*Al-Mustaqbal University*
*Department of Biomedical Engineering*
*Second Stage / 1st Course*
***"Biomaterials Science 1"***
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# Lecture 3
# "Crystal Structure of Biomaterial"

## Introduction:

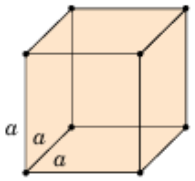
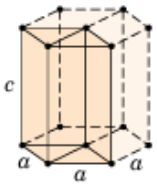
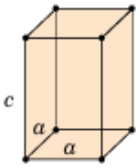
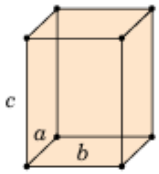
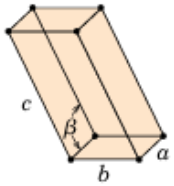
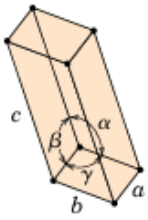
Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. A ***crystalline*** material is one in which the atoms are situated in a repeating or array over large atomic distances, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest neighbor atoms. Crystal structure lattice Some of the properties of crystalline solids depend on the crystal structure of the material, and the manner in which atoms, ions, or molecules are spatially arranged.

When crystalline structures are described, atoms (or ions) are thought of as being solid spheres having well-defined diameters. This is termed the atomic hard-sphere model in which spheres representing nearest-neighbor atoms touch one another. Sometimes the term ***lattice*** is used in the context of crystal structures; in this sense lattice means a three-dimensional array of points coinciding with atom positions (or sphere centers).

## Crystal System:

The crystal system is a grouping of crystal structures that are categorized according to the axial system used to describe their "lattice". A crystal's lattice is a three-dimensional network of atoms that are arranged in a symmetrical pattern. Each crystal system consists of a set of three axes in a particular geometrical arrangement. The seven unique crystal systems, listed in order of decreasing symmetry, are 1. Isometric System, 2. Hexagonal System, 3. Tetragonal System, 4. Rhombohedric (Trigonal)System, 5. Orthorhombic System, 6. Monoclinic System, 7. TriclinicSystem.

**Table 3.2** 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 | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90°$ |  |

## Unit Cell:

The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells.

The unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.

The most common types of crystal structure in solids

**1- Face - centered cubic FCC**

**2- Body - centered cubic BCC**

**3- Hexagonal close - packed HCP Hexagonal system**

For each crystal structure mentioned above, we will determine:

- Position of atoms
- The relation between the length (a) of the cell and the radius of the atom R.
- The coordination number CN.
- Number of atoms/unit cell.
- Atomic packing factor APF.

## Face – Centered Cubic (FCC):

- Atoms are located of the corners and on the centers of all the faces of cubic unit cell.

- Cu, Al, Ag, and Au have this crystal structure.

- The relation between the length (a) and the radius of the atom R:

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

- The coordination number CN = The number of closest neighbors to which an atom is bonded. $CN_{(FCC)} = 12$

- Number of atoms per cell , N, can be computed using the following formula for FCC and BCC:

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

$N_i$ = the number of interior atoms
$N_f$ = the number of face atoms
$N_c$ = the number of corner atoms

$N_{FCC}$= 8x1/8 + 6 x 1/2= 4 atom/ unit cell.

- Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and the volume of the unit cell atoms in a unit cell total unit cell volume

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

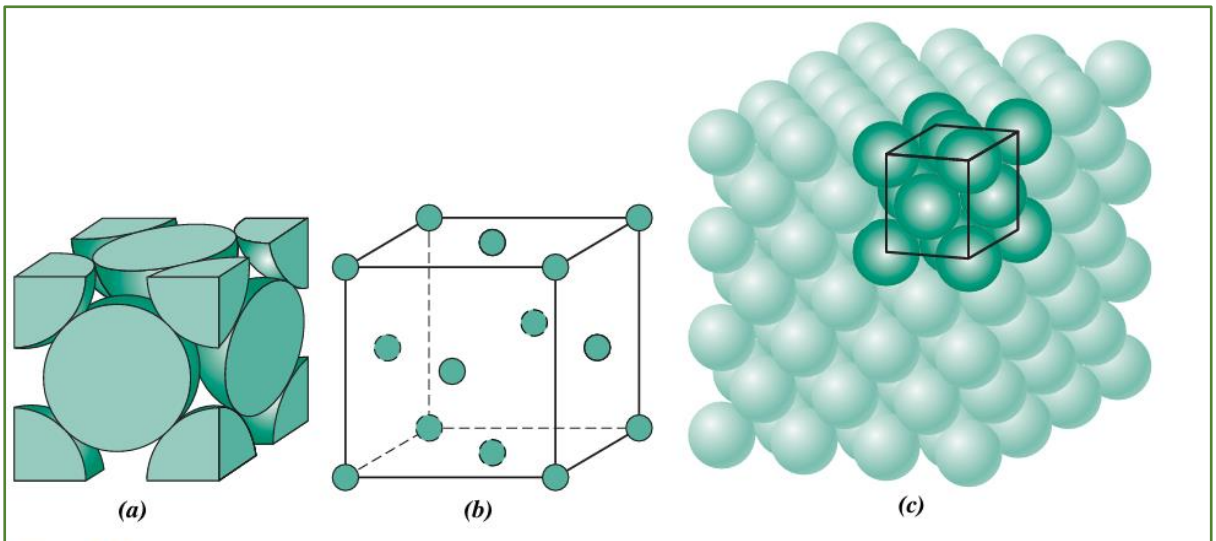



**Figure 3.1** For the face-centered cubic crystal structure, (*a*) a hard-sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms.

## 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 $4R$. Because 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,

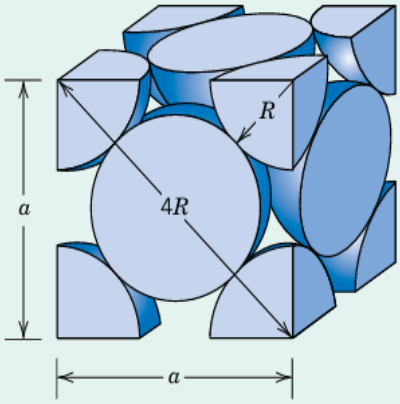
$$a^2 + a^2 = (4R)^2$$

or, solving for $a$,

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

The FCC unit cell volume $V_C$ may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2} \qquad (3.6)$$




## 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 because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

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

From Example Problem 3.1, the total unit cell volume is

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

Therefore, the atomic packing factor is

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

## Body-Centered Cubic (BCC):

- Atoms are located at each corner and at the center of cubic cells.

- Cr, Na, and Fe have this crystal structure.

- The relation between a and R is: $a = \frac{4R}{\sqrt{3}}$

- The coordination number is: $CN_{BCC} = 8$

- Number of atoms per unit cd) n = 8x1/8+ 1=2 atom/ unit cell.

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

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

- Atomic packing factor APF for BCC:

$$\text{APF} = \frac{N_{\text{atoms}} V_{\text{atom}}}{V_{\text{unit cell}}} = \frac{2 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$= \frac{\pi\sqrt{3}}{8} \approx 0.680\,174\,762\,.$$

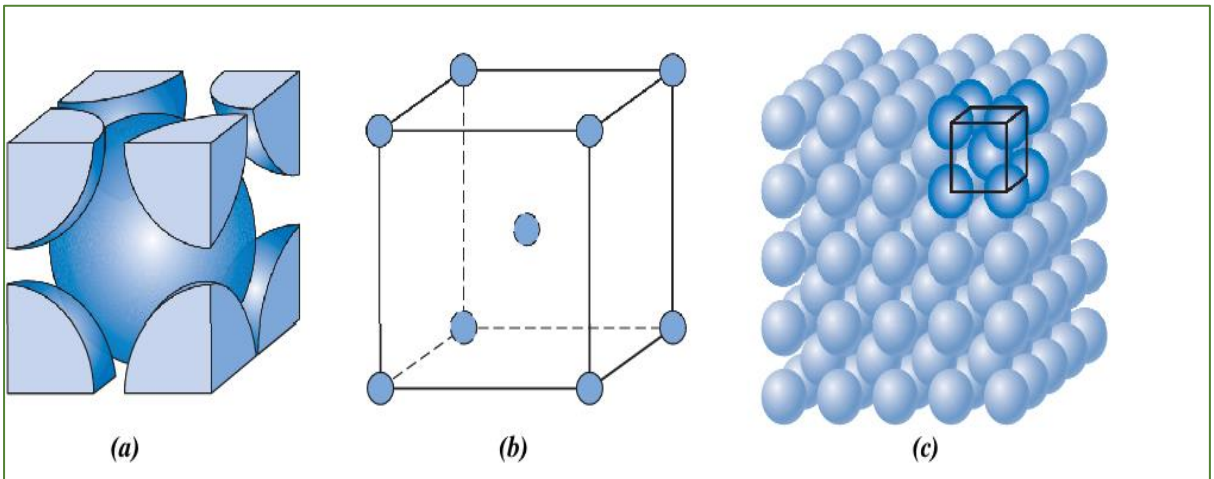
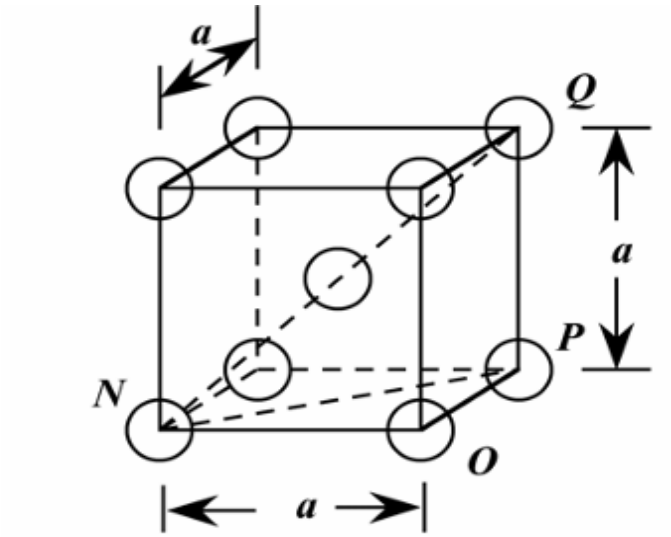



**Figure 3.2** For the body-centered cubic crystal structure, (*a*) a hard-sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms.

**Q/ Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius (R) are related through a =4R/ 3.**




Using the triangle *NOP*

$$(\overline{NP})^2 = a^2 + a^2 = 2a^2$$

And then for triangle *NPQ*,

$$(\overline{NQ})^2 = (\overline{QP})^2 + (\overline{NP})^2$$

But $\overline{NQ} = 4R$, $R$ being the atomic radius. Also, $\overline{QP} = a$. Therefore,

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

or

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

## 3- Hexagonal close packed (HCP)

- Zn, Cd, Mg, etc. Hexagonal closest packed structures in all crystal systems.

-Number of atoms per unit cell for HCP:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{6}$$

$$N = 3 + \frac{2}{2} + \frac{12}{6} = 6$$

- The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively.

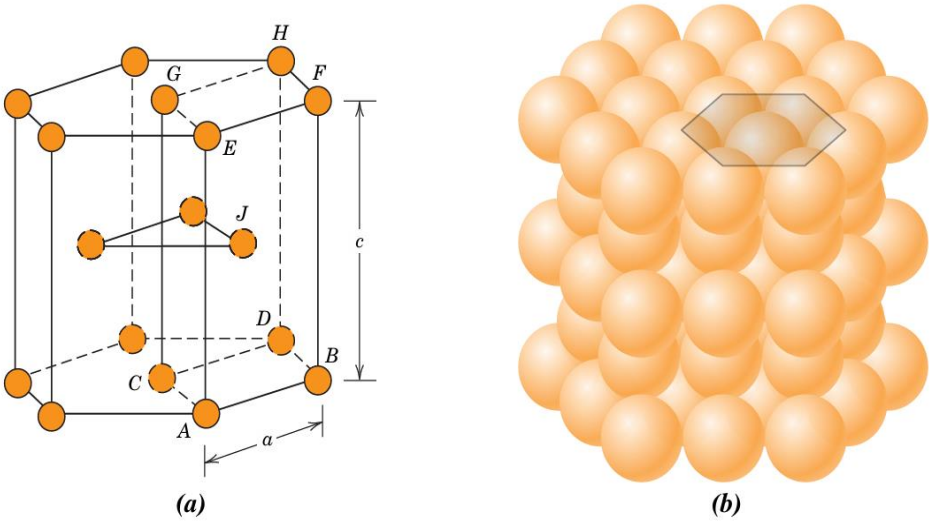



**Figure 3.4** For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell (*a* and *c* represent the short and long edge lengths, respectively), and (*b*) an aggregate of many atoms.

## Density Computations:

A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density $\rho$ through the relationship

$$\rho = \frac{nA}{V_C N_A} \tag{3.8}$$

where

$n$ = number of atoms associated with each unit cell
$A$ = atomic weight
$V_C$ = volume of the unit cell
$N_A$ = Avogadro's number ($6.022 \times 10^{23}$ atoms/mol)

### Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density, and compare the answer with its measured density.

***Solution***

Equation 3.8 is employed in the solution of this problem. Because the crystal structure is FCC, $n$, the number of atoms per unit cell, is 4. Furthermore, the atomic weight $A_{Cu}$ is given as 63.5 g/mol. The unit cell volume $V_C$ for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where $R$, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.8 yields

$$\rho = \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.89 \text{ g/cm}^3$$

The literature value for the density of copper is 8.94 g/cm$^3$, which is in very close agreement with the foregoing result.