Chapter 3: The structure of crystalline solids

Outline

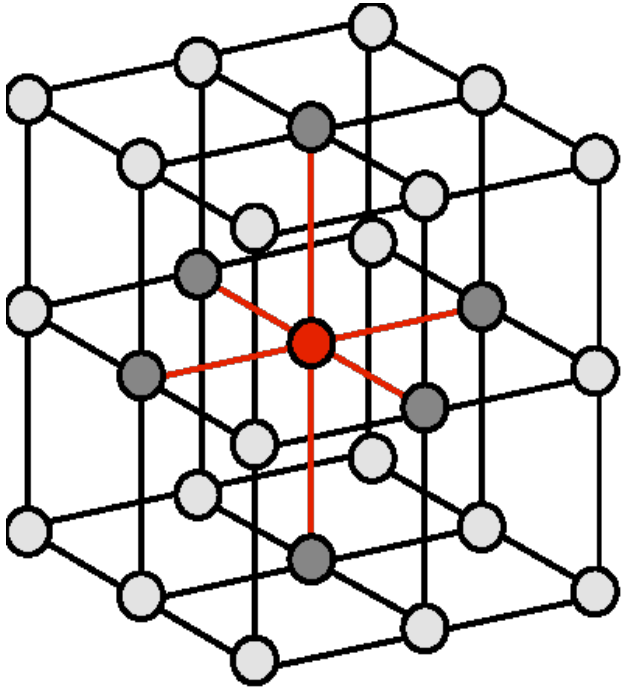
- Fundamental concepts
- Unit cells
- Metallic crystal structure
- Density
- Crystal systems

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.

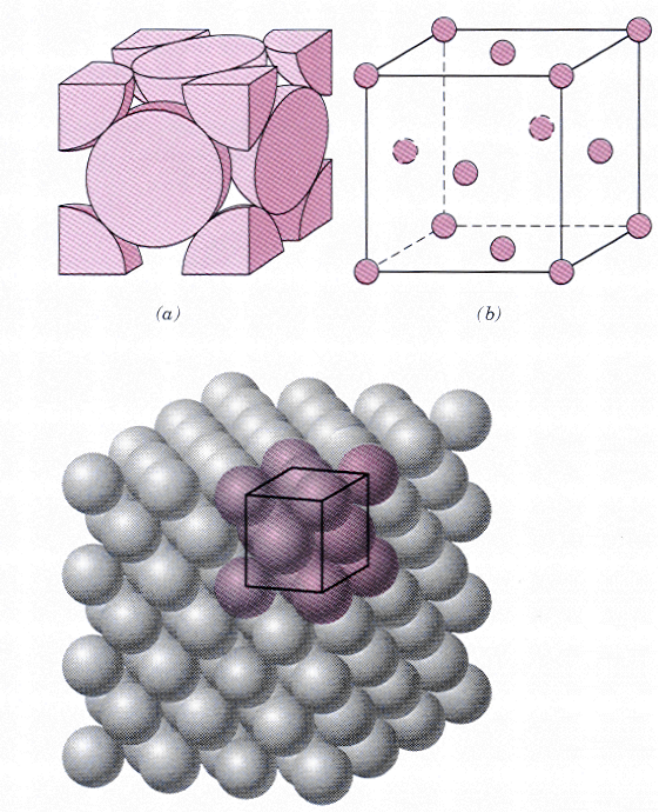


Fig 3.1 (a) a hard sphere unit cell (b) a reduced-sphere unit cell, (c) an aggregate of many atoms

Metallic crystal structures

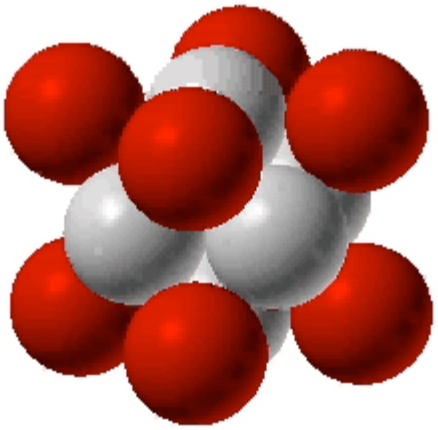
- Features of metallic crystal structures
  - non-directional in nature
  - no restriction on the number and position of nearest-neighbor atoms
  - close-packed: low energy
  - common type:
    - face-centered cubic (FCC)
    - body-centered cubic (BCC)
    - hexagonal closed-packed (HCP)

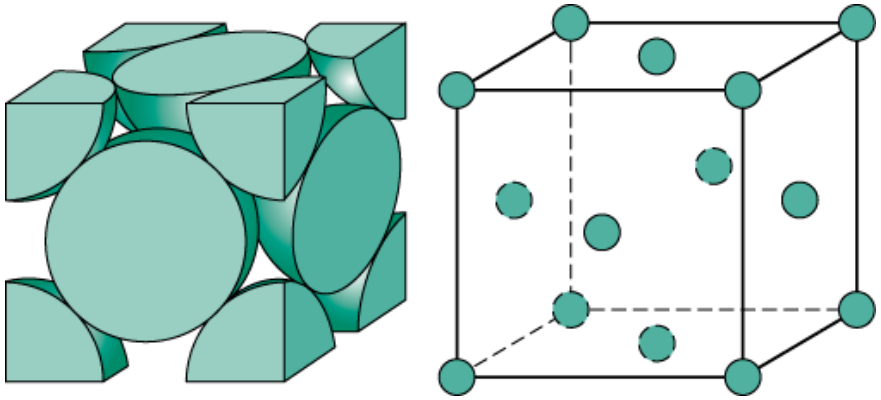
Face Centered Cubic Structure (FCC)

- 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



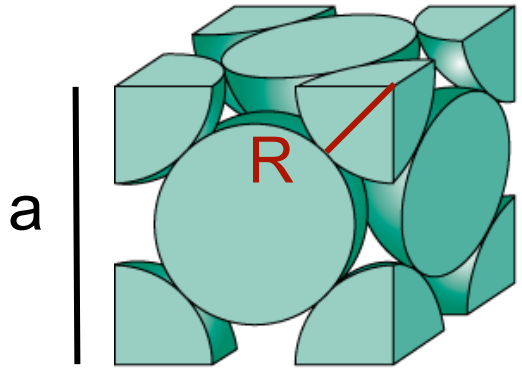


Adapted from Fig. 3.1, *Callister 7e.*

(Courtesy P.M. Anderson)

The FCC crystal structure

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

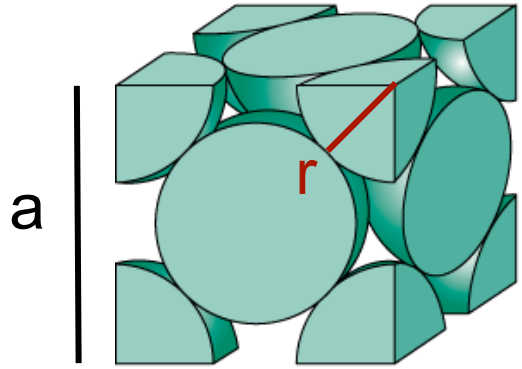


Atomic Packing Factor (APF)

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

*assume hard spheres

- APF for FCC=

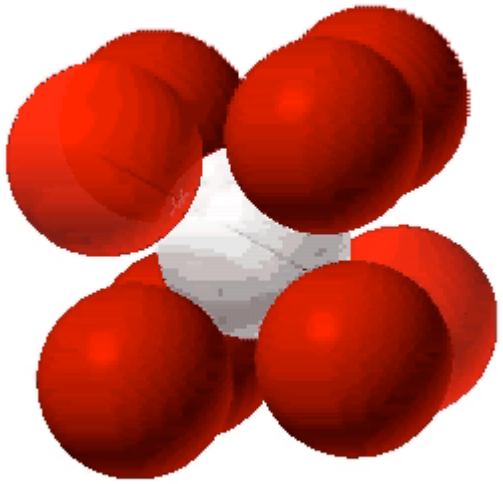


Body Centered Cubic Structure (BCC)

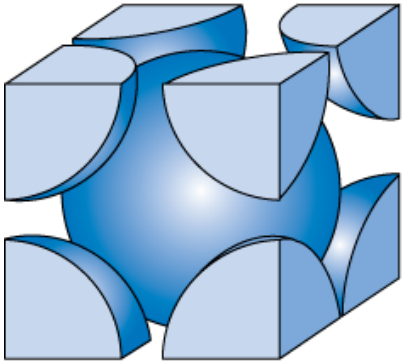
- Atoms touch each other along cube diagonals.
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

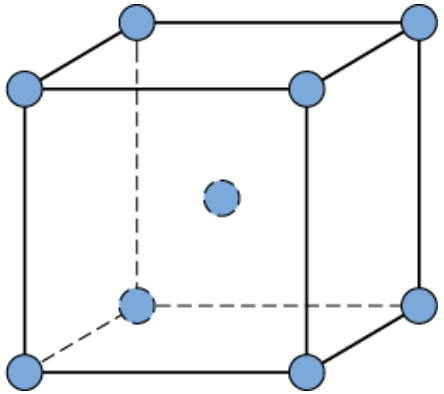
ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8



(Courtesy P.M. Anderson)





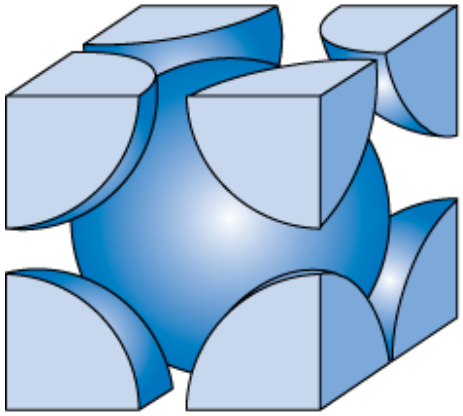
Adapted from Fig. 3.2, *Callister 7e.*

The BCC crystal structure

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

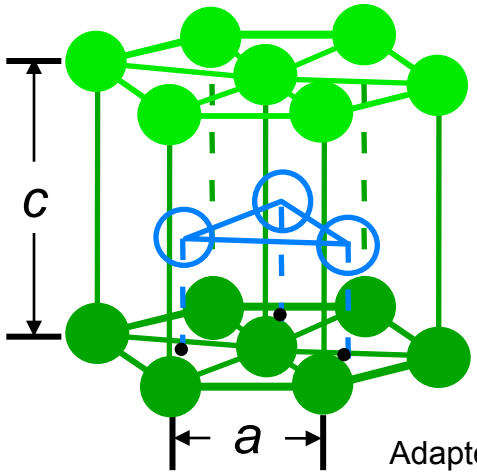
$$a = \frac{4R}{\sqrt{3}}$$

- Atomic packing factor (APF)=0.68



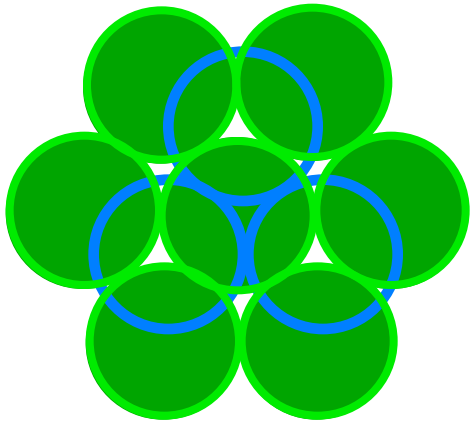
Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a), *Callister 7e.*

- 2D Projection



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

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

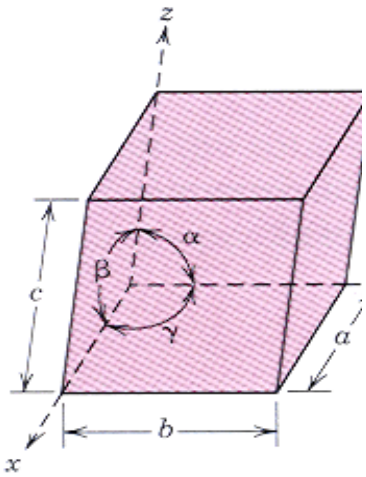
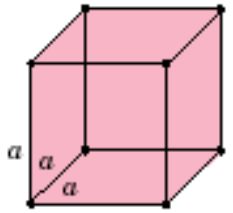
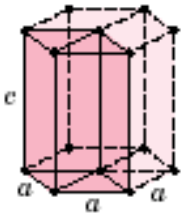
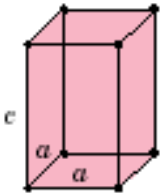
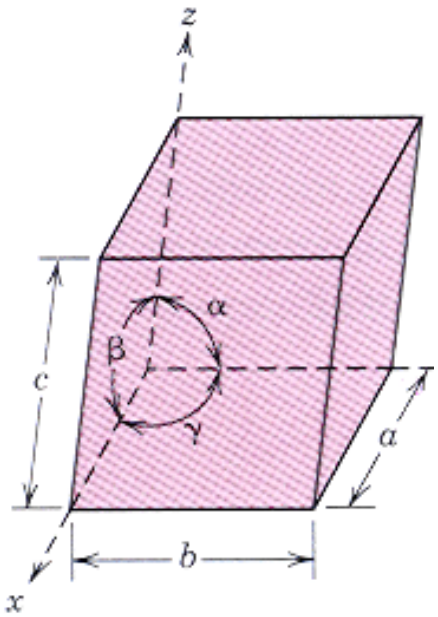


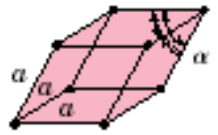
Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

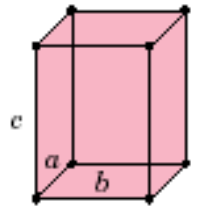
Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	

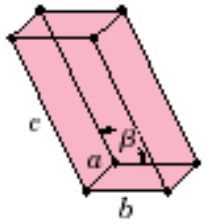
Crystal systems

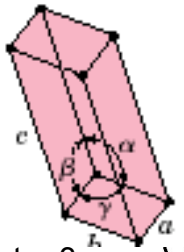


Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$









Crystal Systems

Cubic:
Lead ore

Rhombic:
Topaz

Hexagonal:
Emerald

Tetragonal:
idocrase

Monoclinic:
Gypsum

Triclinic:
Axinite