Materials Science

ME 274

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The Structure of Crystalline Solids

- 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 periodic array over large atomic distances; that is, **long-range** order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbour atoms.

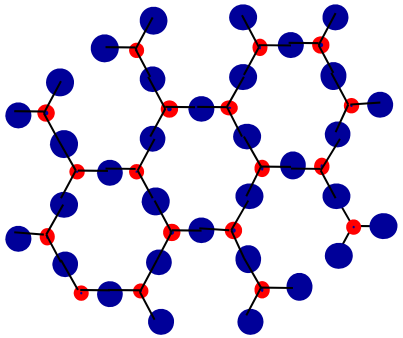
The Structure of Crystalline Solids

- All metals, many ceramic materials, and certain polymers form crystalline structures under normal solidification conditions. For those materials which do not crystallize this long-range order is absent and they are called **amorphous** materials.

Materials and Packing

Crystalline materials...

- atoms pack in periodic, 3D arrays
- typical of: -metals
  -many ceramics
  -some polymers



crystalline SiO_2

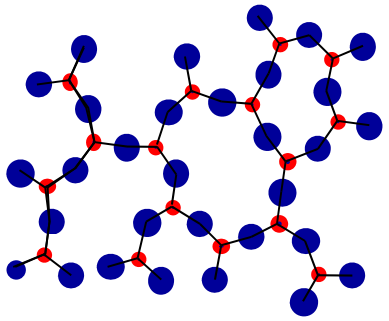
Adapted from Fig. 3.22(a), *Callister 7e.*

• Si • Oxygen

Noncrystalline materials...

- atoms have no periodic packing
- occurs for: - complex structures
  - rapid cooling

"Amorphous" = Noncrystalline



noncrystalline SiO_2

Adapted from Fig. 3.22(b), *Callister 7e.*

Crystal Systems

- The atomic order in crystalline solids indicate that small groups of atoms form a repetitive pattern.
- In describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells.
- **Unit cell**: smallest repetitive volume which contains the complete lattice pattern of a crystal.

Crystal Systems

- A unit cell is chosen to represent symmetry of the crystal structure, wherein all the atom positions in the crystal may be generated by translations of the unit cell integral distances along each of its edges.
- The unit cell is thus 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.

Crystal Systems

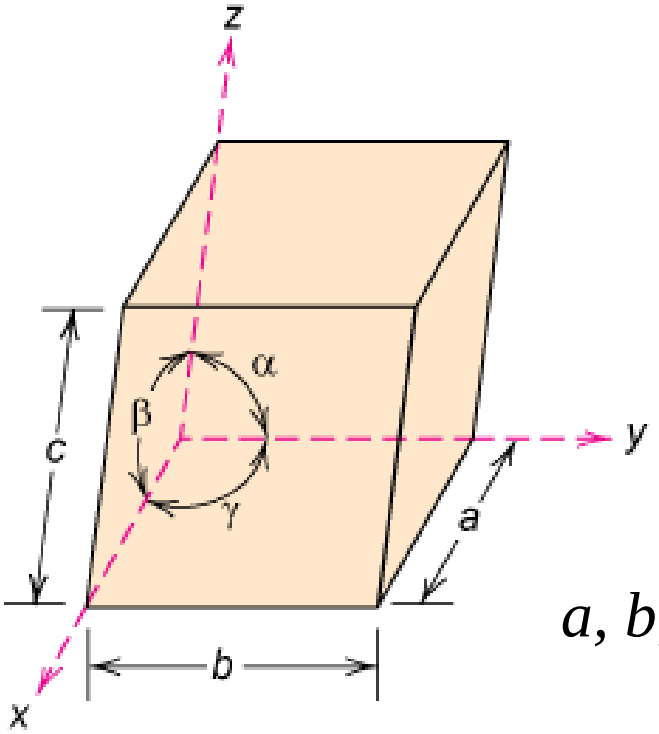


Fig. 3.4, *Callister 7e.*

7 crystal systems

14 crystal lattices

a, *b*, and *c* are the lattice constants

Metallic Crystal Systems

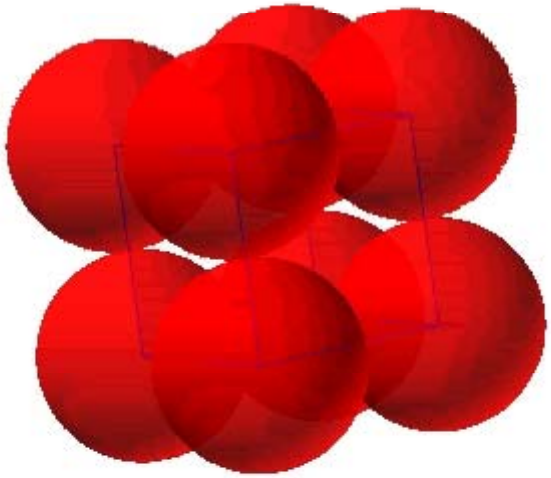
- Tend to be densely packed
- Reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
  - Electron cloud shields cores from each other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

We will examine three such structures…

Simple Cubic Structure (SC)

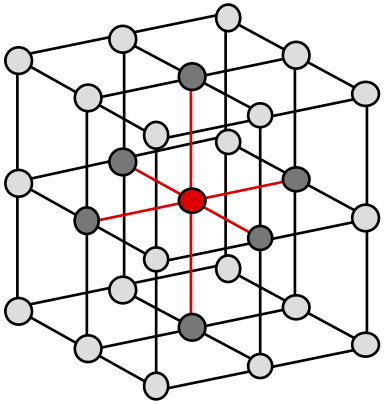
• Rare due to low packing density (only Po has this structure)

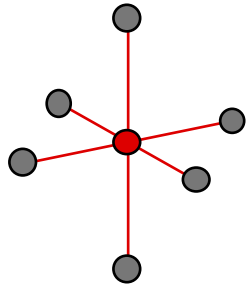
• Close-packed directions are cube edges.



(Courtesy P.M. Anderson)

• Coordination # = 6
(# nearest neighbors)



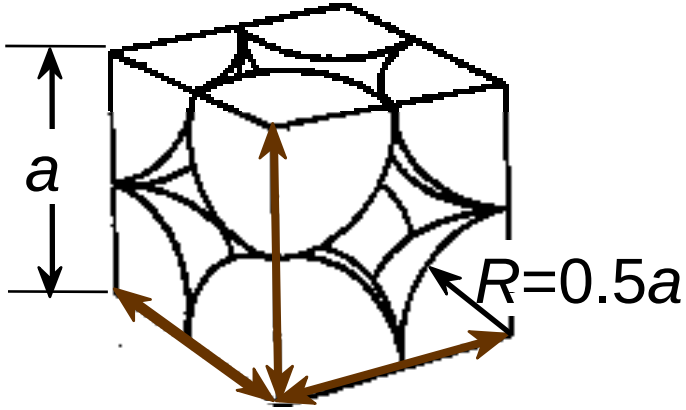


Atomic Packing Factor (APF)

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

*assume hard spheres

- APF for a simple cubic structure = 0.52



close-packed directions

contains 8 x 1/8 =

1 atom/unit cell

$$APF = \frac{\frac{\text{atoms}}{\text{unit cell}} \times \frac{\text{volume}}{\text{atom}}}{\frac{\text{volume}}{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi (0.5a)^3}{a^3}$$

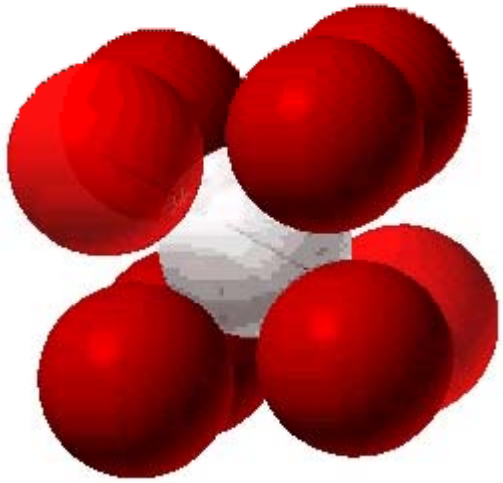
Adapted from Fig. 3.23, *Callister 7e.*

Body Centered Cubic Structure (BCC)

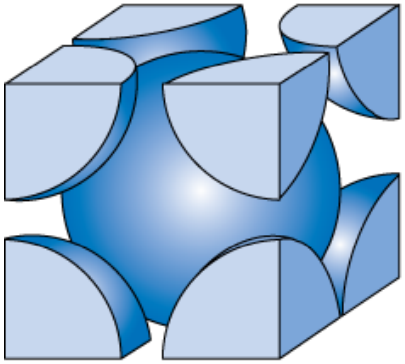
- Atoms touch each other along cube diagonals.
  -Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

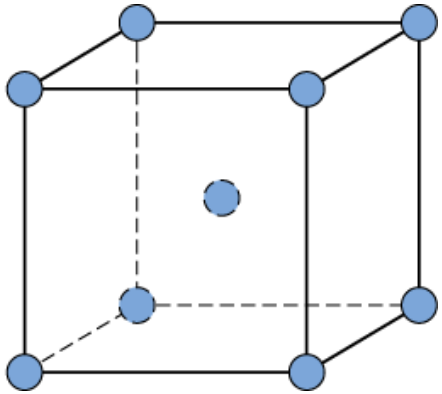
ex: Cr, W, Fe (α), Tantalum, Molybdenum

- Coordination # = 8



(Courtesy P.M. Anderson)



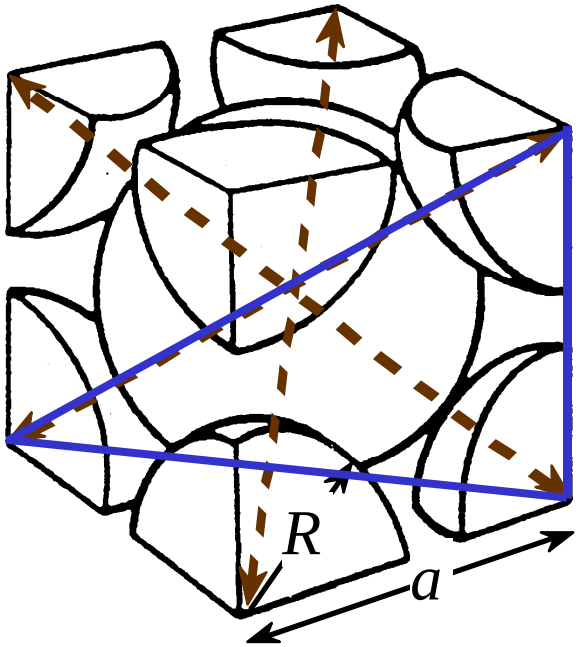


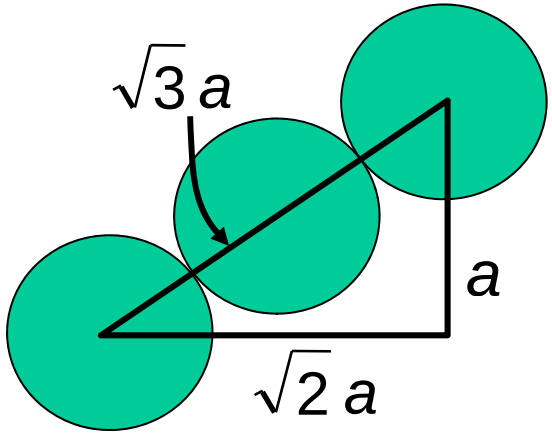
Adapted from Fig. 3.2, *Callister 7e.*

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

Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = 0.68





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

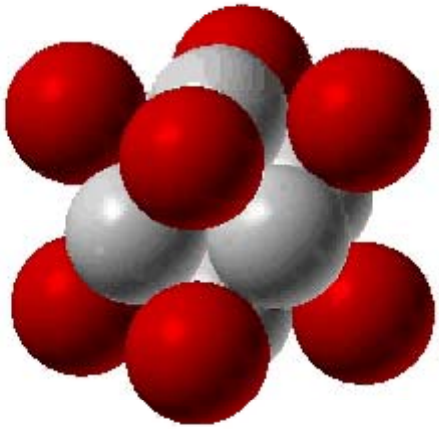
$$\text{APF} = \frac{\left(\frac{\text{atoms}}{\text{unit cell}}\right)\left(\frac{\text{volume}}{\text{atom}}\right)}{\left(\frac{\text{volume}}{\text{unit cell}}\right)} = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3\right)}{a^3}$$

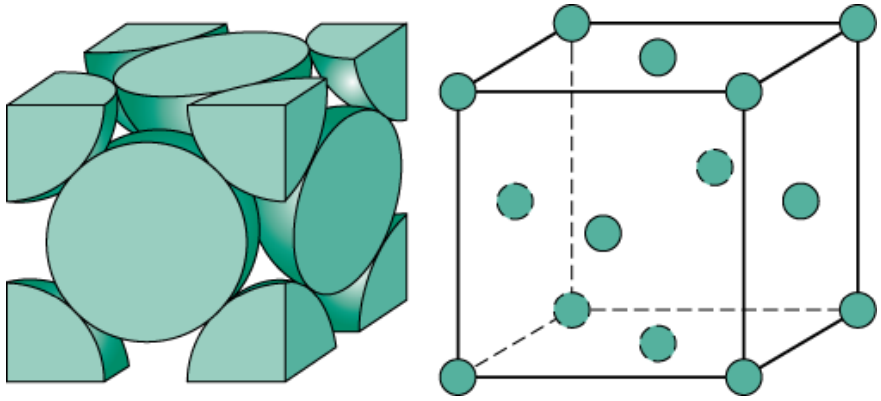
Face Centered Cubic Structure (FCC)

- 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





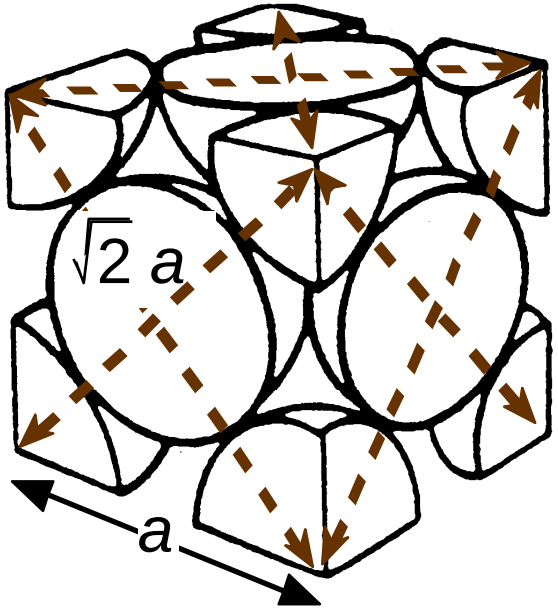
4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

(Courtesy P.M. Anderson)

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

Atomic Packing Factor: FCC

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



Adapted from Fig. 3.1(a), *Callister 7e.*

Close-packed directions:
length = $4R = \sqrt{2}\,a$

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

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

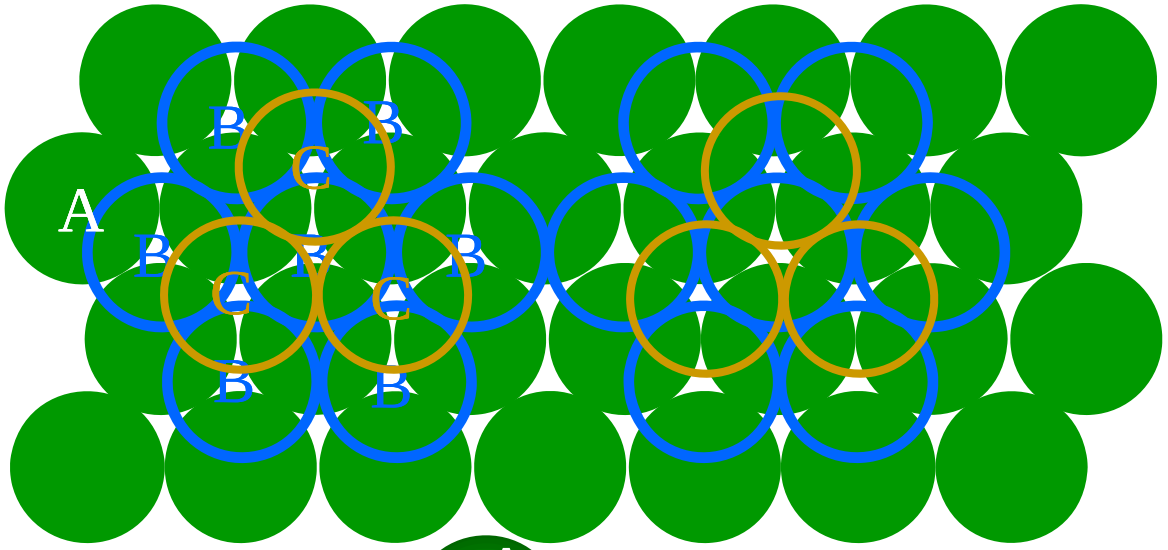
FCC Stacking Sequence

- ABCABC... Stacking Sequence
- 2D Projection

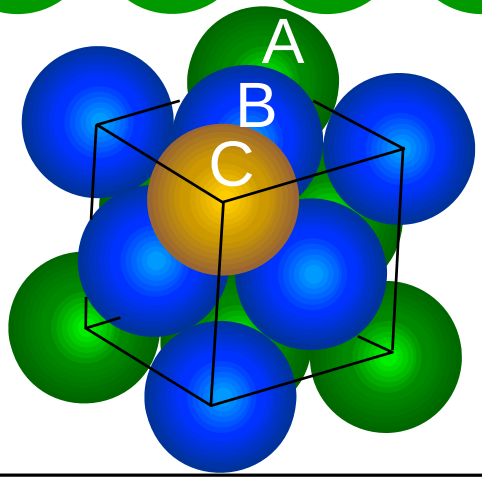
A sites

B sites

C sites

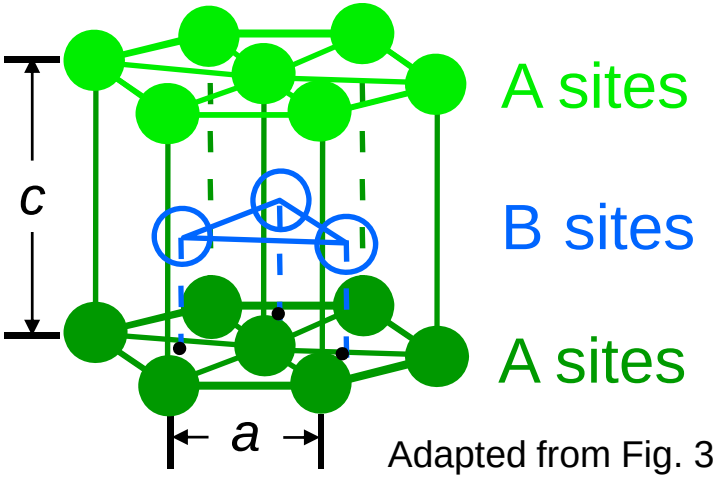


- FCC Unit Cell



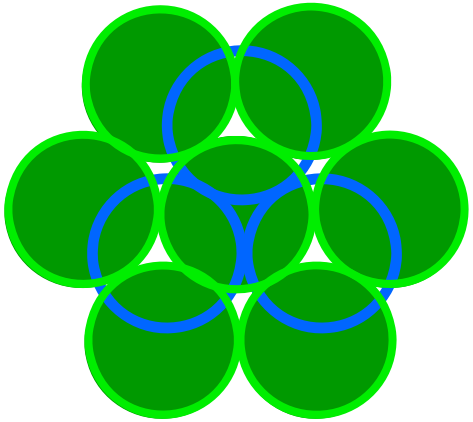
Hexagonal Close-Packed Structure (HCP)

- 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

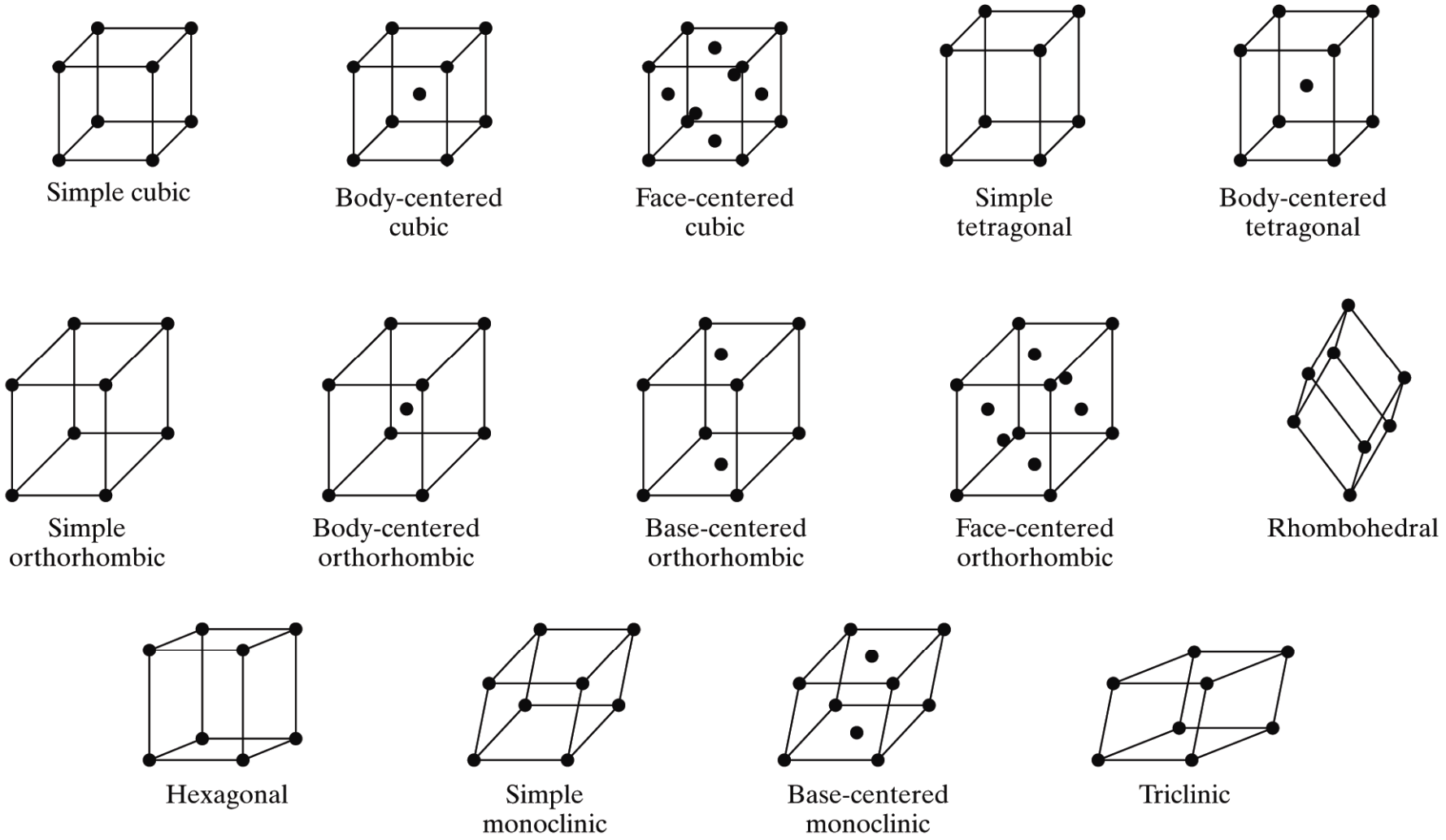


Table 3.2

The 14 Crystal (Bravais) Lattices.

Crystal Systems Relationships

Crystal structure	Relationship between edge length, a, and atomic radius, r
Body-centered cubic (bcc)	$a = 4r/\sqrt{3}$
Face-centered cubic (fcc)	$a = 4r/\sqrt{2}$
Hexagonal close packed (hcp)	$a = 2r$

Table 3.3

Relationship between Unit-Cell Size (Edge Length) and Atomic Radius for the Common Metallic Structures.

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

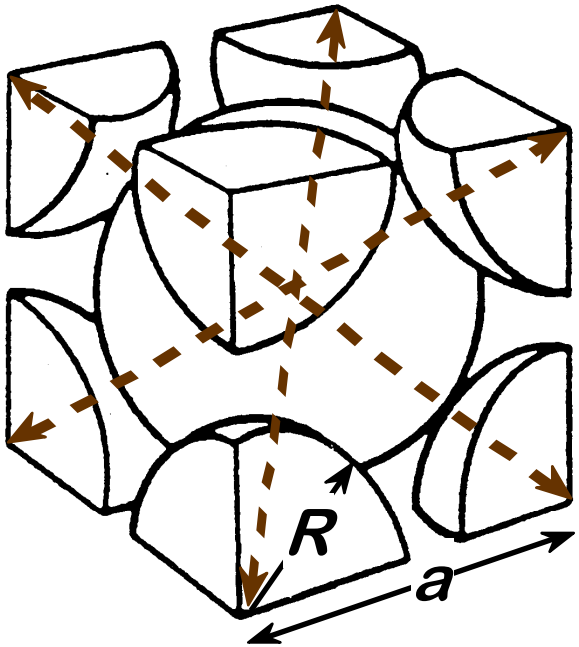
A = atomic weight

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

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol

Theoretical Density, ρ



Ex: Cr (BCC)

A = 52.00 g/mol

R = 0.125 nm

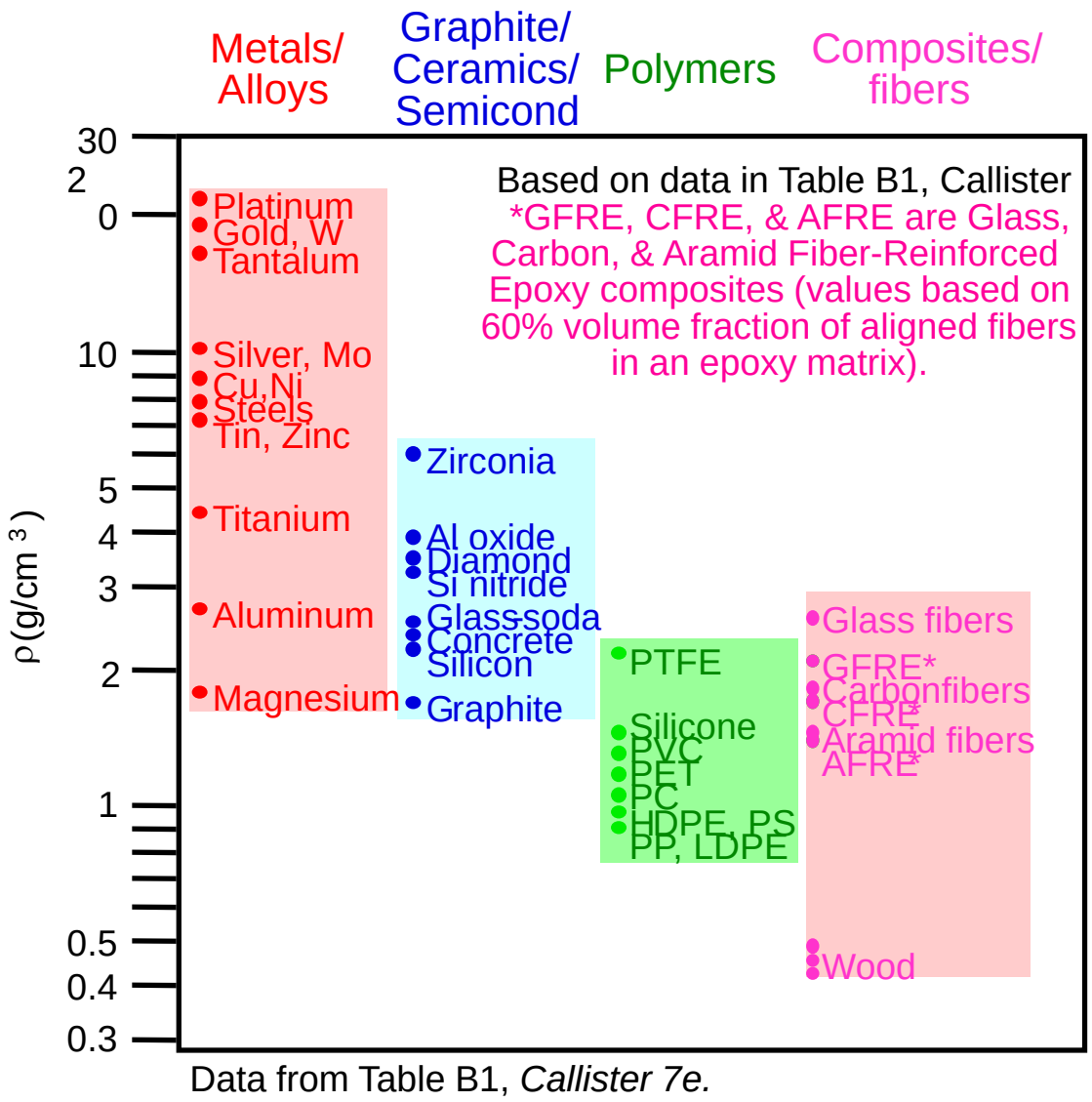
n = 2

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

$$\rho = \frac{\text{unit cell}}{\text{volume}} \cdot \frac{2 \cdot 52.00}{a^3 \cdot 6.023 \times 10^{23}} \cdot \frac{\text{g}}{\text{mol}} \cdot \frac{\text{atoms}}{\text{mol}}$$

$\rho_{theoretical}$	= 7.18 g/cm^3
ρ_{actual}	= 7.19 g/cm^3

Densities of Material Classes



Data from Table B1, *Callister 7e.*

Densities of Material Classes

In general $\rho_{Metals} > \rho_{Ceramics} > \rho_{polymers}$

Why?

Metals have...
- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...
- less dense packing
- often lighter elements

Polymers have...
- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...
- intermediate values