Chemical Engineering 378

Science of Materials Engineering

Lecture 3

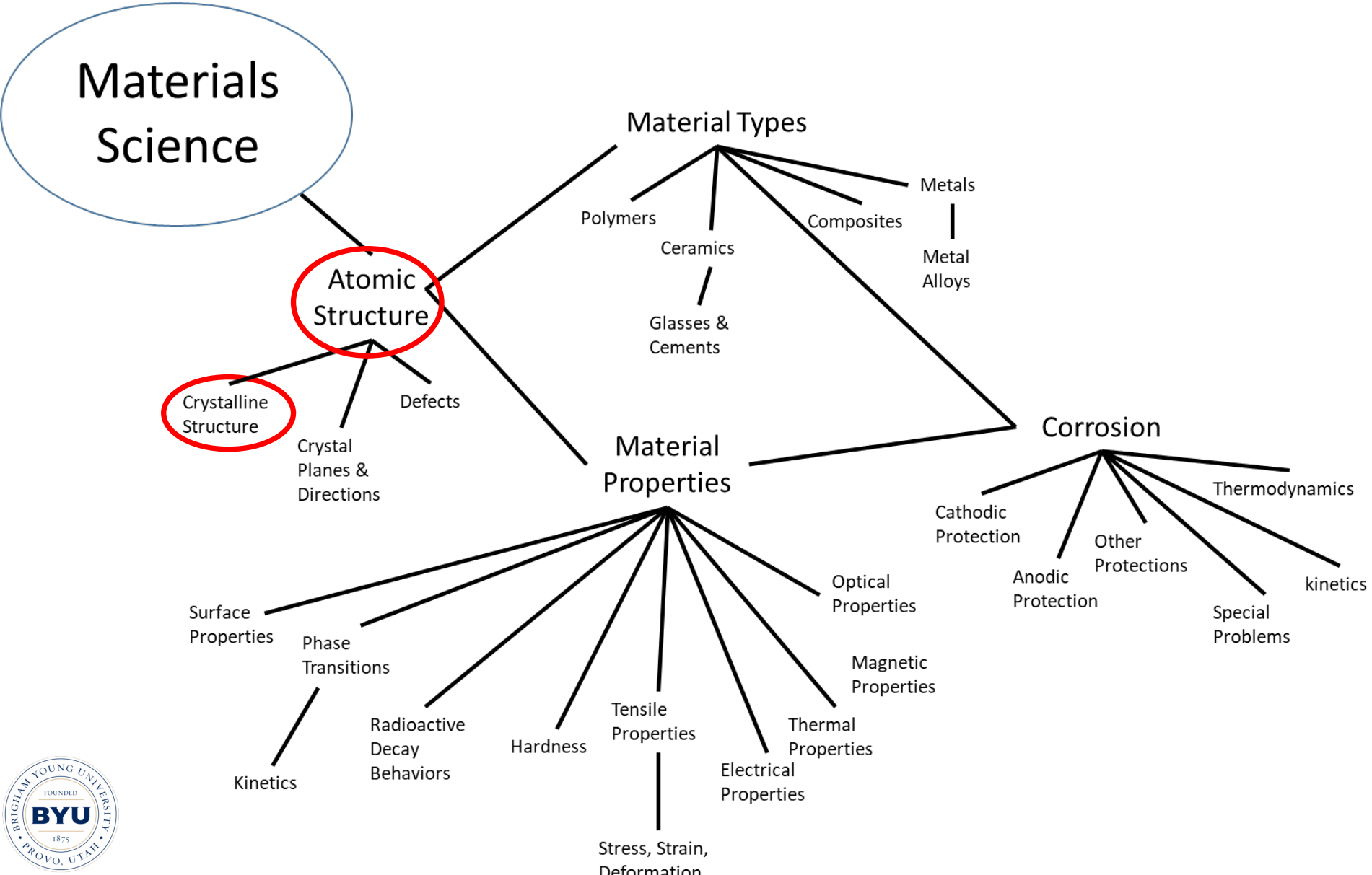
Crystal Structures

Spiritual Thought

"A favorite saying of mine often attributed to St. Francis of Assisi reads, 'Preach the gospel at all times and if necessary, use words.' Implicit in this saying is the understanding that often the most powerful sermons are unspoken."

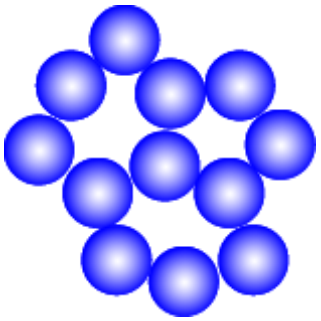
Dieter F. Uchtdorf

Materials Roadmap

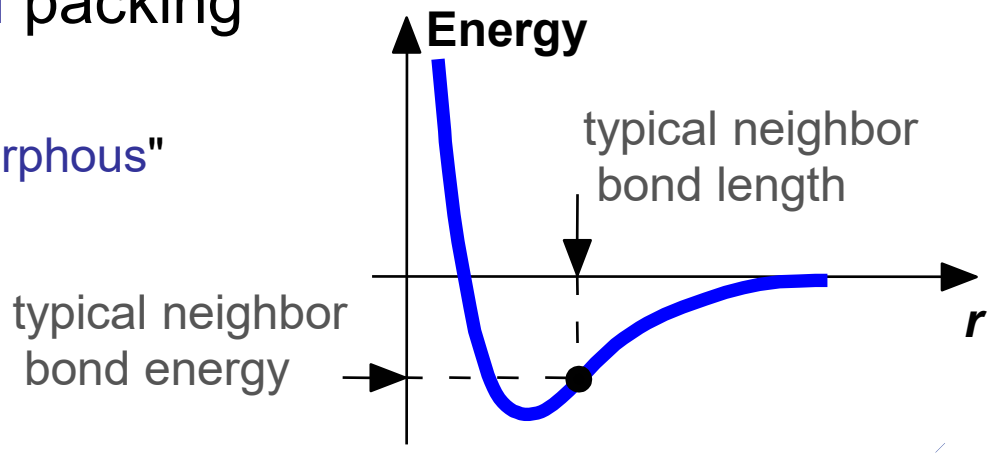


Energy and Packing

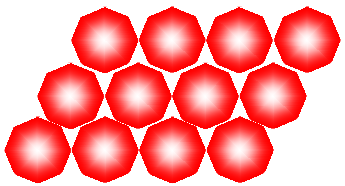
- Non dense, random packing

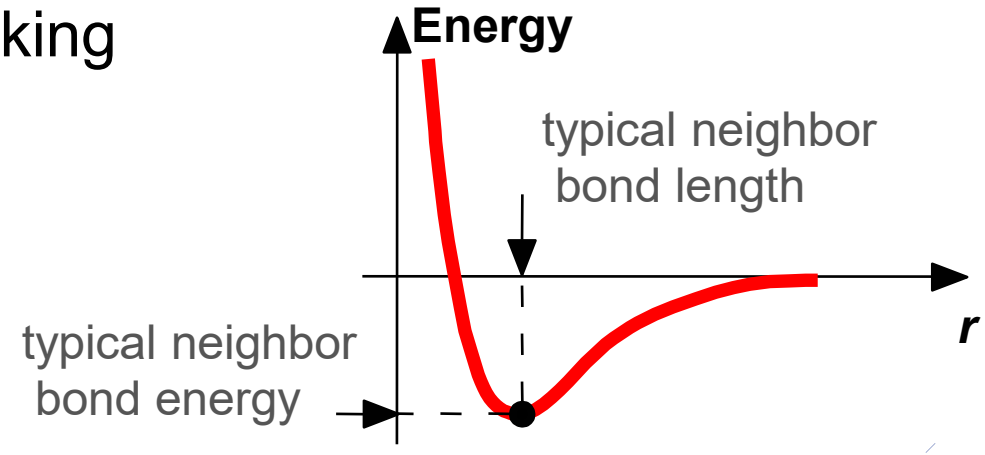


"Amorphous"



- Dense, ordered packing





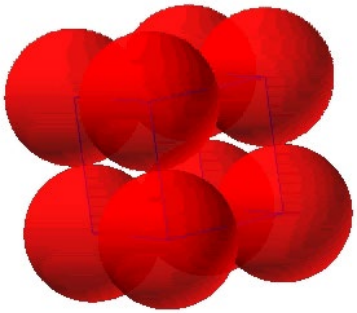
Dense, ordered packed structures tend to have lower energies.

Metallic Crystal Structures

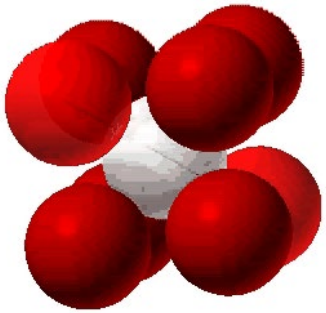
- Tend to be densely packed.
- Reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
  - Electron cloud shields cores from each other
- Have the simplest crystal structures.
- Ceramic and polymers in future lectures

Crystal Structures

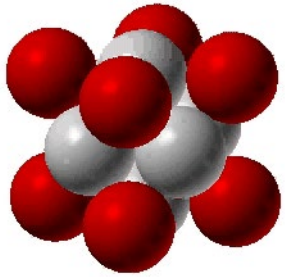
Simple Cubic (SC)	Body Centered Cubic (BCC)	Face Centered Cubic (FCC)	Hexagonal Close Packed (HCP)



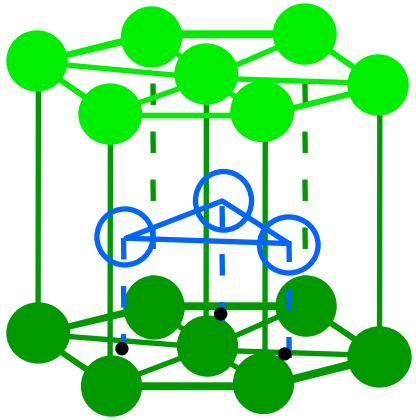
Polonium



Tungsten



Gold



Zinc

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.

https://wileyassets.s3.amazonaws.com/VMSE/index.html

Definitions

Coordination Number

Coordination Number = number of nearest-neighbor or touching atoms

Atoms per unit cell

Number of full atoms contained in a full unit cell

Atomic Packing Factor (APF)

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

*assume hard spheres

Theoretical Density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n A}{V_C N_A} \qquad \frac{\text{How much stuff}}{\text{How much space}}$$

where n = number of atoms/unit cell

A = atomic weight (g/mol)

V_C = Volume of unit cell = a^3 for cubic

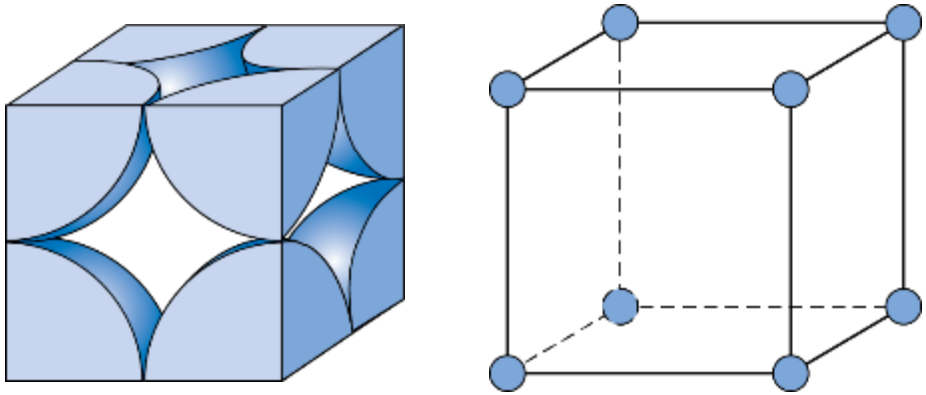
N_A = Avogadro's number

= 6.022×10^{23} atoms/mol

Simple Cubic (SC) Crystal Structure

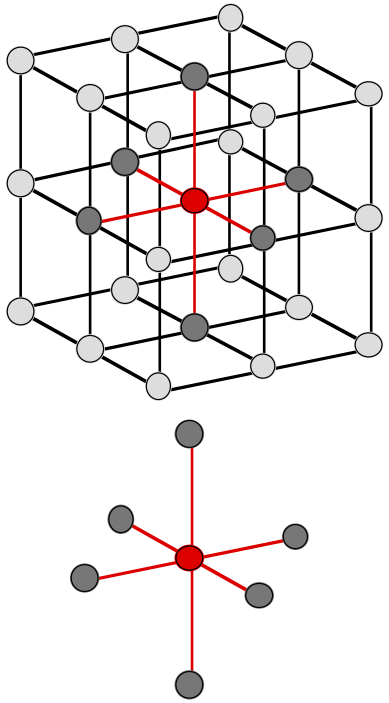
- Centers of atoms located at the eight corners of a cube
- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.

ex: Po



Adapted from Fig. 3.3, *Callister & Rethwisch 10e.*

- Coordination # = 6
  (# nearest neighbors)

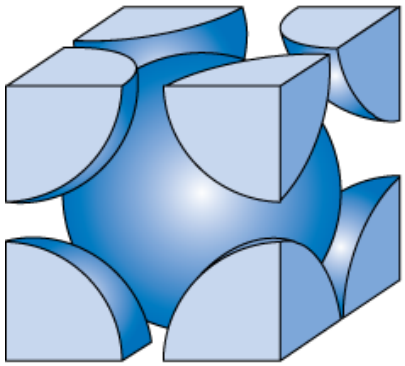


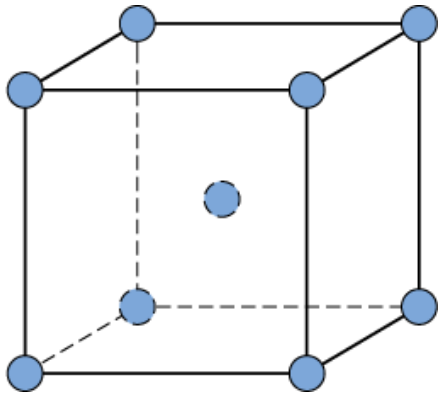
Body-Centered Cubic Structure (BCC)

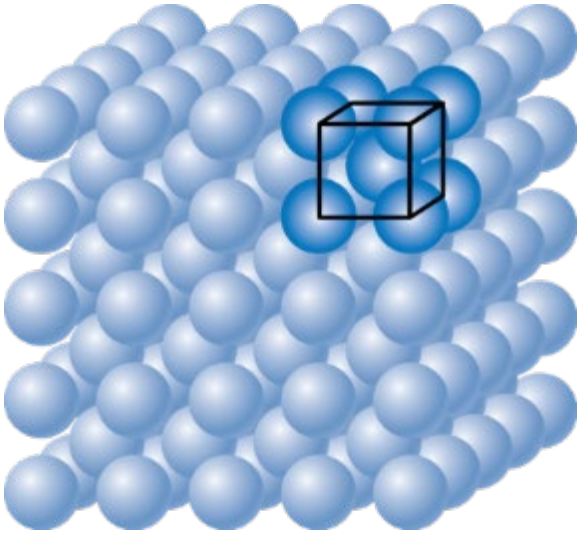
- Atoms located at 8 cube corners with a single atom at cube center.
  --Note: All atoms in the animation are identical; the center atom is shaded differently for ease of viewing.

ex: Cr, W, Ta, Mo

- Coordination # = 8





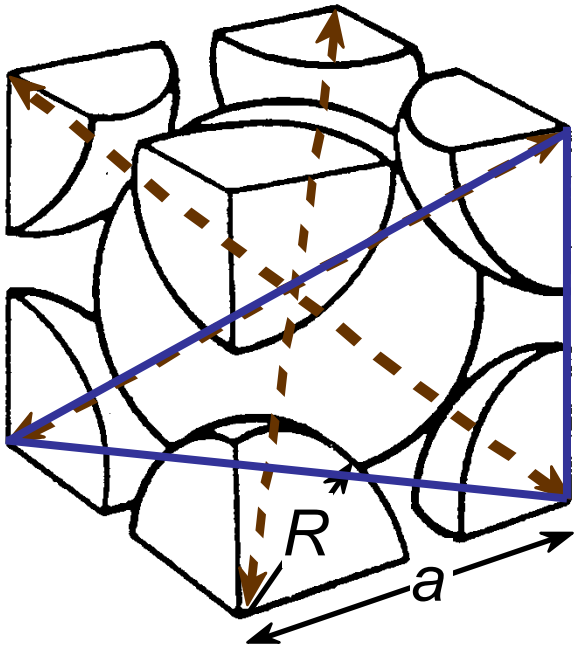


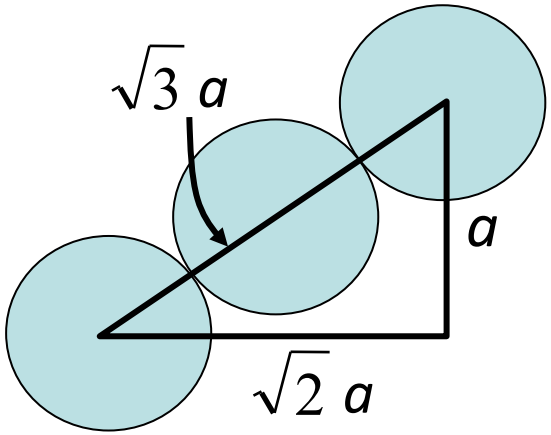
Adapted from Fig. 3.2, *Callister & Rethwisch 10e.*

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

Example: Find the APF for BCC?

- APF for a body-centered cubic structure =

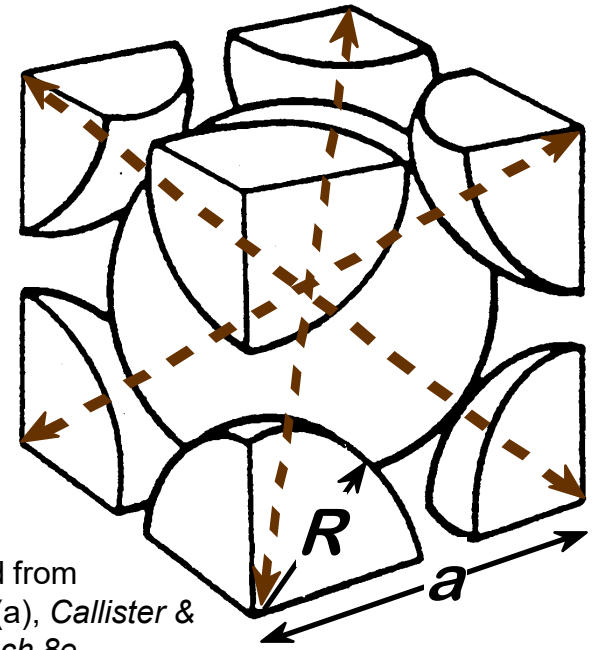




$$4R = \sqrt{3}\,a$$

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

Theoretical Density, ρ



Adapted from Fig. 3.2(a), *Callister & Rethwisch 8e.*

- Ex: Cr (BCC)

  A = 52.00 g/mol — Back of book

  R = 0.125 nm — Table 3.1

  n = 2 atoms/unit cell

$a = 4R/\sqrt{3} = 0.2887$ nm

$$\rho = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{g}}{\text{mol}}}{\frac{\text{volume}}{\text{unit cell}} \cdot \frac{\text{atoms}}{\text{mol}}} = \frac{2 \cdot 52.00}{a^3 \cdot 6.022 \times 10^{23}}$$

$\rho_{theoretical}$ = 7.18 g/cm^3

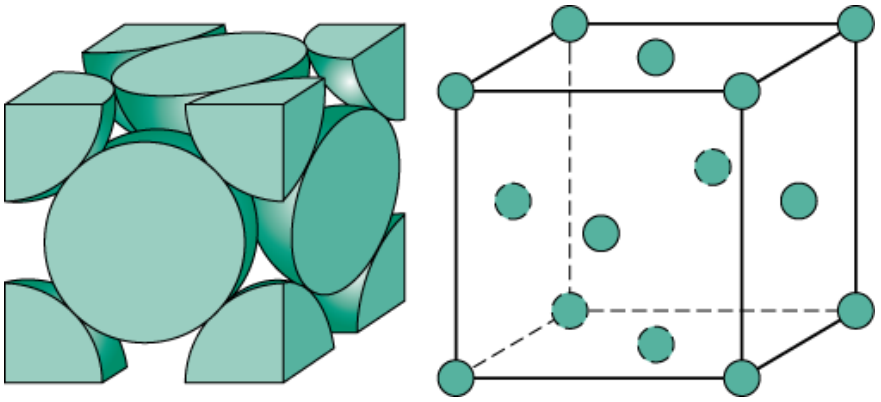
ρ_{actual} = 7.19 g/cm^3

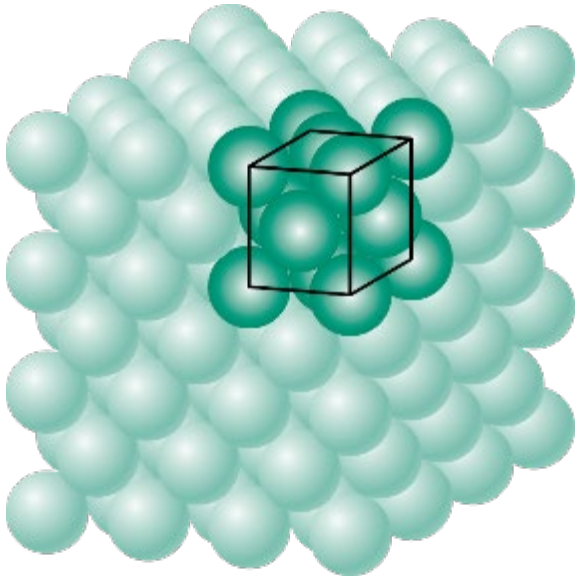
Face-Centered Cubic Structure (FCC)

- Atoms located at 8 cube corners and at the centers of the 6 faces.
  --Note: All atoms in the animation are identical; the face-centered atoms are shaded differently for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12



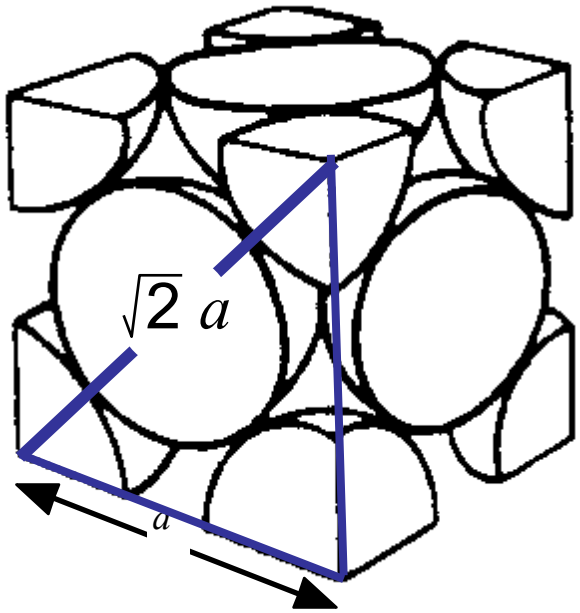


Adapted from Fig. 3.1, *Callister & Rethwisch 10e.*

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

Atomic Packing Factor: FCC

- APF for the face-centered cubic structure = 0.74
  maximum achievable APF



For close-packed directions:

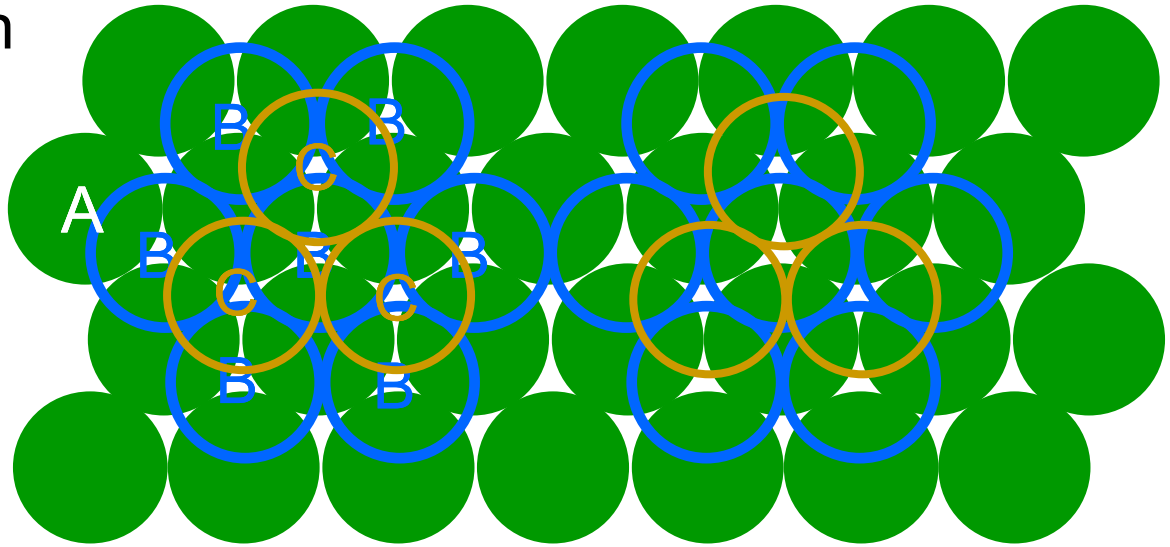
$$4R = \sqrt{2}\,a \quad \left(\text{i.e., } R = \frac{\sqrt{2}a}{4}\right)$$

Unit cell contains: 6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

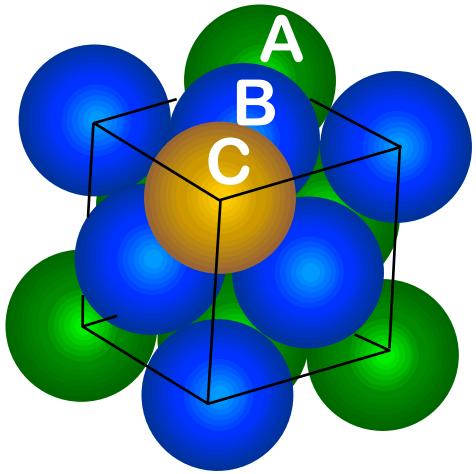
$$\text{APF} = \frac{\dfrac{\text{atoms}}{\text{unit cell}} \cdot \dfrac{\text{volume}}{\text{atom}}}{\dfrac{\text{volume}}{\text{unit cell}}} = \frac{4\left(\frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3\right)}{a^3} = 0.74$$

FCC Stacking Sequence

- ABCABC... Stacking Sequence
- 2D Projection



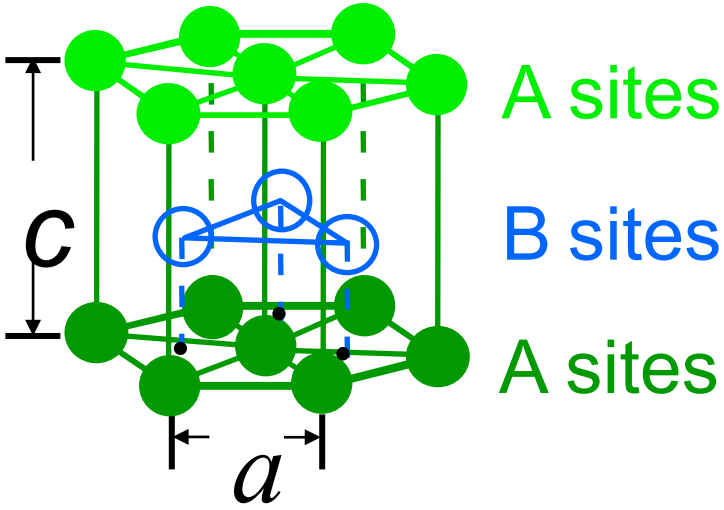
- FCC Unit Cell



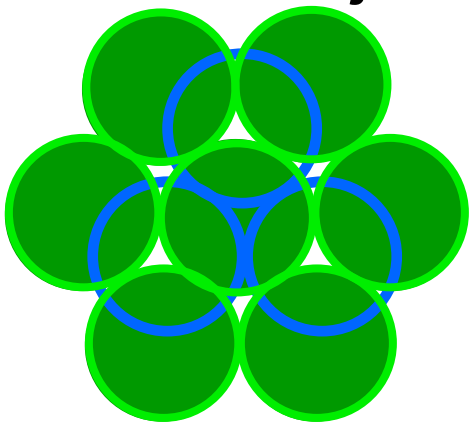
Hexagonal Close-Packed Structure

- ABAB... Stacking Sequence–Close-Packed Planes of Atoms

- 3D Projection



- 2D Projection



- Coordination # = 12
- APF = 0.74
- Ideal c/a = 1.633

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

Crystal System Review

Property	SC	FCC	BCC	HCP
# atoms/cell	1	4	2	6
Lattice Parameter	$a = 2R$	$a = 2\sqrt{2}R$	$a = 4R/\sqrt{3}$	a,c
Coordination #	6	12	8	12
APF	0.52	0.74	0.68	0.74