

Chapter 3: The structure of crystalline solids

Outline

- Fundamental concepts
- Unit cells
- Metallic crystal structure
- Density
- Crystal systems

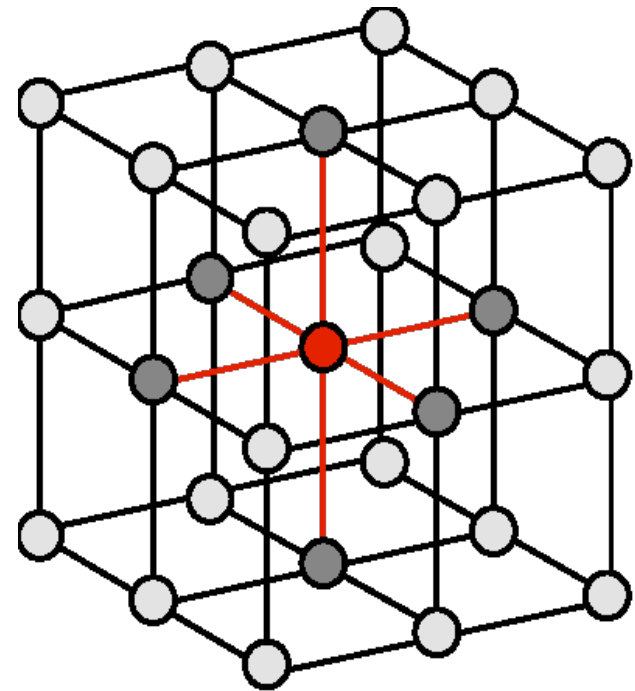


Fundamental concepts

- Crystalline materials: atoms are situated in a repeating or periodic array over large atomic distances-

Long Range Order

- Crystalline structure: how atoms, ions, or molecules are spatially arranged
- Lattice: a three-dimensional array of points coinciding with atom position



Crystal Systems

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

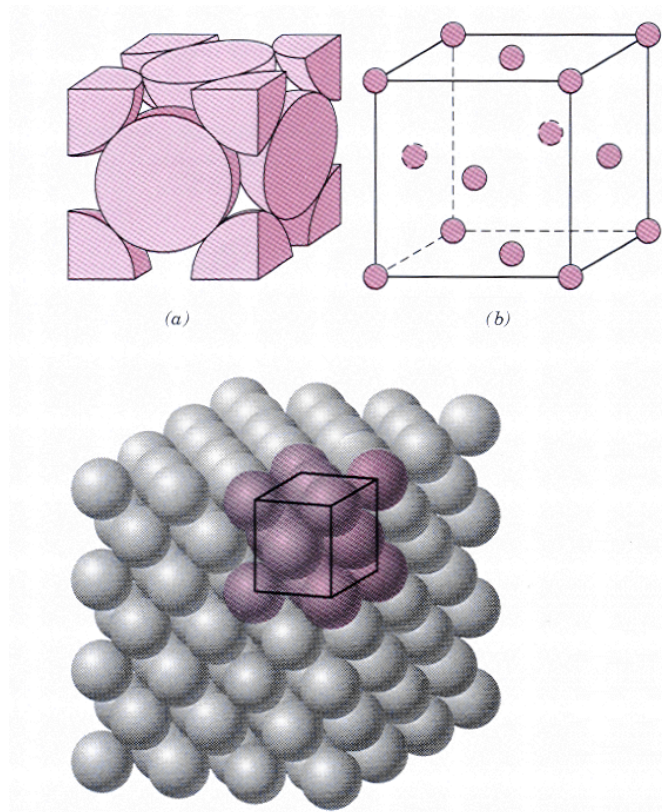


Fig 3.1 (a) a hard sphere unit cell
(b) a reduced-sphere unit cell, (c) an aggregate of many atoms

Metallic crystal structures

- Features of metallic crystal structures
 - non-directional in nature
 - no restriction on the number and position of nearest-neighbor atoms
 - close-packed: low energy
 - common type:
 - face-centered cubic (FCC)
 - body-centered cubic (BCC)
 - hexagonal closed-packed (HCP)

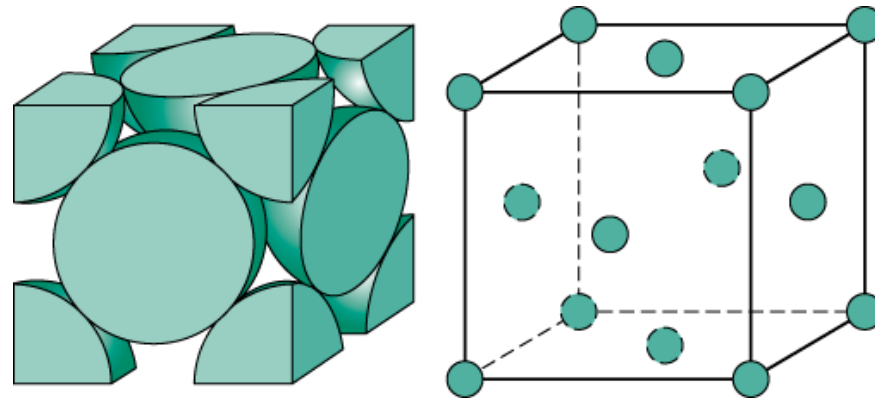
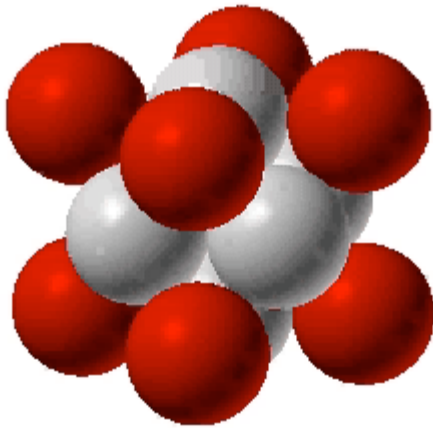


Face Centered Cubic Structure (FCC)

- Atoms touch each other along face diagonals.
 - Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

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

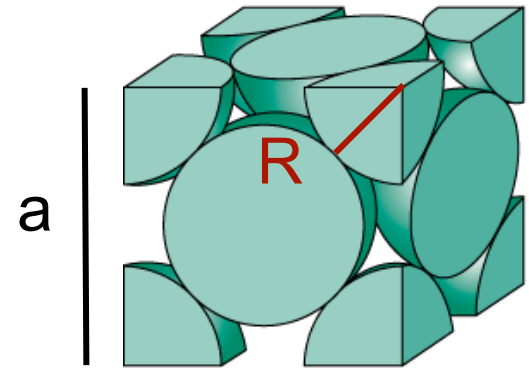
- Coordination # = 12



Adapted from Fig. 3.1, *Callister 7e*.

The FCC crystal structure

- Total atoms per unit cell=
- The relation between cubic edge a and the radius R =

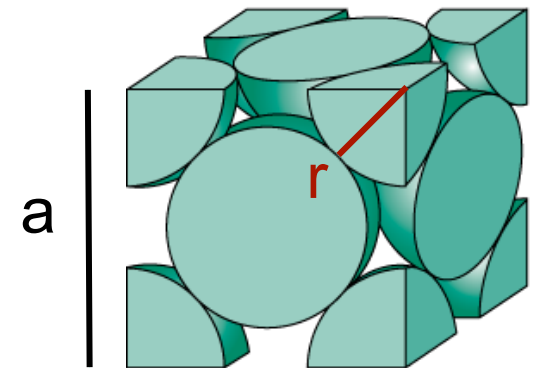


Atomic Packing Factor (APF)

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

*assume hard spheres

- APF for FCC=

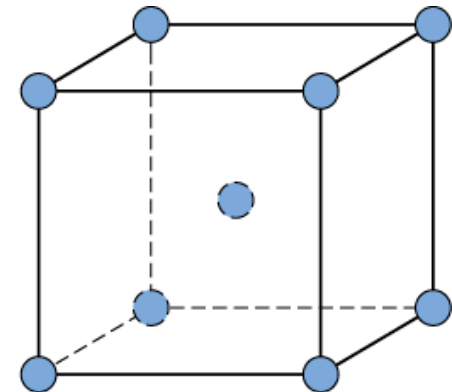
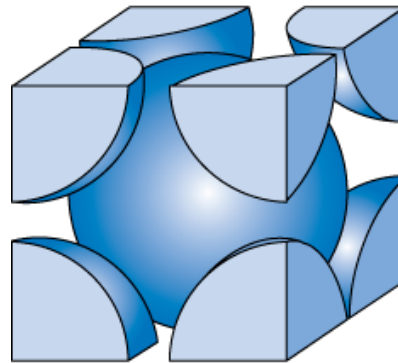
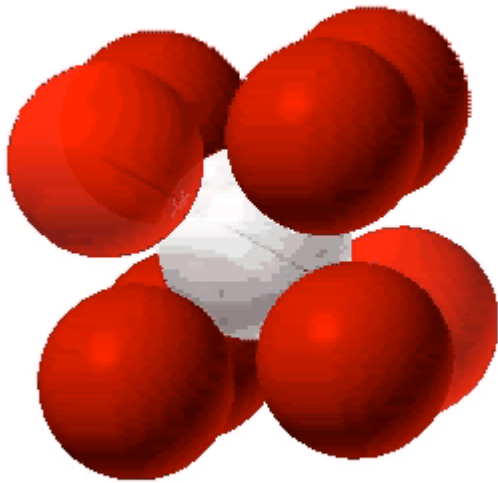


Body Centered Cubic Structure (BCC)

- Atoms touch each other along cube diagonals.
 - Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8



Adapted from Fig. 3.2,
Callister 7e.

(Courtesy P.M. Anderson)

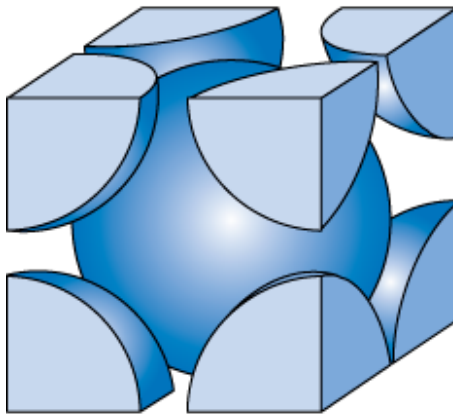


The BCC crystal structure

- Total atoms per unit cell:
- Coordination number:
- The relation between cubic edge a and the radius

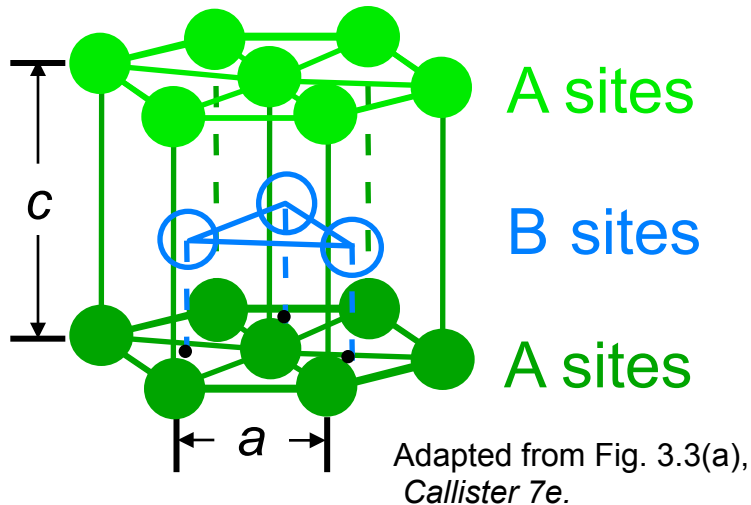
$$a = \frac{4R}{\sqrt{3}}$$

- Atomic packing factor (APF)=0.68



Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



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

- 2D Projection



6 atoms/unit cell

ex: Cd, Mg, Ti, Zn

Theoretical Density, ρ

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

$$\rho = \frac{n A}{V_C N_A}$$

Where

n = number of atoms/unit cell

A = atomic weight

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

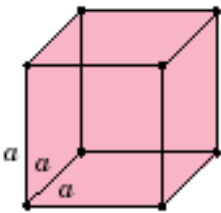
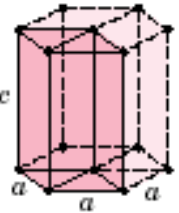
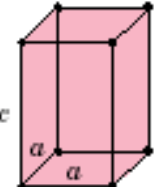
N_A = Avogadro's number

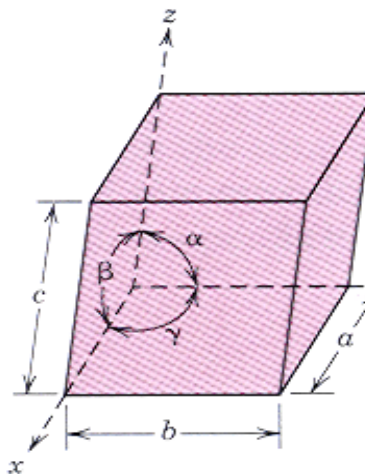
= 6.023×10^{23} atoms/mol



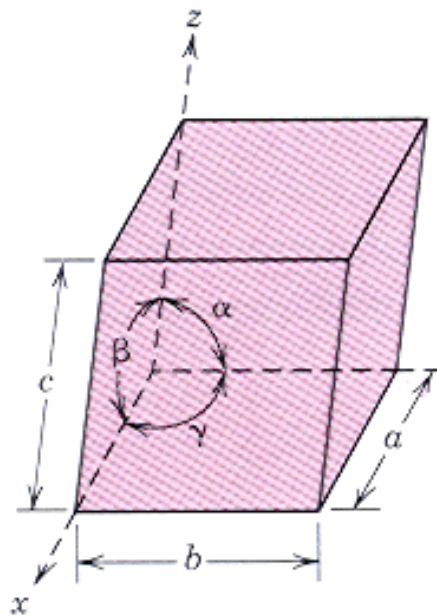
Crystal systems

Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	



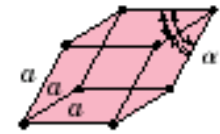
Crystal systems



Rhombohedral

$$a = b = c$$

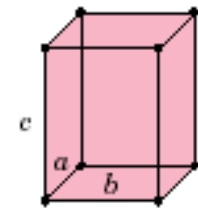
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

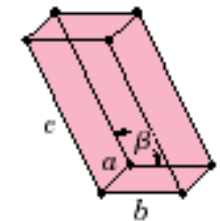
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

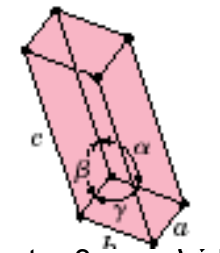
$$\alpha = \gamma = 90^\circ \neq \beta$$



Triclinic

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



Crystal Systems



Cubic:
Lead ore



Rhombic:
Topaz



Hexagonal:
Emerald



Tetragonal:
idocrase



Monoclinic:
Gypsum



Triclinic:
Axinite