Al-Mustaqbal University

Collage of Engineering

Prosthetics and Orthotics Engineering

First Stage

# PHYSICS OF MATERIALS

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## 1st term – Lecture 2

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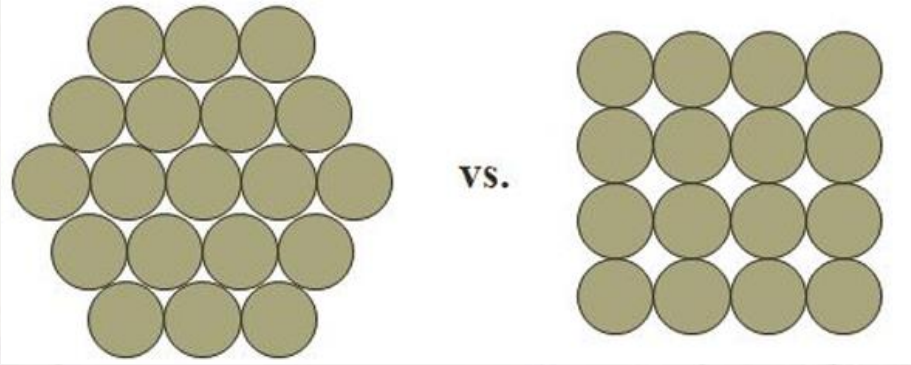
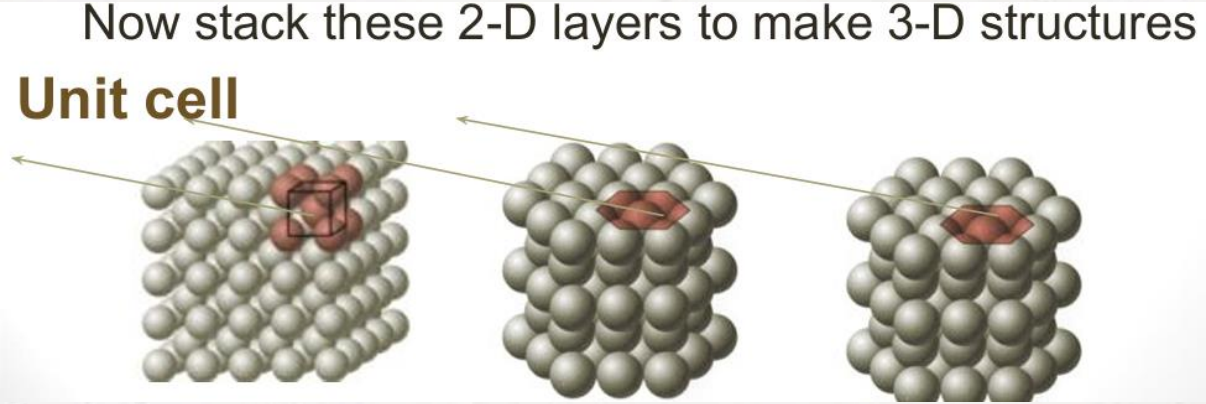
# Metals Structures

**How can we stack metal atoms to minimize empty space?**

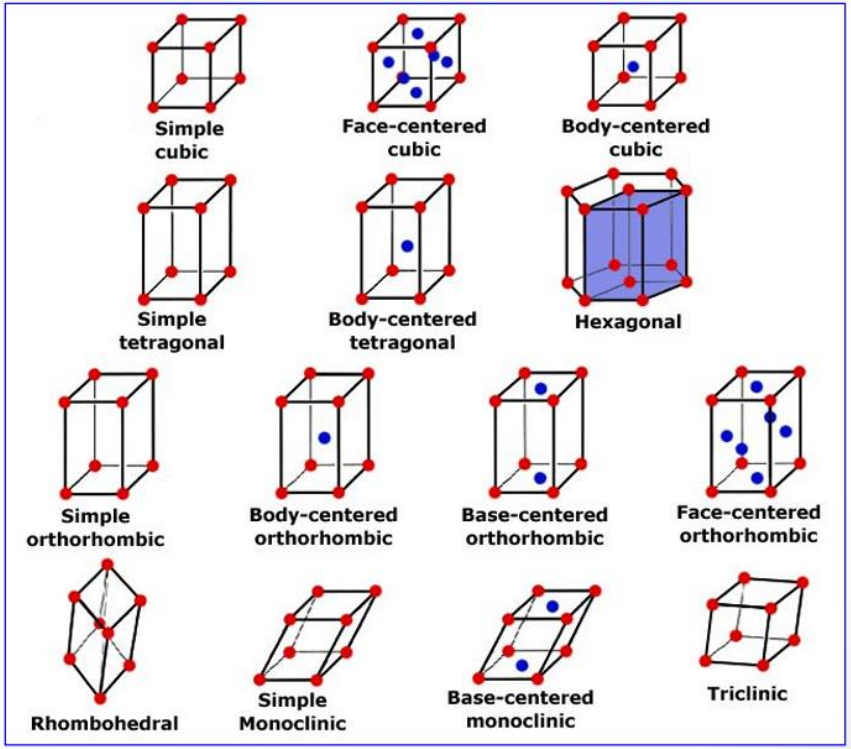


# Crystal structure & Unit Cell

- **Seven different possible geometries for the unit cell.**
- **There are 14 Bravais lattices, with each point representing the same atom or collection of atoms.**

- Pure metals are usually FCC, BCC or HCP.
- Except for hexagonal, number of atoms per unit cell:
  1/8 at corners
  1/2 at face centers
  All of body centered



**Metals form tightly packed crystal structures because:**

**Atoms are equal in size:** This helps them fit together efficiently.

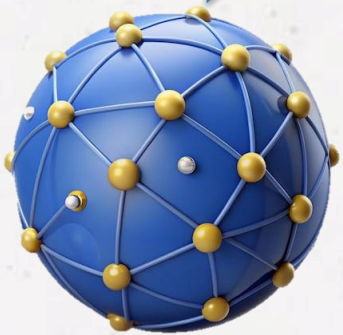
**Energy is reduced:** Atoms are positioned close to reduce bond energy.

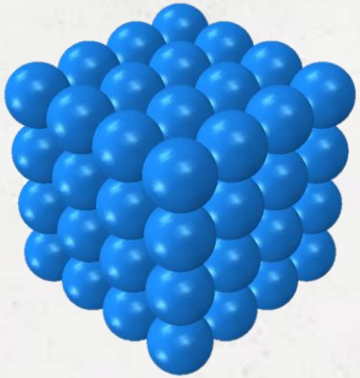
**Electron clouds shield atoms:** This prevents repulsion between atomic cores.

Metals have the simplest crystal structures.

# Atomic Packing Factor (APF)

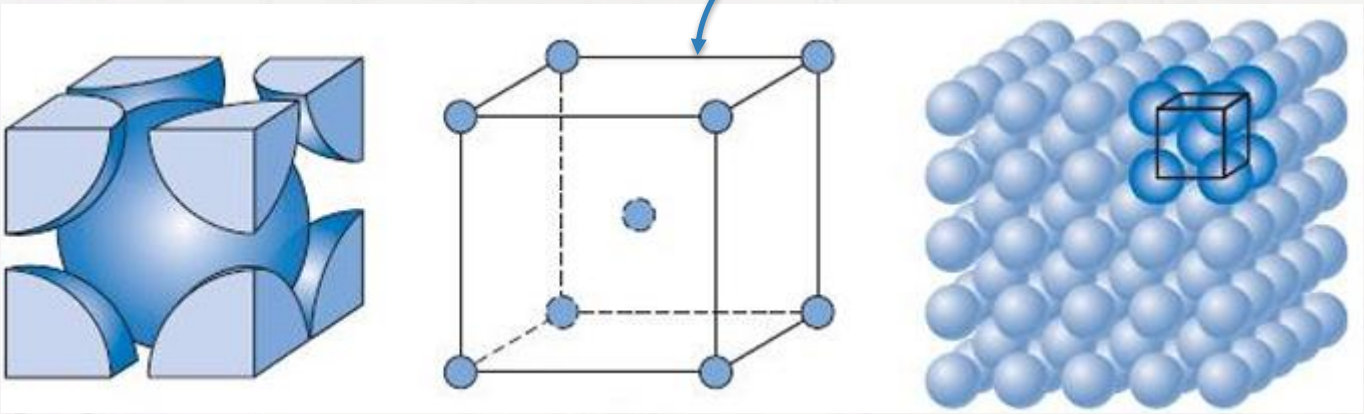
$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$





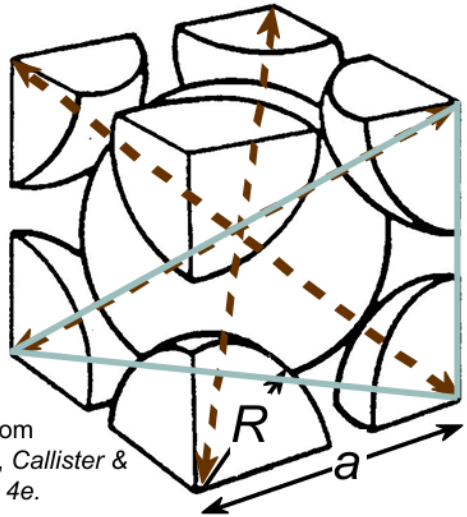
## Body-Centered Cubic (BCC)

Found in metals like iron, chromium, and tungsten. Atoms are less densely packed than FCC, with coordination numbers of 8 and an APF of 0.68.

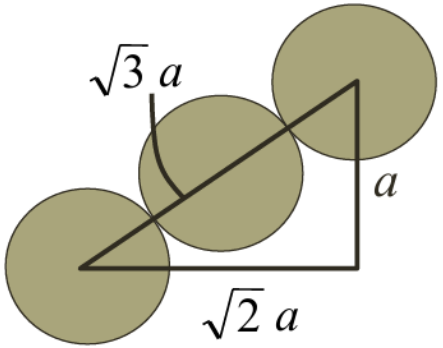


2 atoms/unit cell: 1 center + 8 corners x 1/8

# Body-Centered Cubic (BCC)




Adapted from Fig. 3.2(a), *Callister & Rethwisch 4e.*



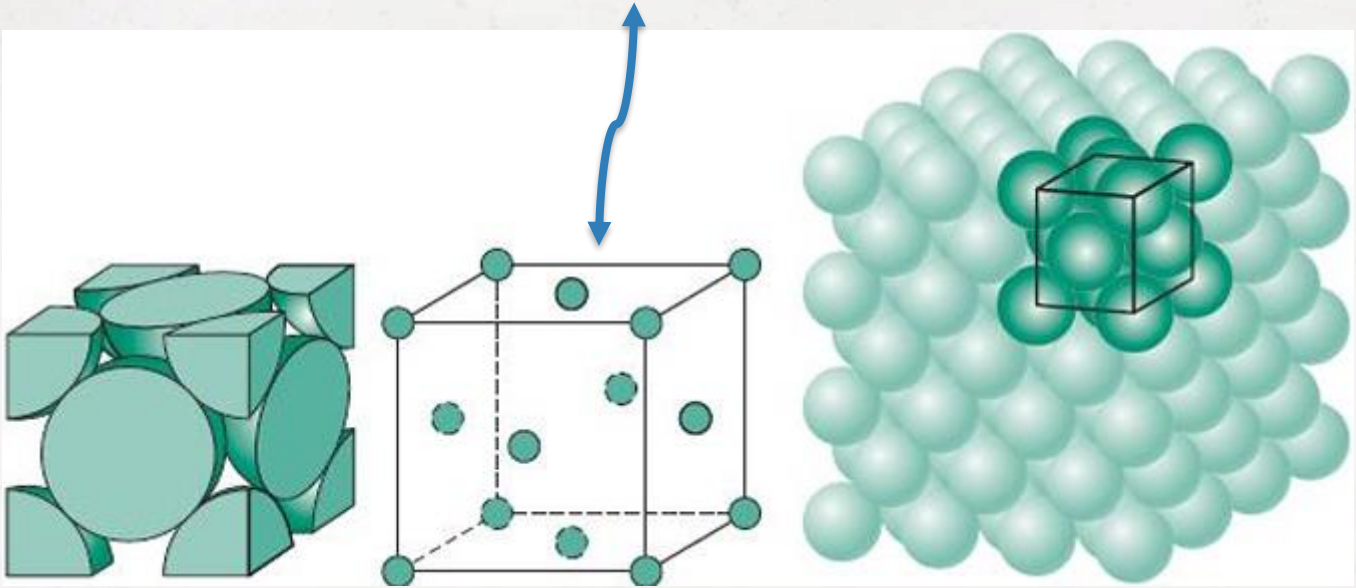

Close-packed direction length = $4R = \sqrt{3}\,a$

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

$$\text{APF} = \frac{\left(\frac{\text{atoms}}{\text{unit cell}}\right)\left(\frac{\text{volume}}{\text{atom}}\right)}{\frac{\text{volume}}{\text{unit cell}}} = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3\right)}{a^3} = 0.68$$

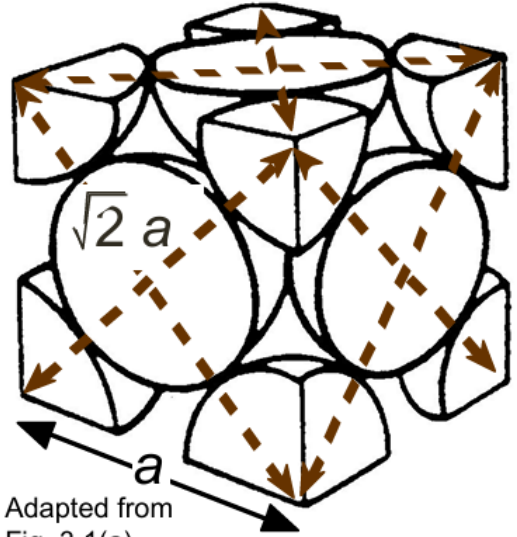
# Face-Centered Cubic (FCC)

Found in metals like copper, aluminum, and silver. Atoms are densely packed, resulting in high coordination numbers (12) and efficient atomic packing (APF: 0.74).



4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

# Face-Centered Cubic (FCC)




Adapted from Fig. 3.1(a), *Callister & Rethwisch 4e.*

Close-packed directions:

length = $4R = \sqrt{2}\,a$

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

Unit cell contains:

$6 \times 1/2 + 8 \times 1/8$

= 4 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}} = \frac{4\left(\frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3\right)}{a^3} = 0.74$$

0.74 is maximum APF

# Face-Centered Cubic (FCC)

## 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

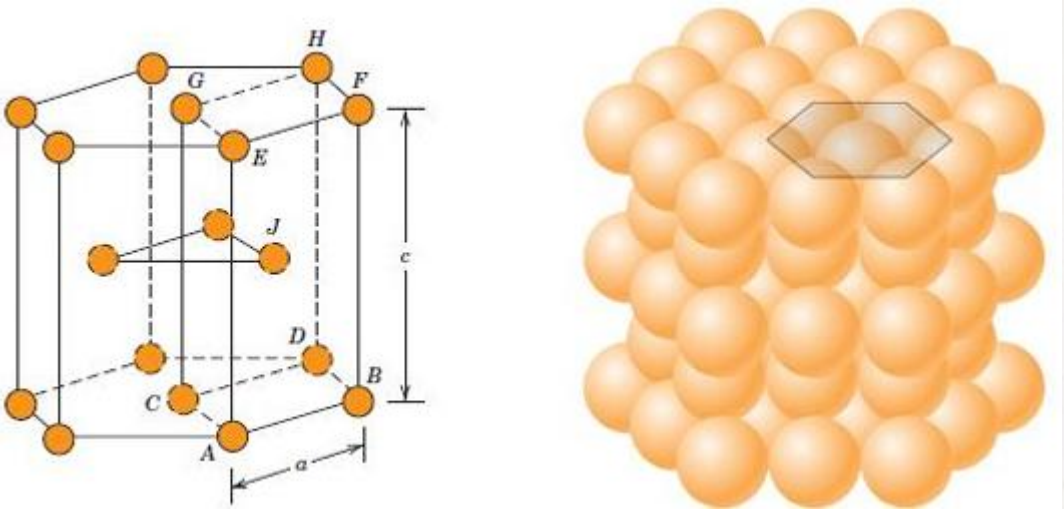
$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

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

# Hexagonal Close-Packed (HCP)

Found in metals like zinc and magnesium. Similar efficiency to FCC with APF: 0.74, and a unique hexagonal structure.




6 atoms/unit cell

**Table. 1** :Atomic Radii and Crystal Structures for 16 Metals.

| *Metal* | *Crystal Structure*[a] | *Atomic Radius*[b] *(nm)* | *Metal* | *Crystal Structure* | *Atomic Radius (nm)* |
|---|---|---|---|---|---|
| Aluminum | FCC | 0.1431 | Molybdenum | BCC | 0.1363 |
| Cadmium | HCP | 0.1490 | Nickel | FCC | 0.1246 |
| Chromium | BCC | 0.1249 | Platinum | FCC | 0.1387 |
| Cobalt | HCP | 0.1253 | Silver | FCC | 0.1445 |
| Copper | FCC | 0.1278 | Tantalum | BCC | 0.1430 |
| Gold | FCC | 0.1442 | Titanium ($\alpha$) | HCP | 0.1445 |
| Iron ($\alpha$) | BCC | 0.1241 | Tungsten | BCC | 0.1371 |
| Lead | FCC | 0.1750 | Zinc | HCP | 0.1332 |

## Density Calculation

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

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

where

$n$ = number of atoms associated with each unit cell
$A$ = atomic weight
$VC$ = volume of the unit cell
$NA$ = Avogadro>s number ($6.022 * 10^{23}$ atoms/mol)

# Density Calculation

## 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.


Thank
you