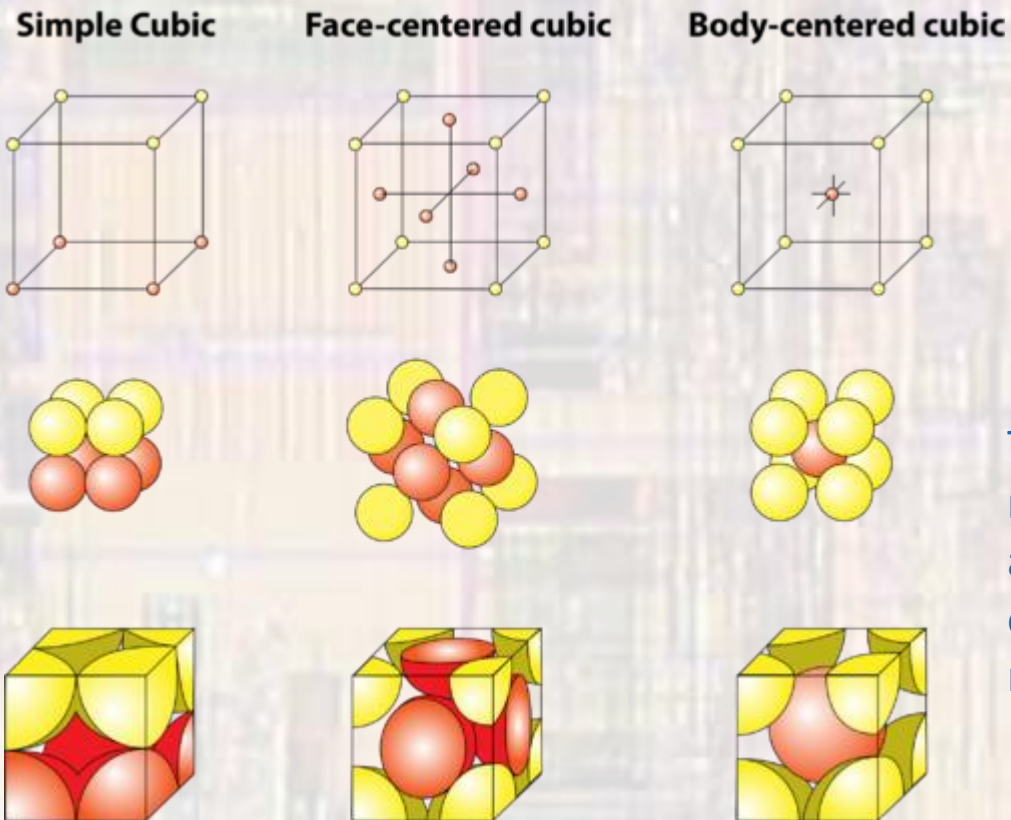# Silicon Crystal Structure

Last updated 2/26/22

These concepts have been greatly simplified

Silicon Crystal Structure
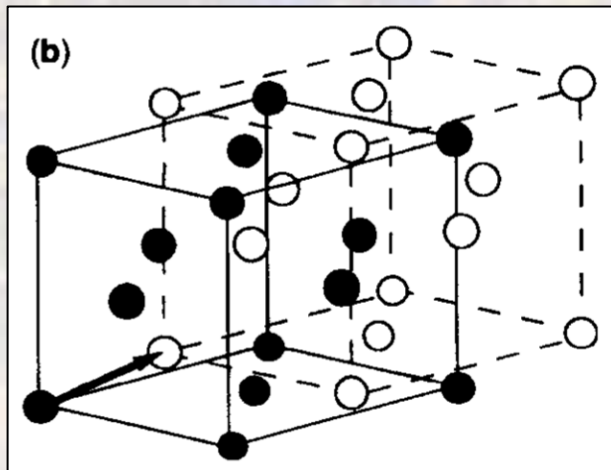
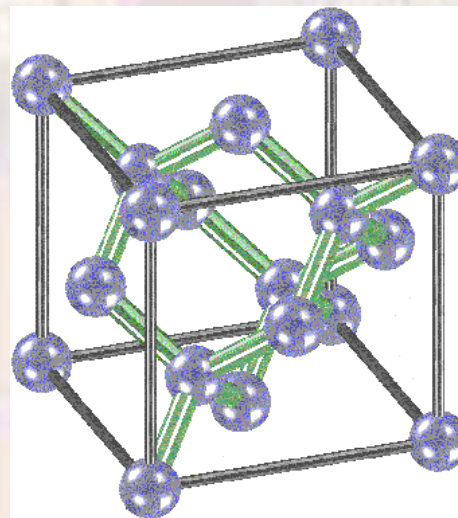- Crystals are characterized with 3d geometric structures (unit cell)

Simple Cubic **Face-centered cubic** **Body-centered cubic**

The spheres here represent the approximate extents of the atom, not the nuclei
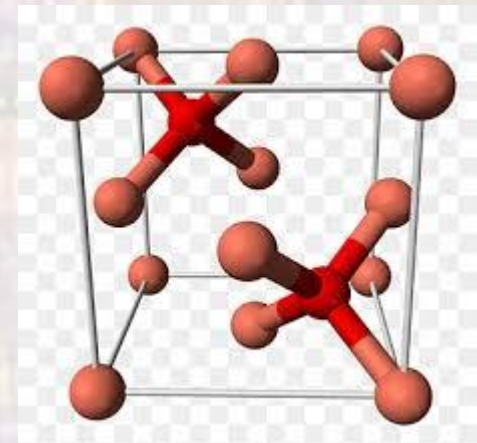
Silicon Crystal Structure

- ## Silicon unit cell
  - ### 2 interpenetrating Face Centered Cubic Cells

2 FCC cells
1 shifted ¼ of the way
along the major diagonal

Resulting diamond
cubic lattice

Atoms showing
4 nearest neighbor
structure

Lattice parameter (edge length) of 0.543 nm
Nearest neighbor distance is 0.235 nm.

Silicon Crystal Structure

- Silicon unit cell
  - Corners: 8, 1/8 atoms/unit cell
  - Faces: 6, 1/2 atoms/unit cell
  - Inside: 4 full atoms/unit cell
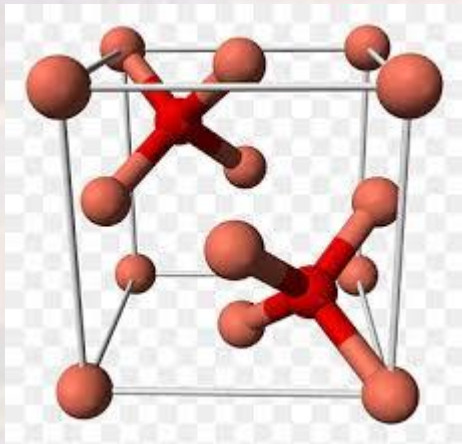
1
3
<u>4</u>
8 atoms/unit cell

Cell volume:

$$(.543 \text{ nm})^3 = 1.6 \times 10^{-22} \text{ cm}^3$$
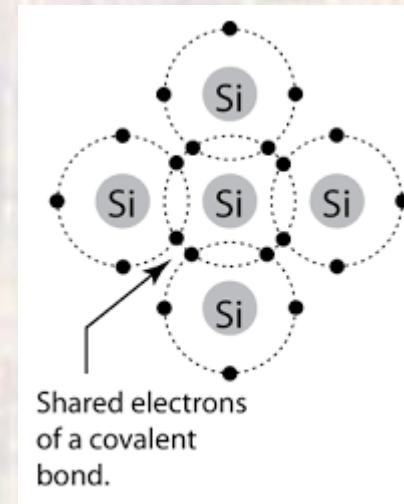
Density of silicon atoms

$$= (8 \text{ atoms}) / (\text{cell volume}) = 5 \times 10^{22} \text{ atoms/cm}^3$$

Silicon Crystal Structure

- Silicon unit cell – bonding model
  - Si has a half full outer electron shell (4 / 8)
  - Lowest energy state is the Diamond Lattice
   - 4 electrons are shared between 4 nearest neighbors

Atoms showing
4 nearest neighbor
structure

Each atom appears to have a full
valence band → very stable

Silicon Crystal Structure

- Silicon Crystal – binding energies
  - The net effect of combining into the crystal structure is that the allowed energy states are modified
    - A group of allowed low energy states is formed
      - Valence Band
      - At 0K, all of the electrons are in these bands
    - A group of allowed high energy states is formed
      - Conduction Band
      - At 0K, no electrons are in these bands
    - A gap, where no allowed energy states exist is created
      - Bandgap
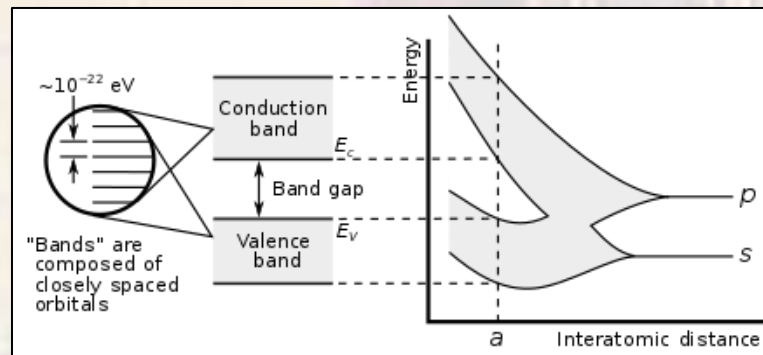
4 allowed states / atom in each band

Silicon Crystal Structure

- Silicon Crystal – binding energies
  - As temperature is increased – some electrons acquire enough energy to "jump" the bandgap and move from a valence band state to a conduction band state
  - These electrons can move freely through the crystal while in the conduction band

  - Once an electron has left the valence band, there is a missing bond (electron) in the structure (Hole)
  - These holes can move freely through the crystal while in the valence band

Silicon Crystal Structure

- Intrinsic carrier density
  - How many electrons have moved from the valence band to the conduction band

$$n_i = BT^{3/2}\, e^{\frac{-E_g}{2kT}}$$

B – semiconductor specific coefficient
T – temperature in Kelvin
E_g – semiconductor band gap energy in eV
k – Boltzmann's constant (86×10^{-6} eV/K)

For Si:
  B = 5.23×10^{15} cm^{-3}K$^{-3/2}$
  E_g = 1.2eV(0K), 1.1eV(300K)

at 300K (room temp?) → n_i = 1.5×10^{10}/cm^3

Silicon Crystal Structure

- Intrinsic carrier density

5×10^{22} atoms/cm^3

1.5×10^{10} electrons/cm^3

one in 3.3×10^{12} electrons has been elevated
1 in 3 Trillion

resistivity $\rho = 3.4 \times 10^5$ Ω-cm