraction of volume occupied by atoms.

Fraction of empty space = 1 – APF

APF = (Total volume of atoms in the unit cell / Volume of the unit cell)

All these parameters will calculated in detail for each structure.

I. The Simple Cubic Crystal Structure (SC)

Simple Cubic Structure (SC): Rare due to low packing density (only ***Po*** (***Polonium***) has this structure. Close-packed directions are cube edges.

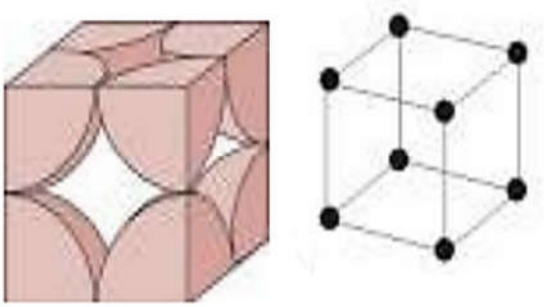
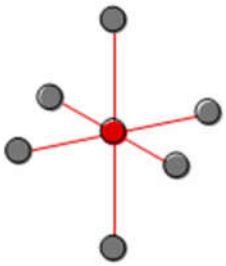
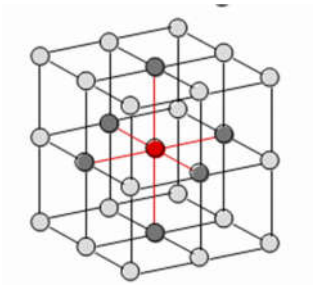


Figure 3. A Simple Cubic Crystal Structure

1) ***Coordination NO. = 6***
(#** nearest neighbors**)





2) **N:** *is the total number of lattice points (atoms) for cubic unit cell is:*

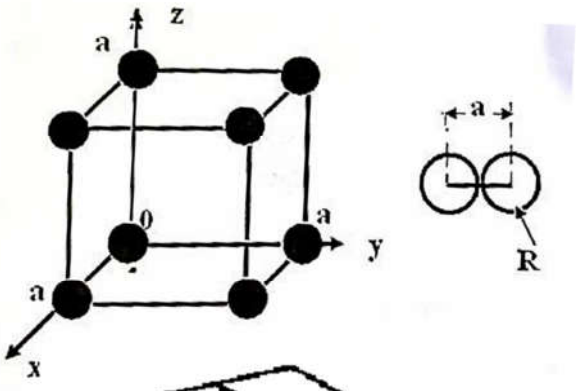
$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

***Ni** = 0 atoms at interior of the unit cell.*
***Nf** = 0 atoms on the face of the unit cell.*
***Nc** = 8 atoms at the corner of the unit cell*

$$N = 0 + \frac{0}{2} + \frac{8}{8} = 1\ atom$$

3) *The relationship between the cube edge length **(a)** and the atomic radius **(R)***

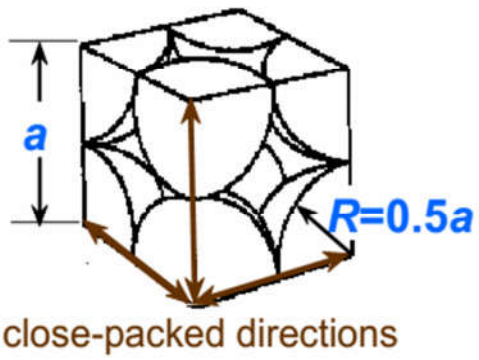
$$a = 2R$$



4) APF = (Total volume of atoms in the unit cell / Volume of the unit cell)

$$\text{APF} = \frac{N \times (\frac{4}{3}\Pi R^3)}{a^3}$$

$$\text{APF} = \frac{1 \times (\frac{4}{3}\Pi R^3)}{(2R)^3} = 0.52$$



II. The Face-Centered Cubic Crystal Structure (FCC)

- *Atoms located at each of the corners and the centers of all the cube faces.*
- *Some of the familiar metals having this crystal structure are Al, Cu, Au, Pb, Ni, Pt, Ag*
- *Atoms touch each other along face diagonals.*

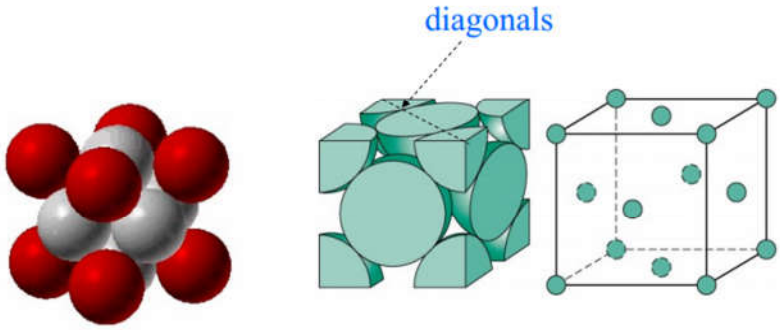


Figure 4. Face-Centered Cubic Crystal Structure

1) ***Coordination NO. = 12 (**# nearest neighbors**)***

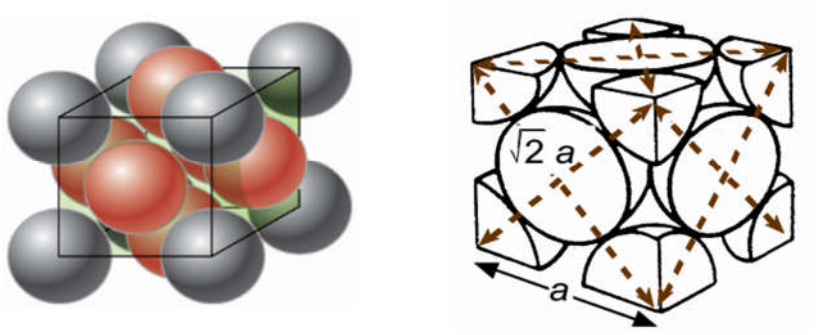
2) **N:** *is the total number of lattice points (atoms) for cubic unit cell is:*

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

***Ni = 0** atoms at interior of the unit cell.*
***Nf = 6** atoms on the face of the unit cell.*
***Nc = 8** atoms at the corner of the unit cell*

$$N = 0 + \frac{6}{2} + \frac{8}{8} = 4\ atoms$$

3) *The relationship between the cube edge length **(a)** and the atomic radius **(R)***

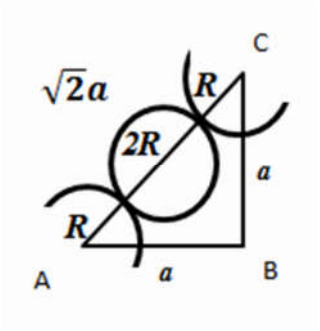


$$(4R)^2 = a^2 + a^2$$

$$16R^2 = 2a^2$$

$$8R^2 = a^2$$

$$a = 2R\sqrt{2}$$



4) APF = (Total volume of atoms in the unit cell / Volume of the unit cell)

$$\text{APF} = \frac{N \times Vatom}{V_c} = \frac{N \times (\frac{4}{3}\Pi R^3)}{a^3}$$

$N = 4\ atoms$

$$Vatom = 4 \times \left(\frac{4}{3}\Pi R^3\right) = 16\Pi R^3/3$$

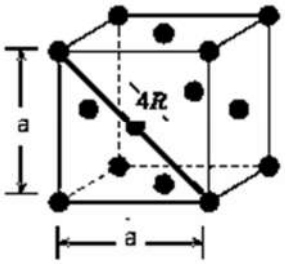
$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

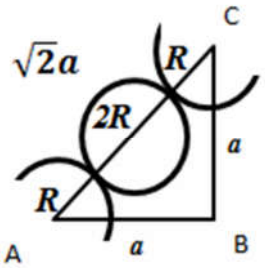
$$\text{APF} = \frac{16\Pi R^3/3}{16R^3\sqrt{2}} = 0.74$$

EXAMPLE:

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.





Because the unit cell is a cube, its volume is a^3 ($V_C = a^3$) (a is the cell edge length). From the right triangle on the face,

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

The FCC unit cell volume V_C may be computed from

$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

H.W (2) *Show that the atomic packing factor for the FCC crystal structure is 0.74?*

III. The Body-Centered Cubic Crystal Structure (BCC)

- *Atoms located at all eight corners and a single atom at the cube center.*
- *Examples: Iron (α), Cr: Chromium, W: Tungsten, Ta: Tantalum, Mo: Molybdenum.*
- *Atoms touch each other along cube diagonals.*

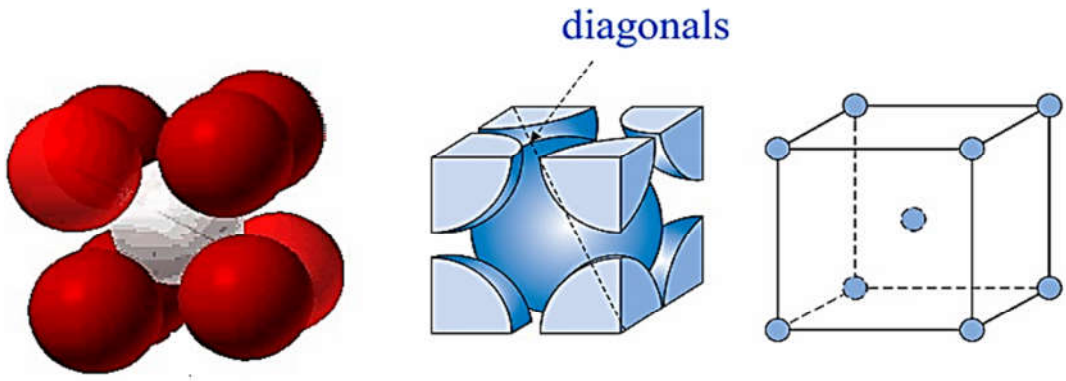


Figure 5. Body-Centered Cubic Crystal Structure

1) ***Coordination NO. = 8 (#** nearest neighbors**)***

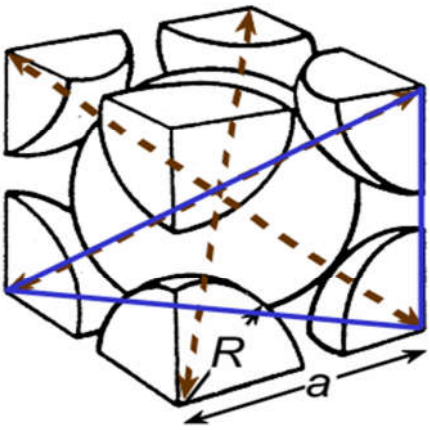
2) **N:** *is the total number of lattice points (atoms) for cubic unit cell is:*

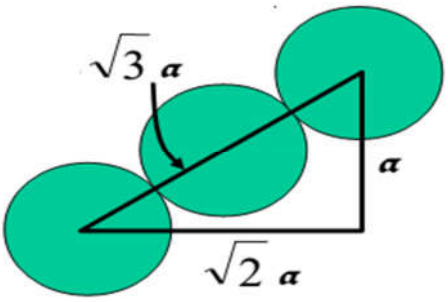
$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

***Ni =** **1** atoms at interior of the unit cell.*
***Nf = 0** atoms on the face of the unit cell.*
***Nc =** **8** atoms at the corner of the unit cell*

$$N = 1 + \frac{0}{2} + \frac{8}{8} = 2\ atoms$$

3) *The relationship between the cube edge length **(a)** and the atomic radius **(R)***

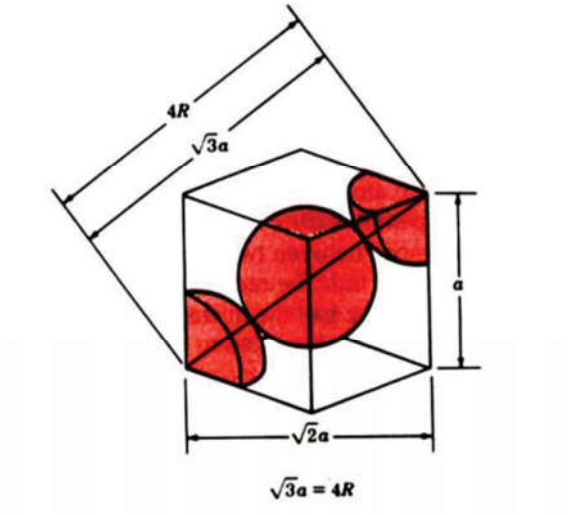




$$(4R)^2 = a^2 + (\sqrt{2a})^2$$

$$16R^2 = 3a^2$$

$$\mathbf{a} = \frac{\mathbf{4R}}{\sqrt{\mathbf{3}}}$$



4) APF = (Total volume of atoms in the unit cell / Volume of the unit cell)

$$\text{APF} = \frac{\boldsymbol{N} \times (\frac{\mathbf{4}}{\mathbf{3}}\boldsymbol{\Pi R^3})}{\boldsymbol{a^3}}$$

$$\text{APF} = \frac{\mathbf{2} \times (\frac{\mathbf{4}}{\mathbf{3}}\boldsymbol{\Pi R^3})}{(\frac{\mathbf{4R}}{\sqrt{\mathbf{3}}})^{\mathbf{3}}} = \mathbf{0.68}$$

- ***N0TE***: The coordination number for the BCC crystal structure is 8; each center atom has as nearest neighbors its eight corner atoms. Because the coordination number is less for BCC than FCC, so also is the atomic packing factor for BCC lower = 0.68 versus 0.74.
- A face-centered cubic crystal structure will exhibit more ductility (deform more readily under load before breaking) than a body-centered cubic

structure. [i.e., lattice structures with closely packed planes allow more plastic deformation than those that are not closely packed. Additionally, cubic lattice structures allow slippage to occur more easily than non-cubic lattices]. The BCC lattice, although cubic, is not closely packed and forms strong metals. Alpha-iron and tungsten have the BCC form. Gamma-iron, silver, gold, and lead have FCC structures. Finally, HCP lattices are closely packed, but not cubic. HCP metals like cobalt and zinc are not as ductile as the FCC metals.

Hexagonal System Structure

I. The Hexagonal Close-Packed Crystal Structure (HCP)

- Not all metals have unit cells with cubic symmetry; the final common metallic crystal structure to be discussed has a unit cell that is hexagonal.
- There are **six atoms in HCP unit cell calculated as follows:**
  1) 3 mid-plane atoms shared by no other cells: (***3×1= atoms***).
  2) 12 hexagonal corner atoms shared by six cells: (***12×1/6 = 2 atoms***).
  3) 2 atoms in the center of hexagon of both the top and bottom layers each contribute 1/2 atom: (***2×1/2= 1 atom***).

  N: *is the total number of lattice points (atoms) for* **HCP unit cell** *is:*

  N = 3+2+1 = 6 atoms

- **HCP unit cell** has two lattice parameters **a** and **c, the ideal ratio is (c/a =1.633).**
- ***Coordination NO.*** *of atoms in* HCP unit cell *= 12, which is the same as FCC structure.* ***(a =2R)***
- The HCP metals include cadmium Cd, magnesium Mg, titanium Ti, and zinc Zn.

H.W. (3) *Show that the atomic packing factor for HCP is 0.74?*

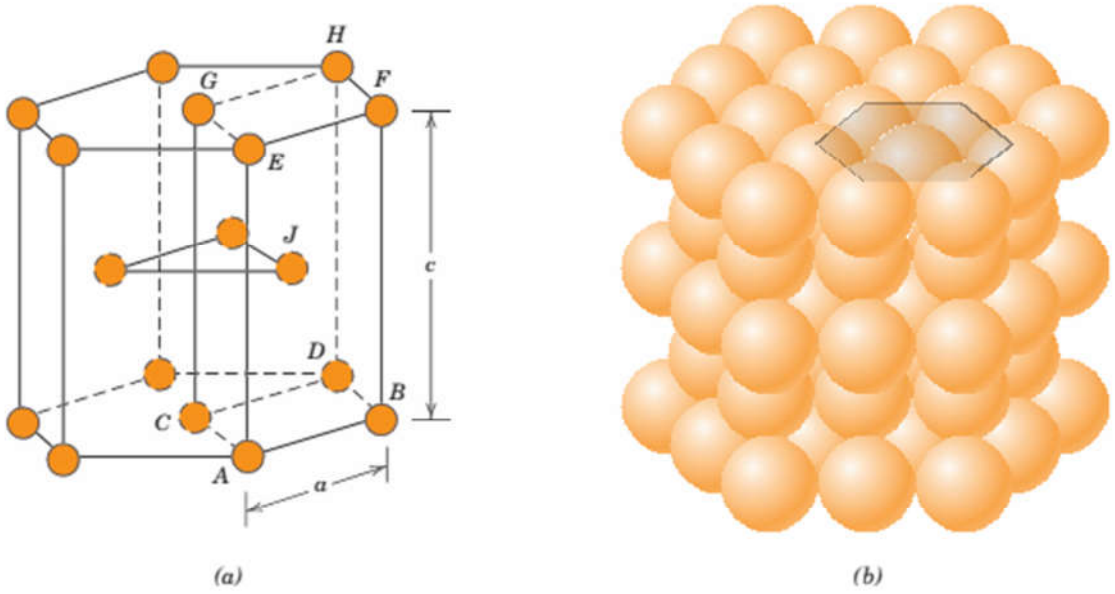
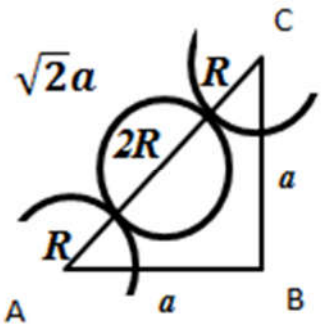


Figure 6. For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell (a and c represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms.

Examples: *If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters?*

Solution:

Aluminum has an FCC crystal structure;



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

$$16R^2 = 2a^2$$

$$8R^2 = a^2$$

$$a = 2R\sqrt{2}$$

$$V_c = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

If R =0.143 nm;

$$V_c = (16) \times (0.143 \times 10^{-9}\text{m})^3 \times (\sqrt{2})$$

$$V_c = 6.62 \times 10^{-29}\, m^3$$