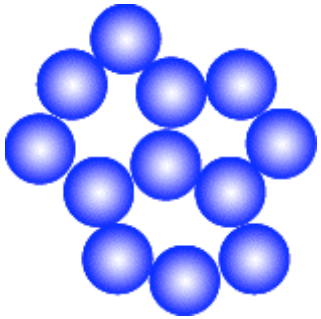
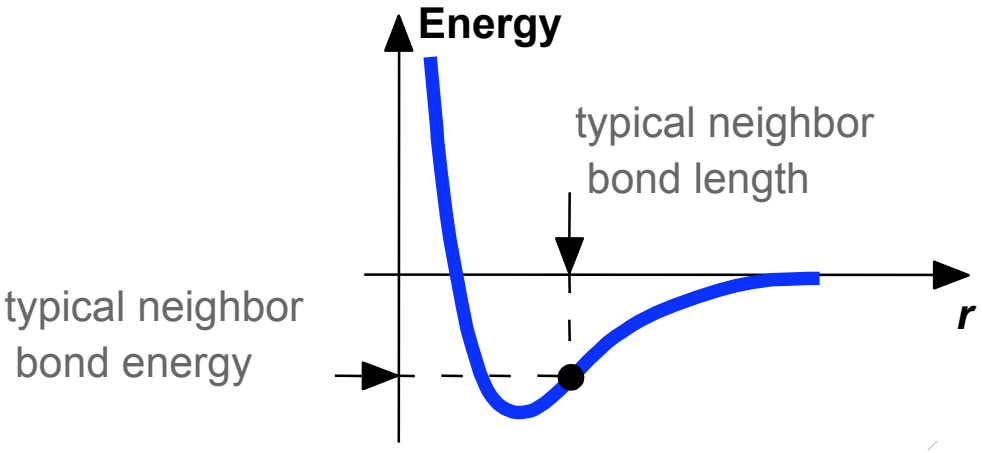
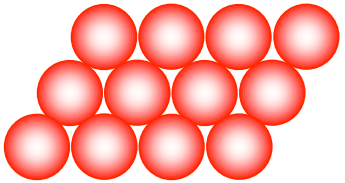
Energy and packing

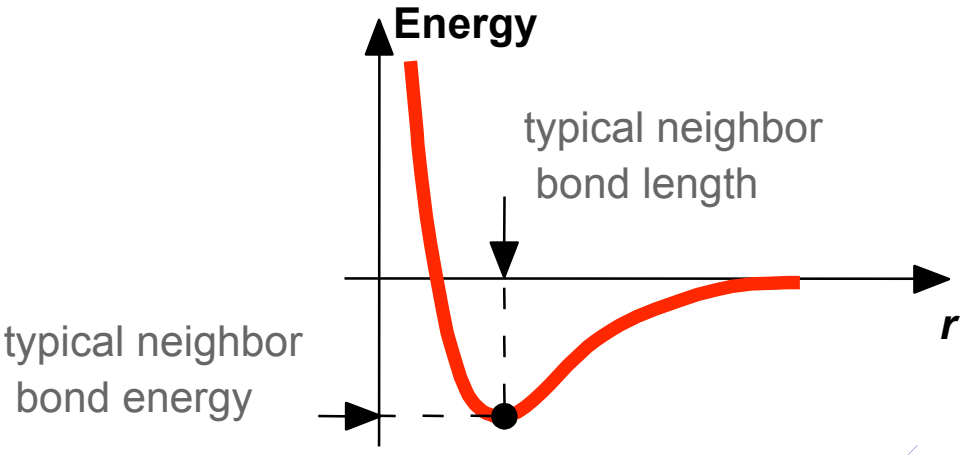
- Non dense, random packing





- Dense, ordered packing

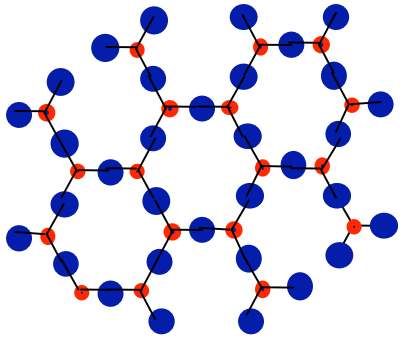




Dense, ordered packed structures tend to have lower energies.

Materials and packing

Crystalline materials...

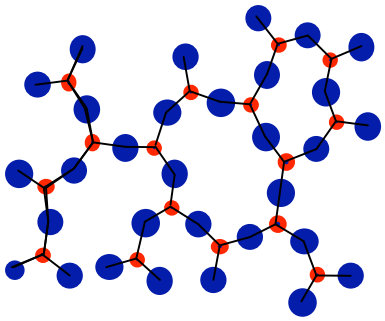


crystalline SiO_2

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

● **Si** ● **Oxygen**

Noncrystalline materials...



noncrystalline SiO_2

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

Crystals

Unit cell:

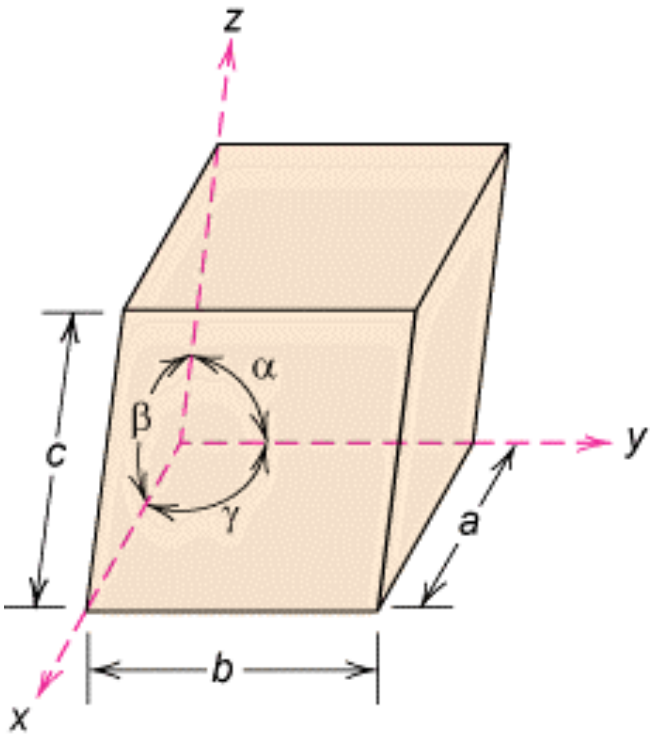
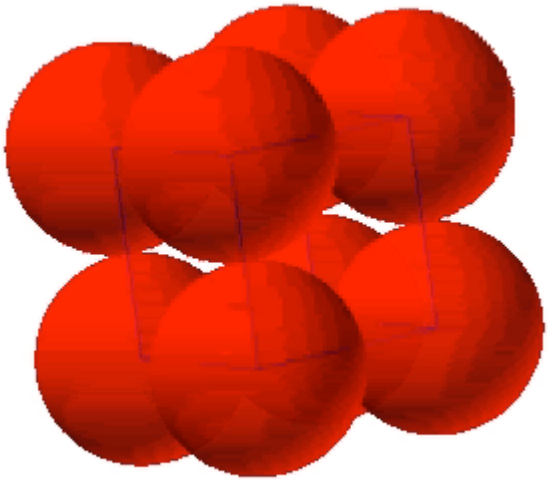


Fig. 3.4, *Callister 7e.*

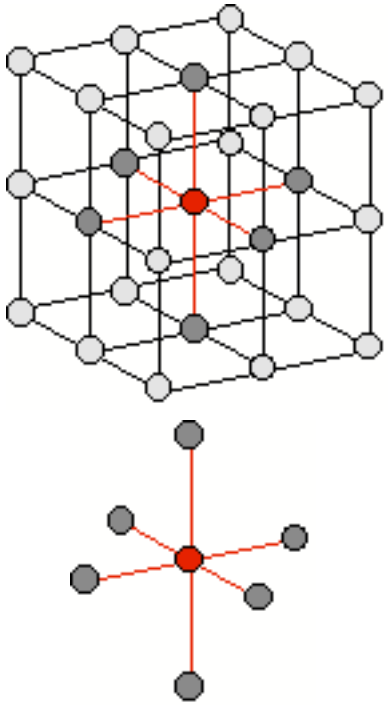
a, b, and *c* are the lattice constants

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)

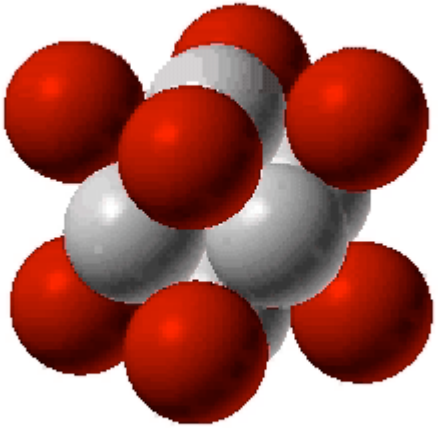


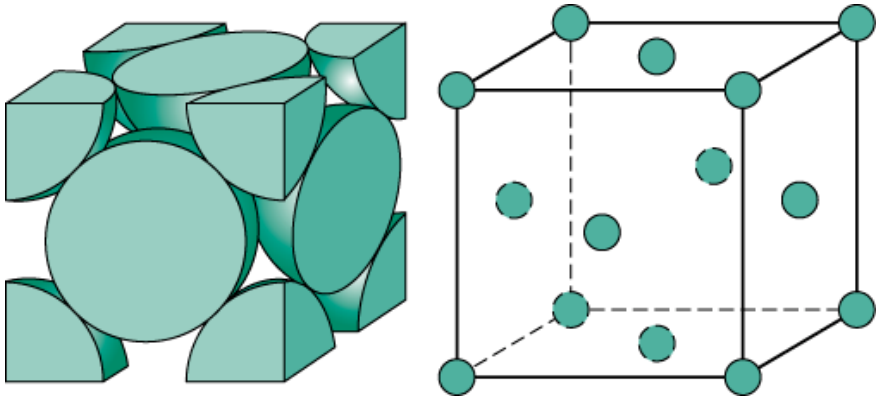
Face centered cubic structure (FCC)

- 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

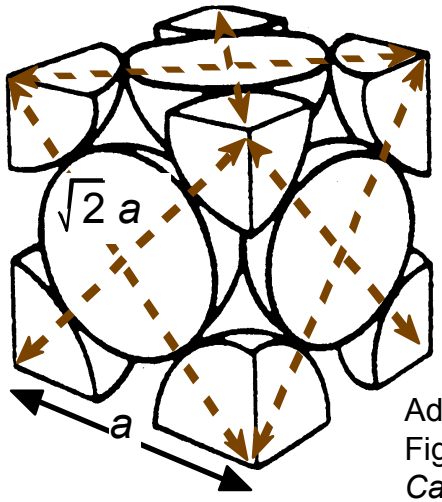




Adapted from Fig. 3.1, *Callister 7e.*

(Courtesy P.M. Anderson)

Atomic packing factor (APF): FCC



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

close-packed directions

contains 6 x 1/2 + 8 x 1/8 =

4 atoms/unit cell

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

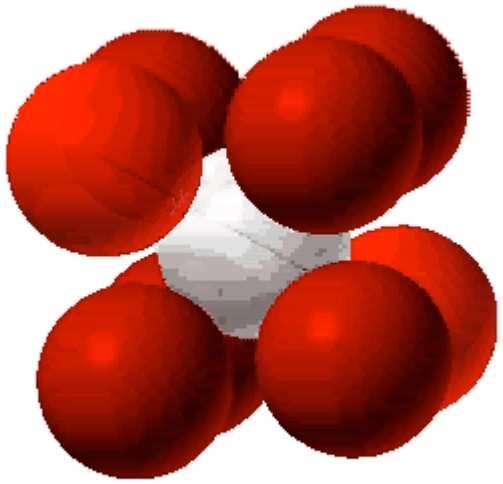
n = number of atoms/unit cell
A = atomic weight
V_C = Volume of unit cell = a^3 for cubic
N_A = Avogadro's number
= 6.023×10^{23} atoms/mol

Body centered cubic structure (BCC)

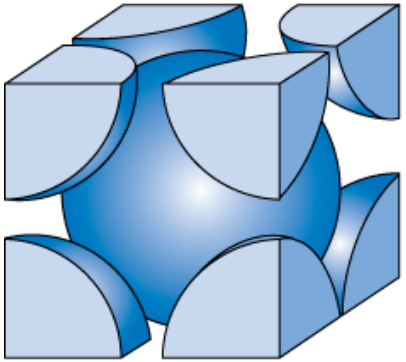
- Atoms touch each other along cube diagonals.

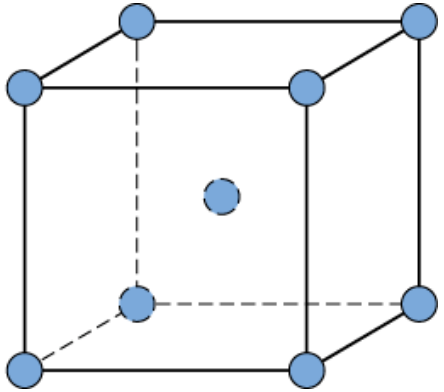
  --Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

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



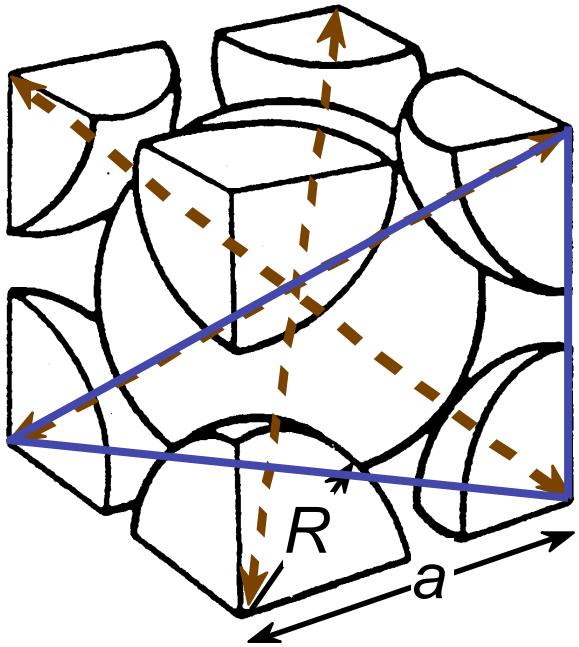
(Courtesy P.M. Anderson)





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

Atomic packing factor (APF): BCC



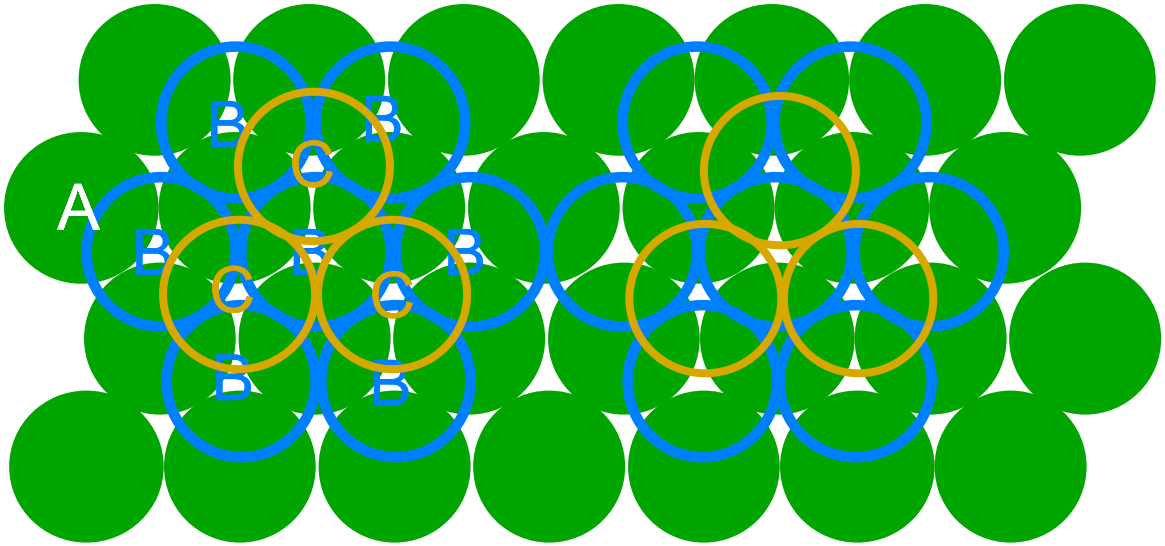
FCC stacking sequence

- ABCABC... Stacking Sequence
- 2D Projection

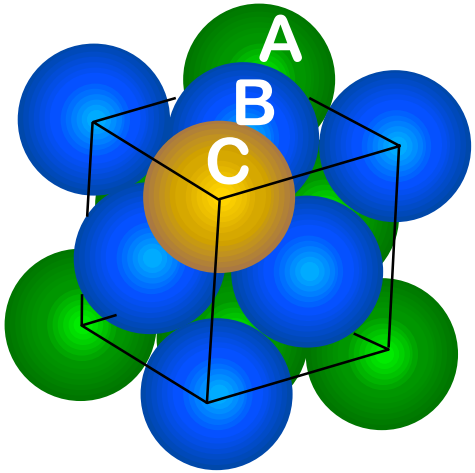
A sites

B sites

C sites



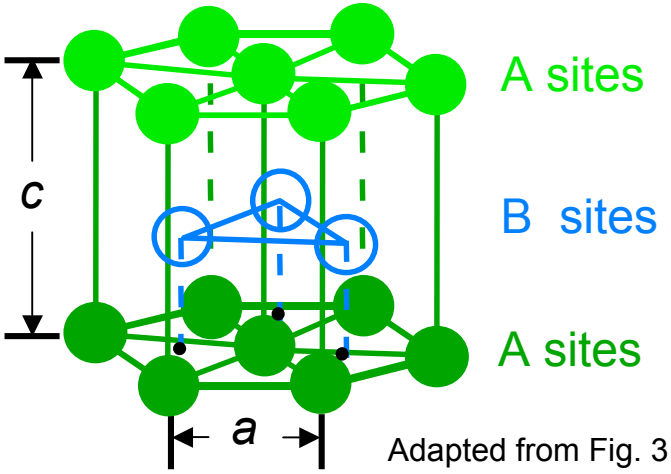
- FCC Unit Cell



Hexagonal close-packed structure (hcp)

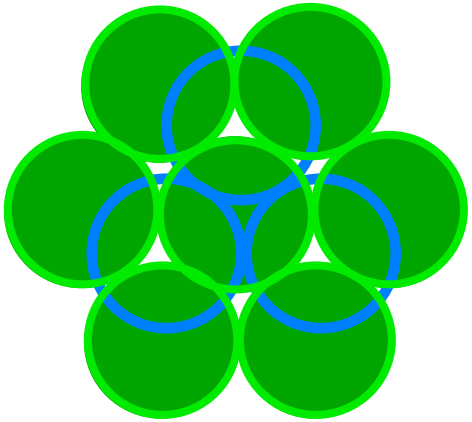
- ABAB... Stacking Sequence

- 3D Projection



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

- 2D Projection



6 atoms/unit cell

ex: Cd, Mg, Ti, Zn