# MSE 170: Introduction to Materials Science and Engineering

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|---|---|
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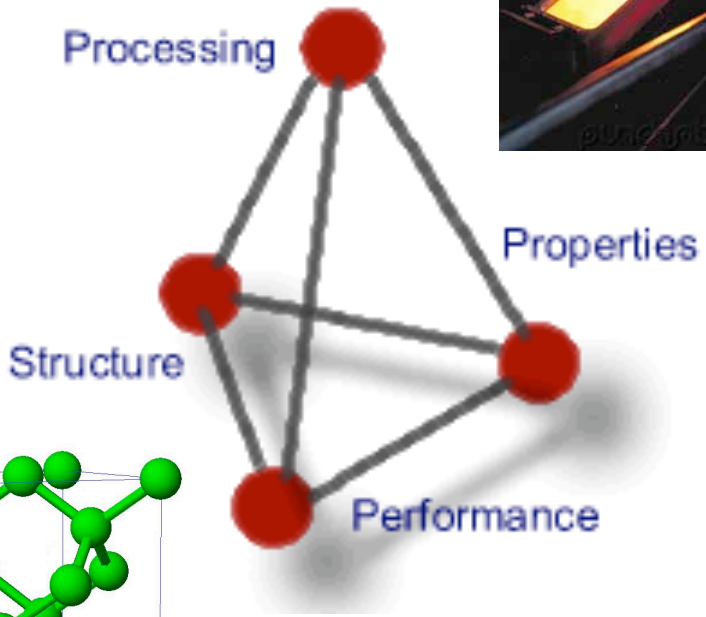
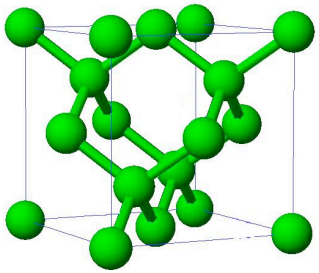
# What is Materials Science and Engineering?

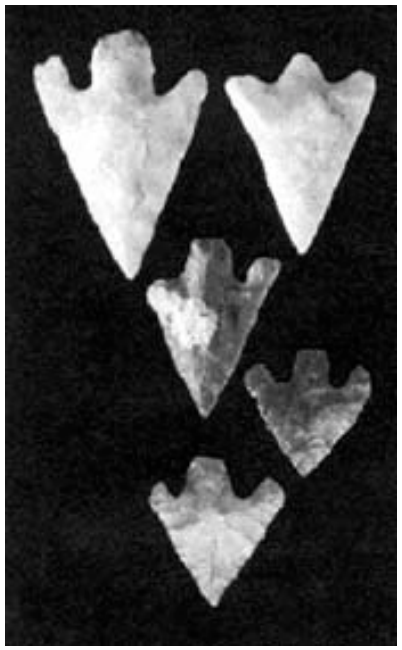


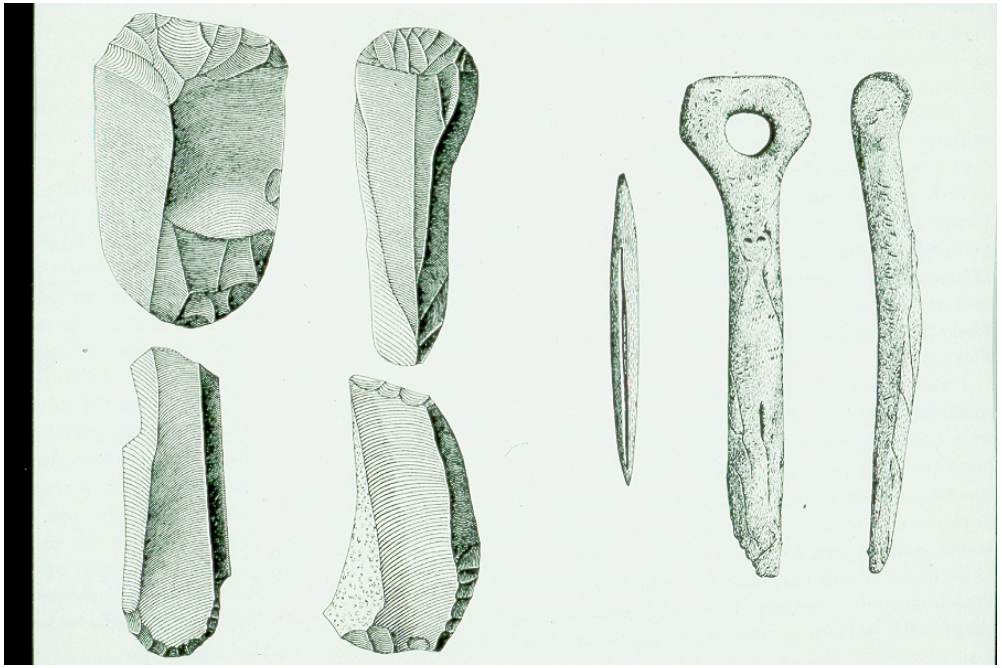



An interdisciplinary field that addresses the fundamental relationships between the Processing, Structure and Properties of materials and develops them for the desired technological application (Performance).

# Materials through the ages

**Stone Age (beginning of life – 3000 BC)**





Feature: Using naturally occurring materials with only changes in shape

# Materials through the ages

**Bronze Age (3000 BC – 1200 BC)**

*Copper and Tin alloy*

Ability to modify materials by refining (using heat), chemical modifications (alloying) and mechanical deformation (cold working)

Imperfection (Ch. 4)
Diffusion (Ch. 5)
Phase diagram (Ch. 9)
Metal Processing (Ch. 11)

# Materials through the ages

**Iron Age (1200 BC – Present)**

Casting and alloying wasn't perfected until 16th century

Mastery of Steel (Iron alloy) technology enables Industrial Revolution in the 18th and 19th century

Ability to heat treat at high temperature, control microstructure at different length scale and ability to design specific microstructures for specific properties

Phase transformation (Ch. 10)

# Materials through the ages

**Plastic Age (1940 - Present)**

Discovery of polymers, and the ability to synthesize and process polymers.

# Materials through the ages

**Silicon Age (1950 - Present)**

Commercialization of silicon technology (integrated circuits, electronic devices, etc…) leads to the information age, which gives boost to human productivity

Electronic Prop. (Ch.18)
Thermal Prop. (Ch.19)
Magnetic Prop. (Ch.20)
Optical Prop. (Ch.21)

Ability to control alloying accurately, ability to make thin films

# Future

**1. Nanotechnology**

- Synthesis and characterizations of nanomaterials and nanostructure

**2. Biotechnology**

- biomimetics and biomaterials

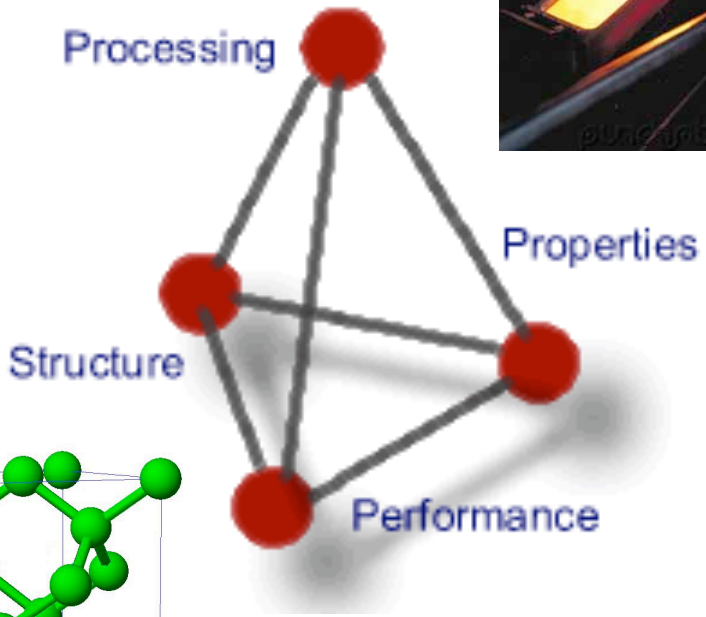
**3. Energy/Environmental**

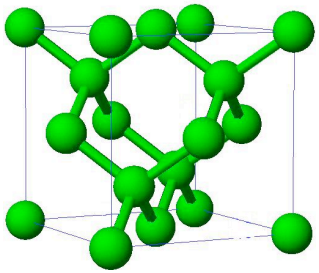
- Next generation energy conversion

**4. Information Technology**

- Materials informatics

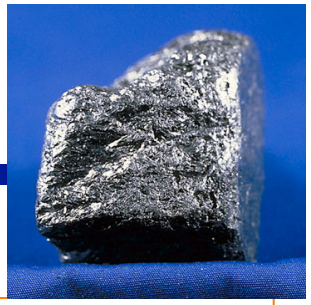
# What is Materials Science and Engineering?

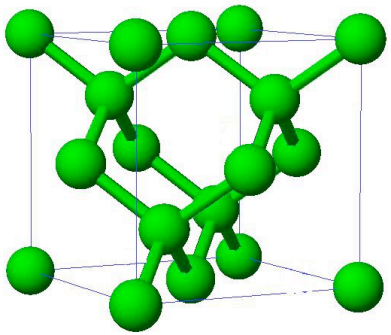


An interdisciplinary field that addresses the fundamental relationships between the Processing, Structure and Properties of materials and develops them for the desired technological application (Performance).

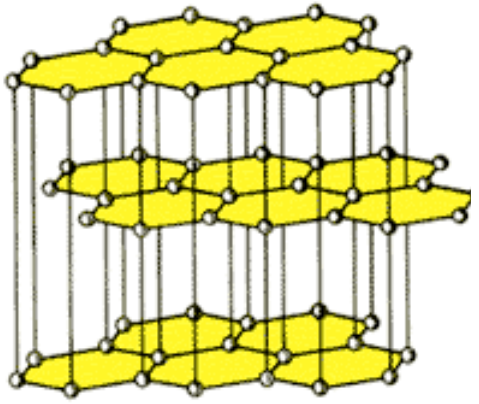
# Two Forms of Carbon





**Diamond**

VS.

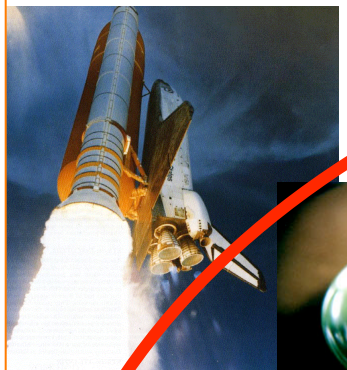


**Graphite**

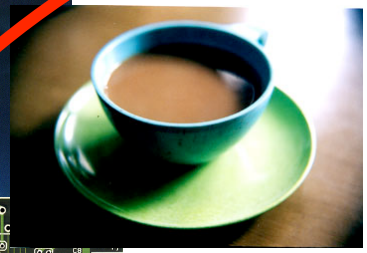
- A structure of carbon only produced at high temperature and pressure.
- The hardest known material.

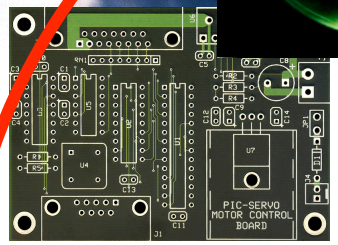
- A structure of carbon that is in equilibrium (it is stable and will not change form over time).
- It is soft.

# Materials

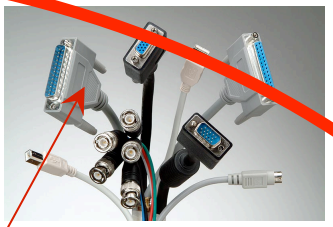


Ceramics
Ch. 12

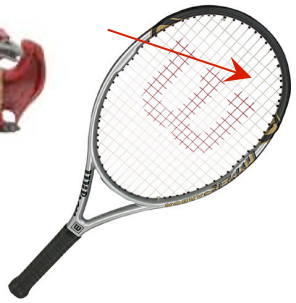










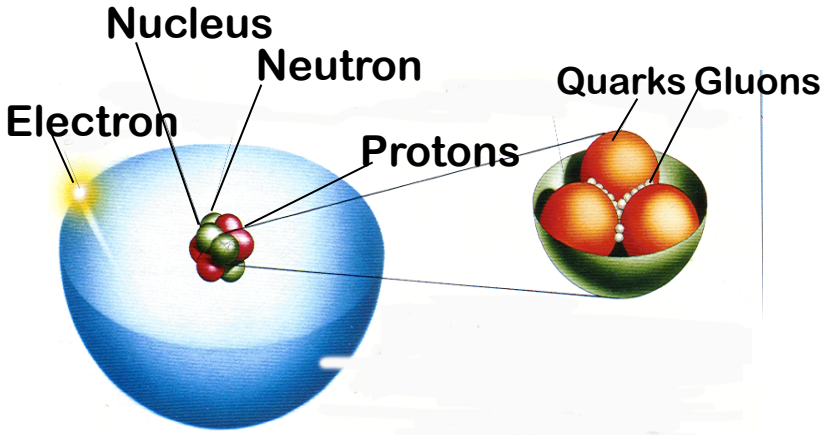


Polymers
Ch.14 and 15

Metals
Ch. 11

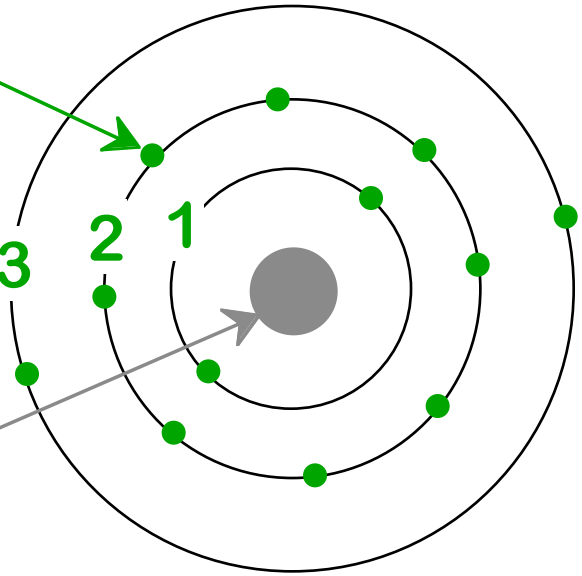
Composite
Ch. 16

# Atomic structure




**BOHR ATOM**

**orbital electrons:**
**n = principal quantum number**




Nucleus: Z = # protons

= 1 for hydrogen to 94 for plutonium

Atomic mass A ≈ Z + N  N = # neutrons

# Electronic structure

Valence electrons determine all of the following properties:

- Chemical
- Electrical
- Thermal
- Optical

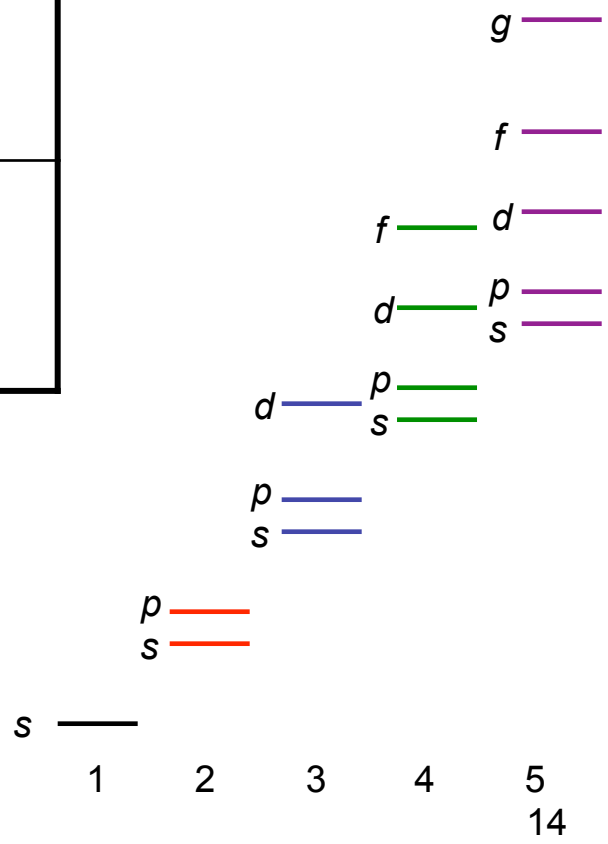
Electrons have wavelike and particulate properties.

- This means that electrons are in orbitals defined by a probability.
- Each orbital at discrete energy level determined by quantum numbers.

| Quantum # | Designation |
|---|---|
| $n$ = principal (energy level-shell) | $K$, $L$, $M$, $N$, $O$ (1, 2, 3, etc.) |
| l = subsidiary (orbitals) | $s$, $p$, $d$, $f$ (0, 1, 2, 3,…, $n$ -1) |
| $m_l$ = magnetic | 1, 3, 5, 7 (-l to +l) |
| $m_s$ = spin | ½, -½ |

# Electronic structure

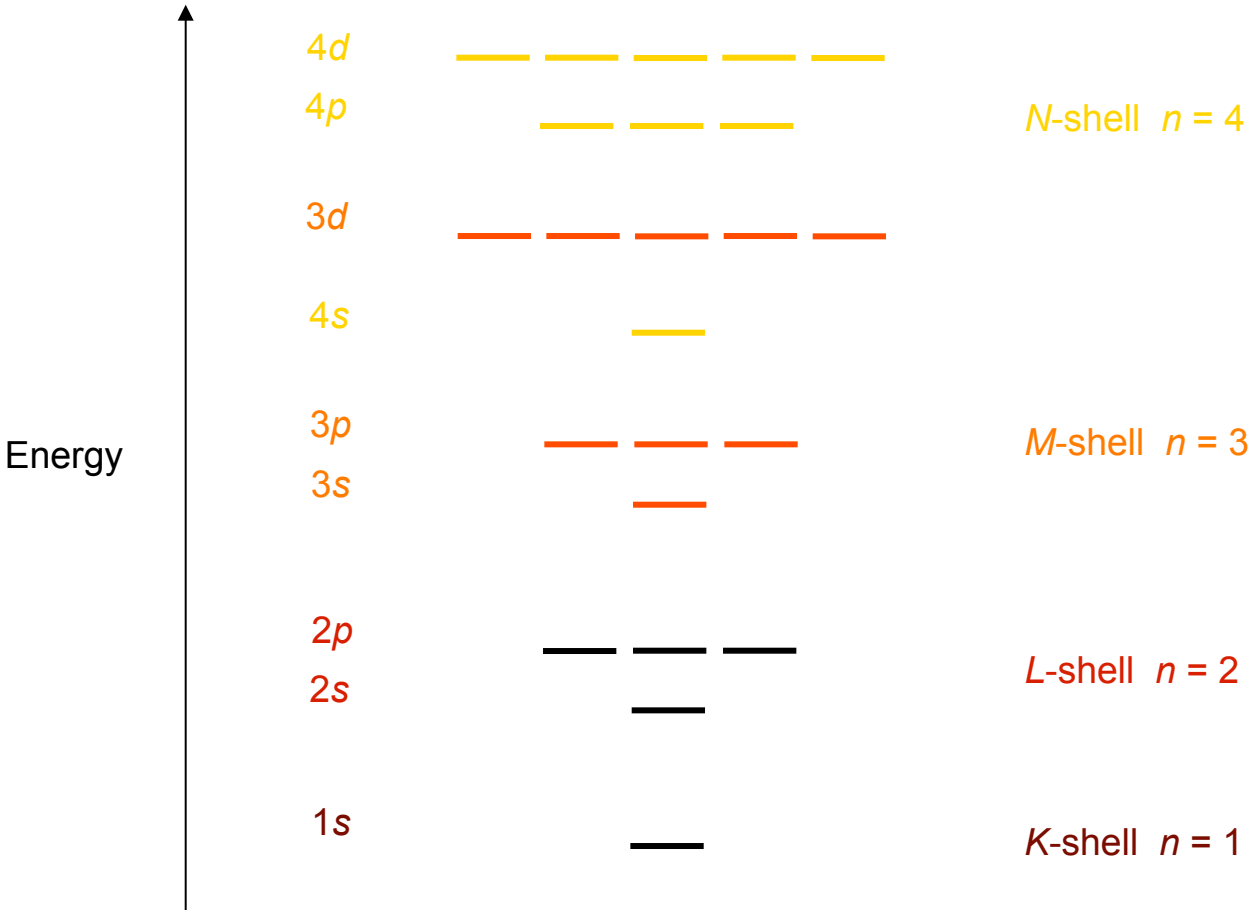
| Principal quantum no. | Shell designation | Subshells | No. of states | Number of electrons | |
|---|---|---|---|---|---|
| | | | | Per subshell | Per shell |
| 1 | *K* | *s* | 1 | 2 | 2 |
| 2 | *L* | *s* | 1 | 2 | 8 |
| | | *p* | 3 | 6 | |
| 3 | *M* | *s* | 1 | 2 | 18 |
| | | *p* | 3 | 6 | |
| | | *d* | 5 | 10 | |
| 4 | *N* | *s* | 1 | 2 | 32 |
| | | *p* | 3 | 6 | |
| | | *d* | 5 | 10 | |
| | | *f* | 7 | 14 | |



# Electron energy states

Electrons...

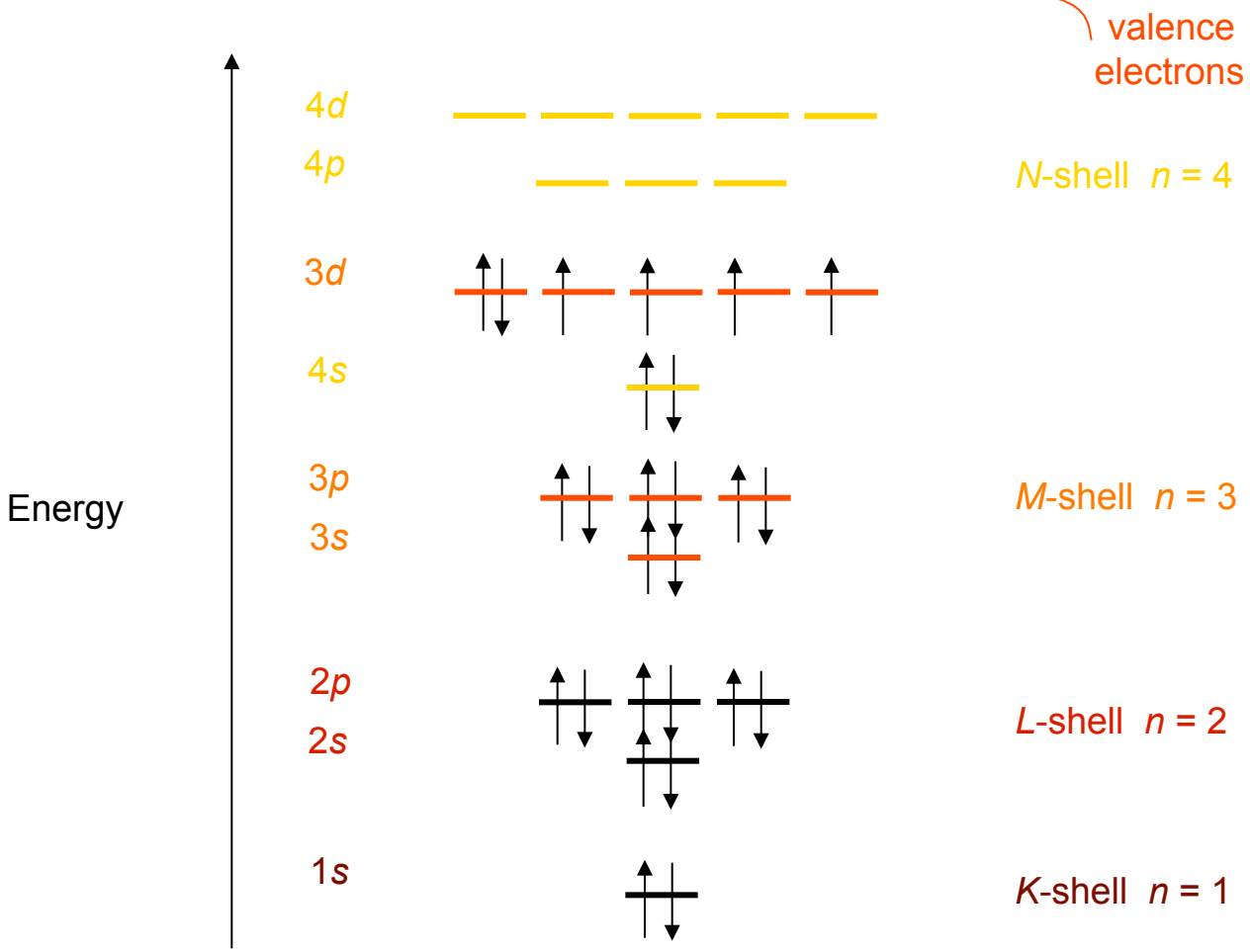
- have discrete energy states
- tend to occupy lowest available energy state.




Adapted from Fig. 2.4, *Callister 7e.*

# Electronic configuration

ex: Fe - atomic # = 26 $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^6$ $4s^2$




Adapted from Fig. 2.4, *Callister 7e.*

# Survey of elements

- Most elements: Electron configuration not stable.

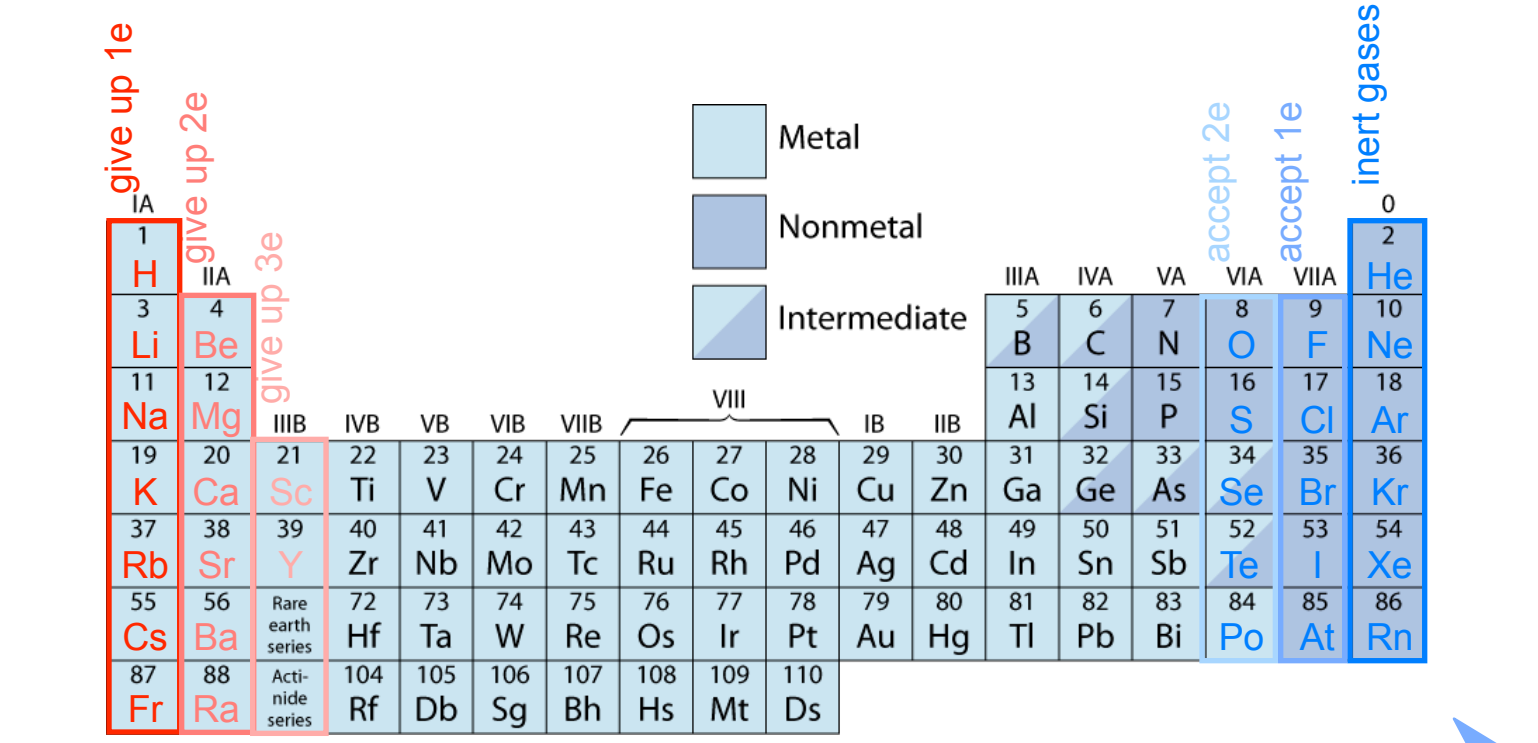
| Element | Atomic # | Electron configuration | |
|---|---|---|---|
| Hydrogen | 1 | $1s^1$ | |
| Helium | 2 | $1s^2$ | (stable) |
| Lithium | 3 | $1s^2 2s^1$ | |
| Beryllium | 4 | $1s^2 2s^2$ | |
| Boron | 5 | $1s^2 2s^2 2p^1$ | |
| Carbon | 6 | $1s^2 2s^2 2p^2$ | |
| ... | | ... | |
| Neon | 10 | $1s^2 2s^2 2p^6$ | (stable) |
| Sodium | 11 | $1s^2 2s^2 2p^6 3s^1$ | |
| Magnesium | 12 | $1s^2 2s^2 2p^6 3s^2$ | |
| Aluminum | 13 | $1s^2 2s^2 2p^6 3s^2 3p^1$ | |
| ... | | ... | |
| Argon | 18 | $1s^2 2s^2 2p^6 3s^2 3p^6$ | (stable) |
| ... | ... | ... | |
| Krypton | 36 | $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ | (stable) |

- Why? Valence (outer) shell usually not filled completely.

Adapted from Table 2.2, *Callister 7e.*

# The periodic table

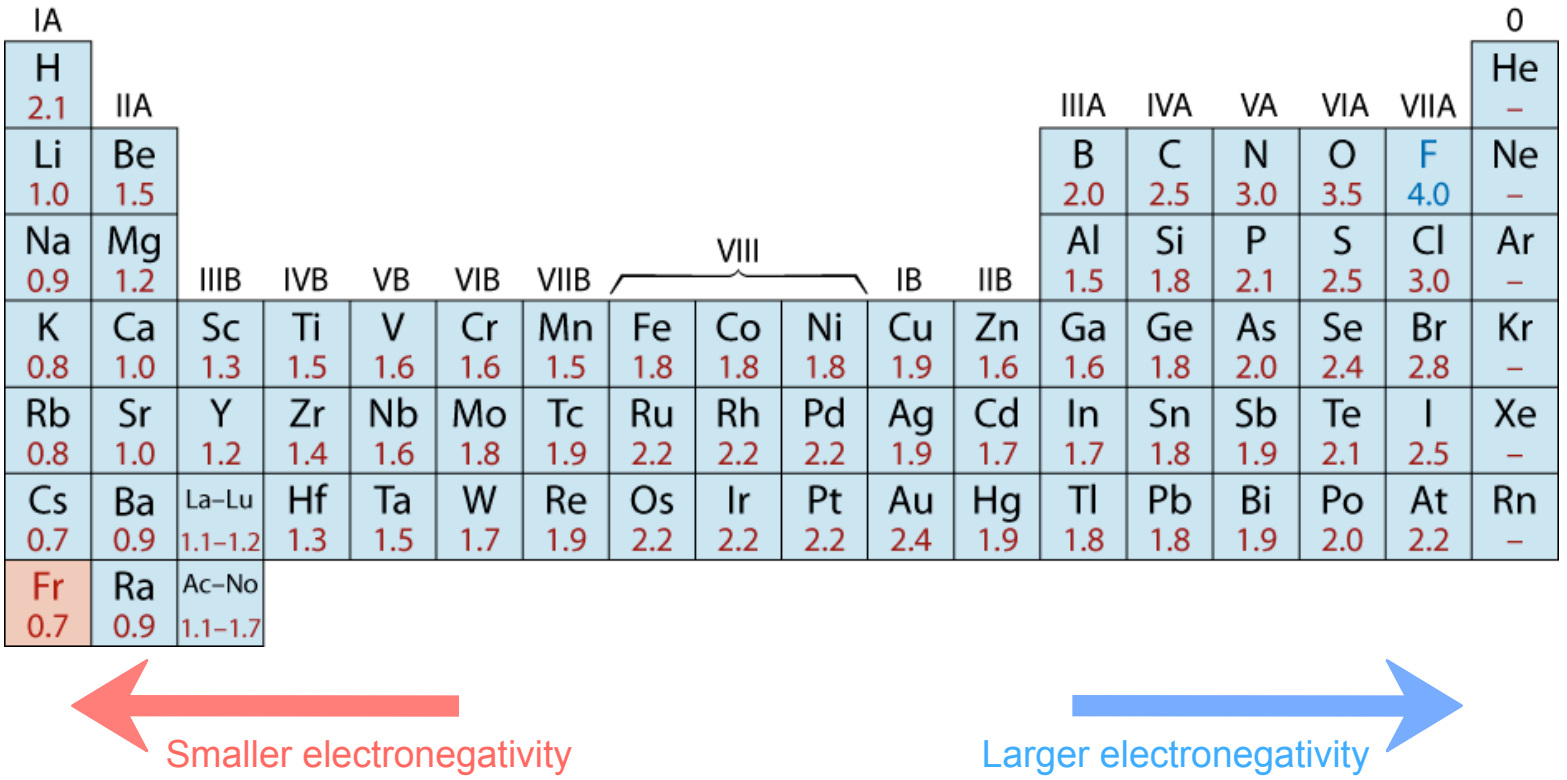
- Columns: Similar Valence Structure




Adapted from Fig. 2.6, *Callister 7e.*

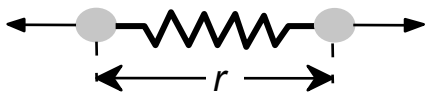
# Electronegativity

- Ranges from 0.7 to 4.0,
- Large values: tendency to acquire electrons.

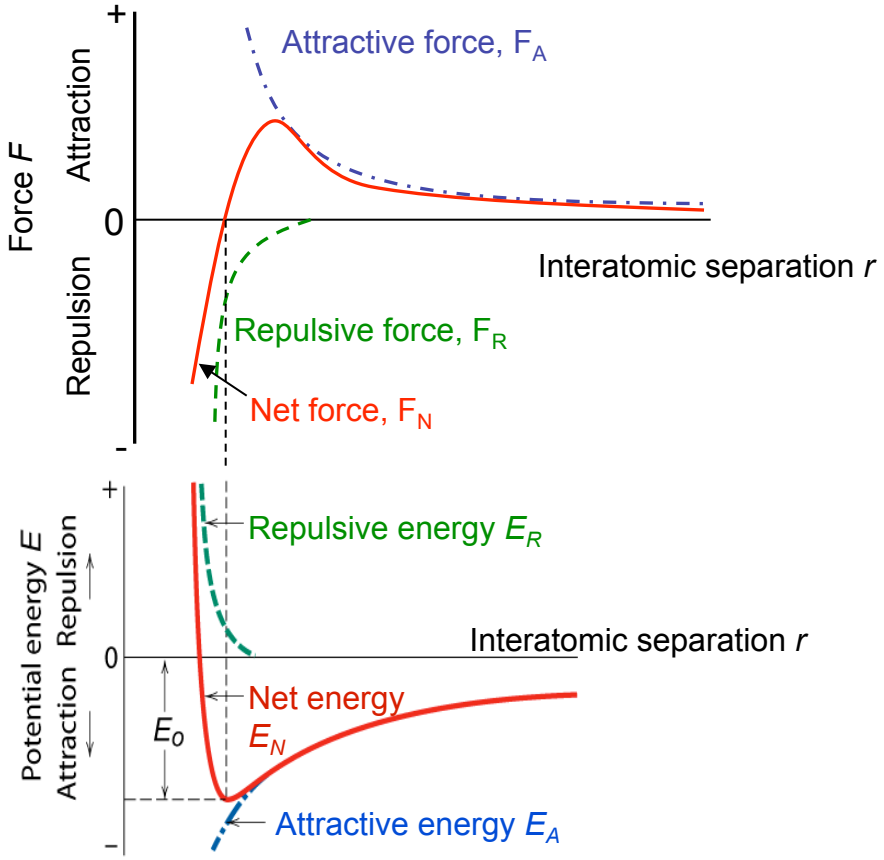



Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

# Bonding forces and energies




- Attractive force, $F_A$
- Repulsive force, $F_R$



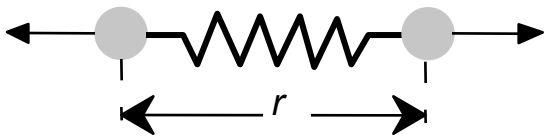

$$E = \int F dr$$

$$E_N = \int_{\infty}^{r} F_N dr = \int_{\infty}^{r} F_A dr + \int_{\infty}^{r} F_R dr$$

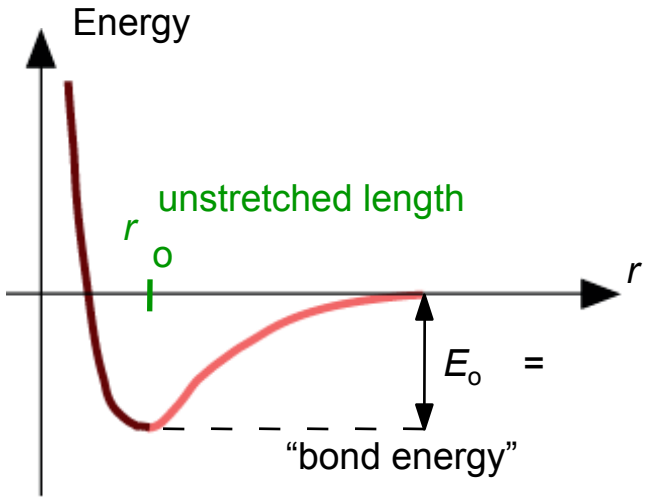
$$= E_A + E_R$$

# Properties from bonding

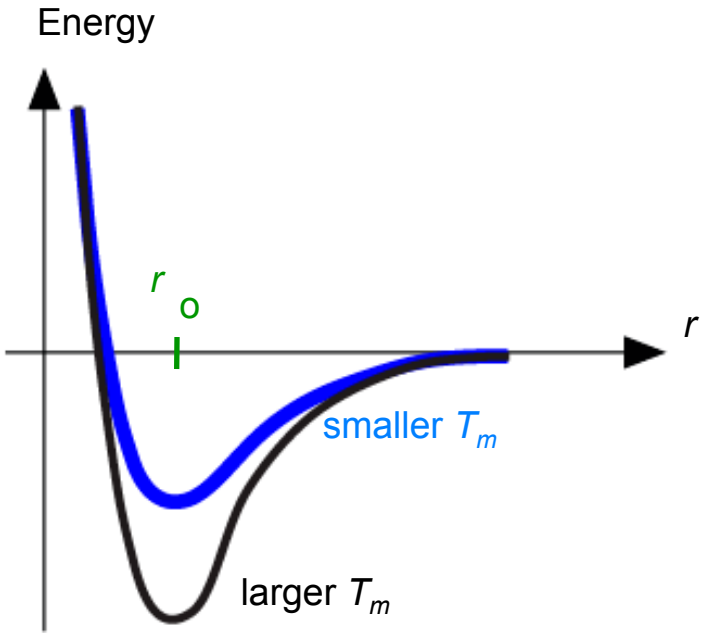
- Bond length, $r$




- Bond energy, $E_o$



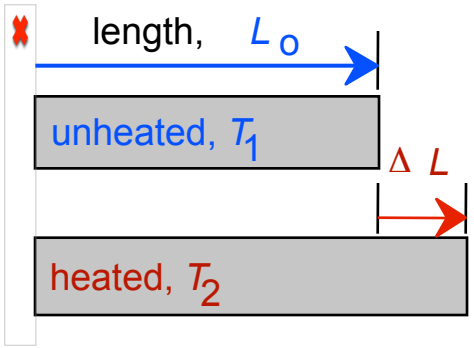

- Melting Temperature, $T_m$




$T_m$ is larger if $E_o$ is larger.

# Properties from bonding: thermal expansion coefficient

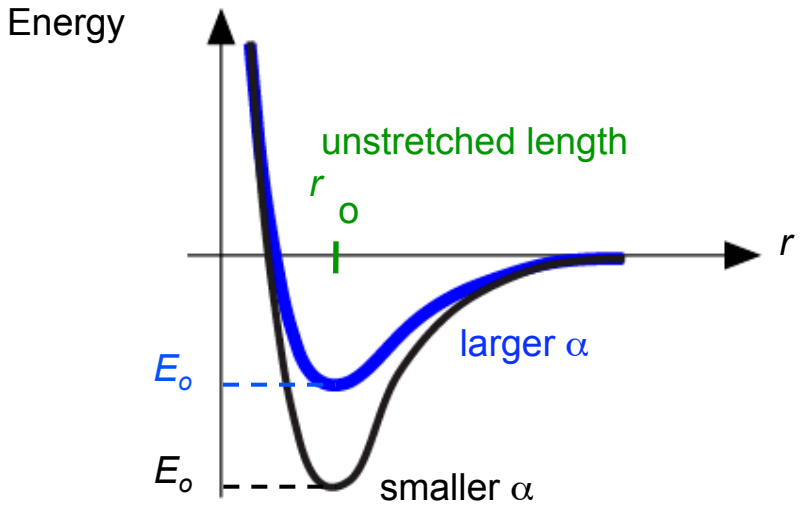
- Coefficient of thermal expansion, $\alpha$




coeff. thermal expansion

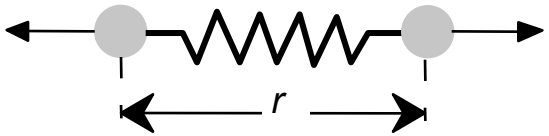
$$\frac{\Delta L}{L_o} = \alpha (T_2 - T_1)$$

- $\alpha$ ~ symmetry at $r_o$

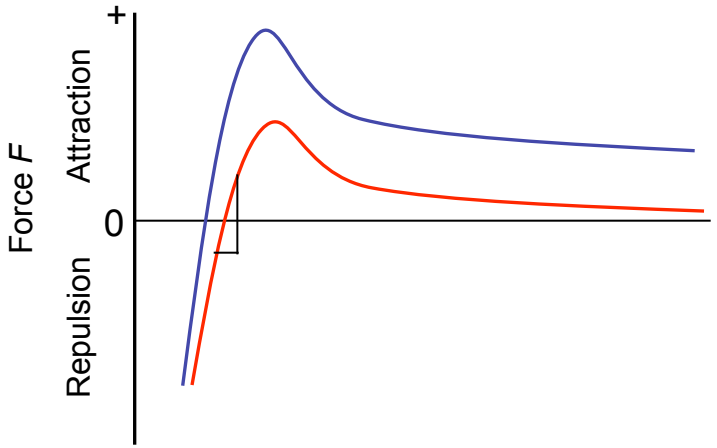



$\alpha$ is larger if $E_o$ is smaller.

# Properties from bonding: modulus *E*

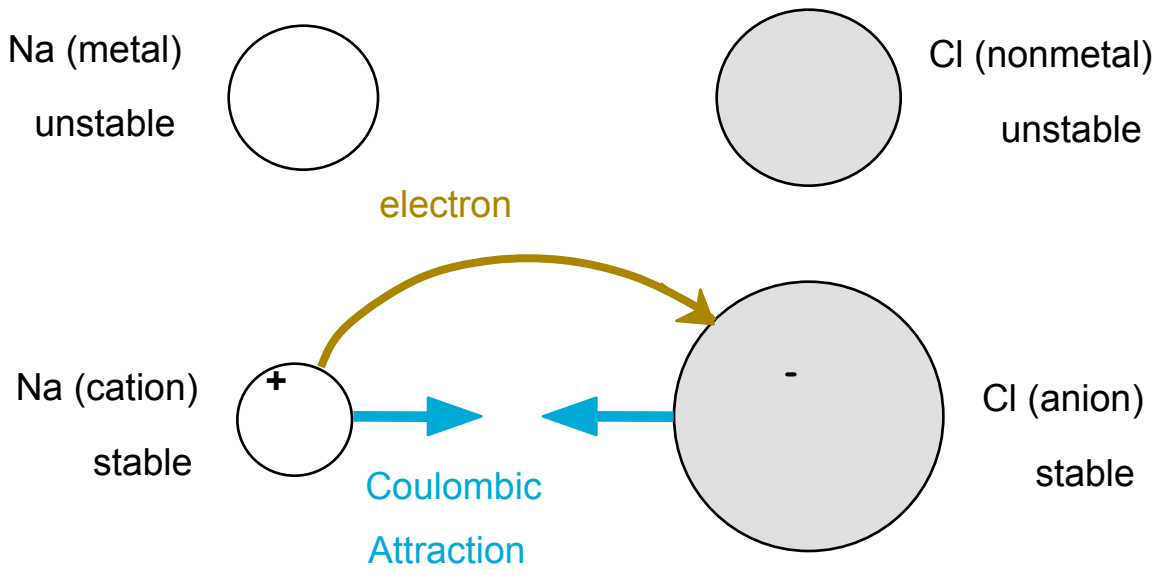



F = kx



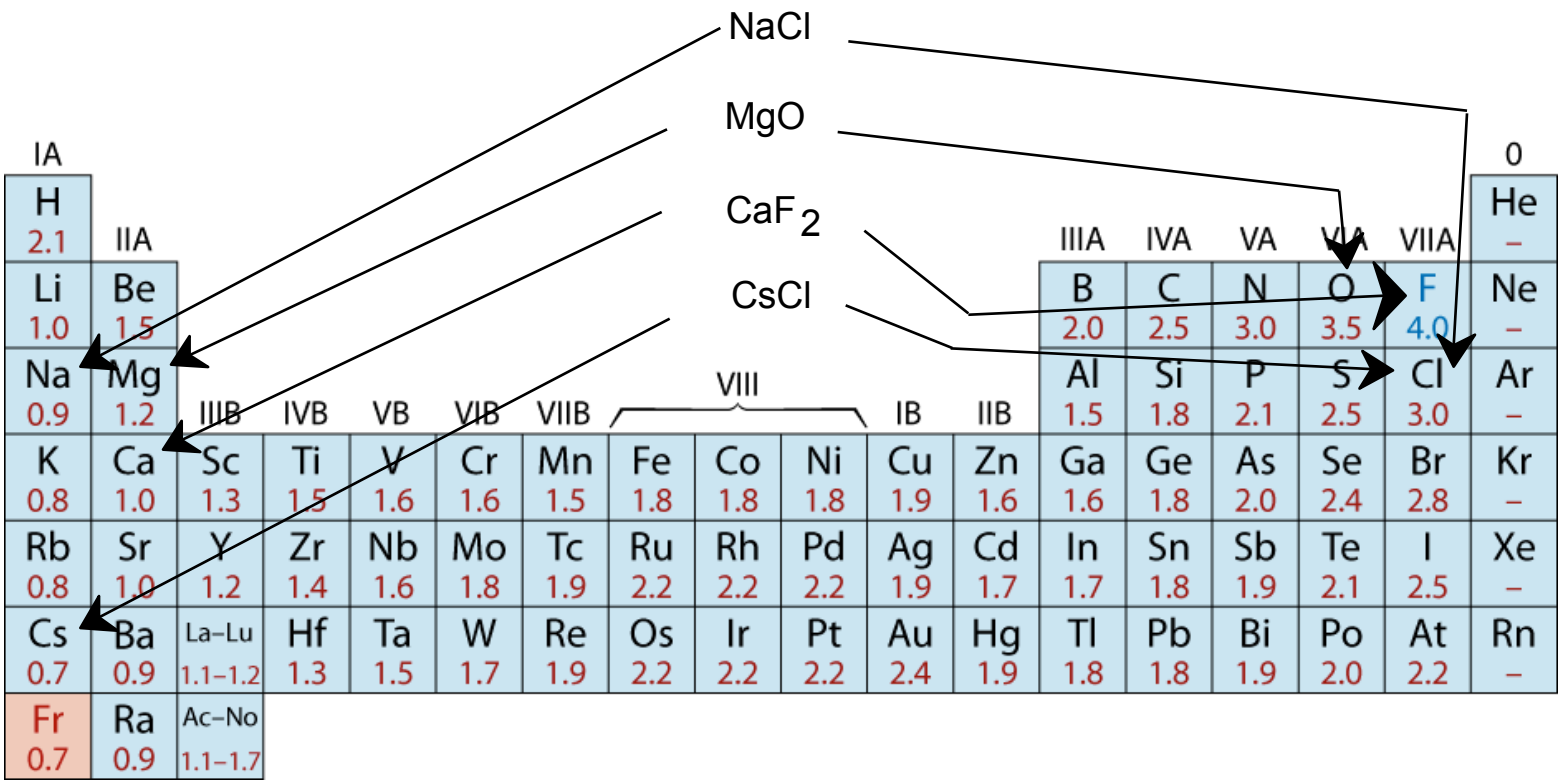
# Types of bonding: ionic

- Occurs between + and - ions.
- Requires electron transfer.
- Large difference in electronegativity required.
- Example:  NaCl



# Examples of ionic bonding

- Predominant bonding in Ceramics




Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

# Covalent bonding

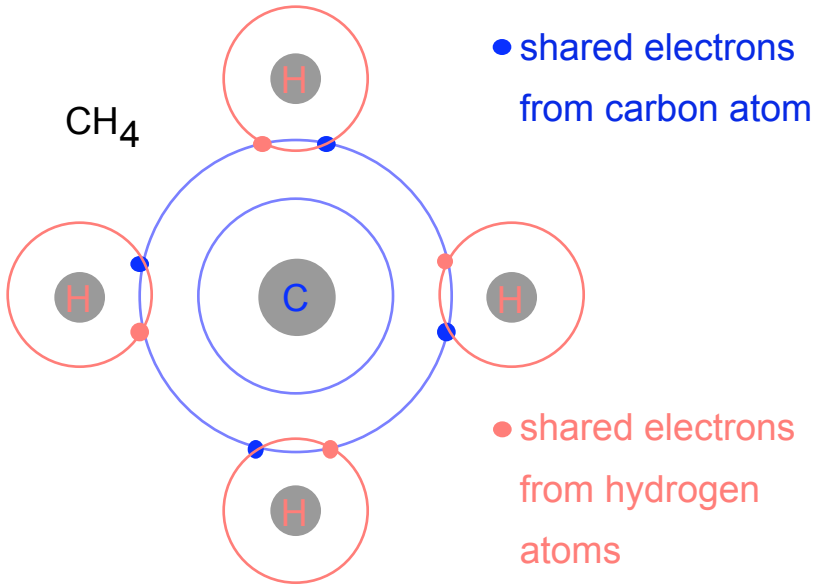
- similar electronegativity ∴ share electrons
- bonds determined by valence – *s* & *p* orbitals dominate bonding

- Example: $CH_4$

C: has 4 valence $e^-$, needs 4 more

H: has 1 valence $e^-$, needs 1 more

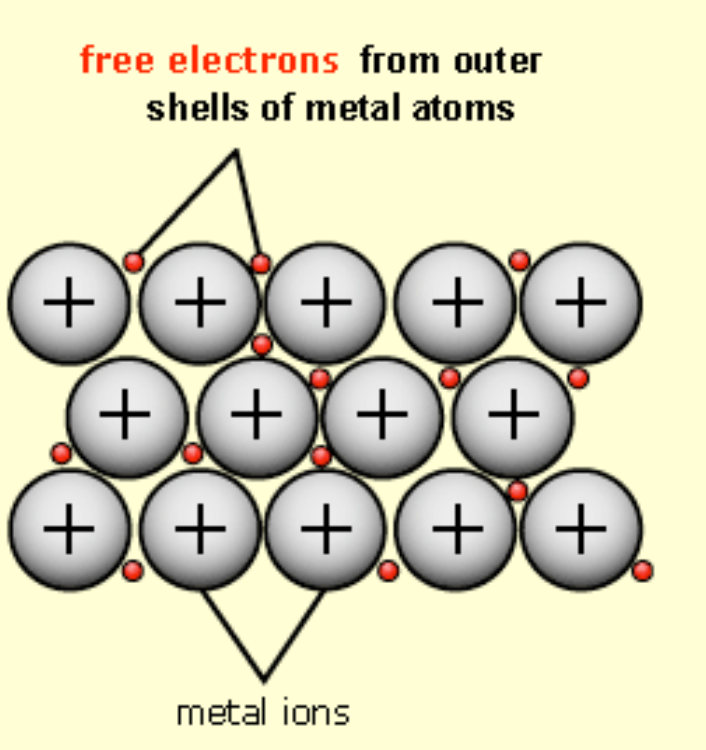
Electronegativities are comparable.




Adapted from Fig. 2.10, *Callister 7e.*

# Metallic bonding

- Ions in a sea of electrons
- Attraction between free electrons and metal ions



# Ionic-covalent mixed bonding

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(X_A - X_B)^2}{4}}\right) \times (100\ \%)$$

where $X_A$ & $X_B$ are Pauling electronegativities

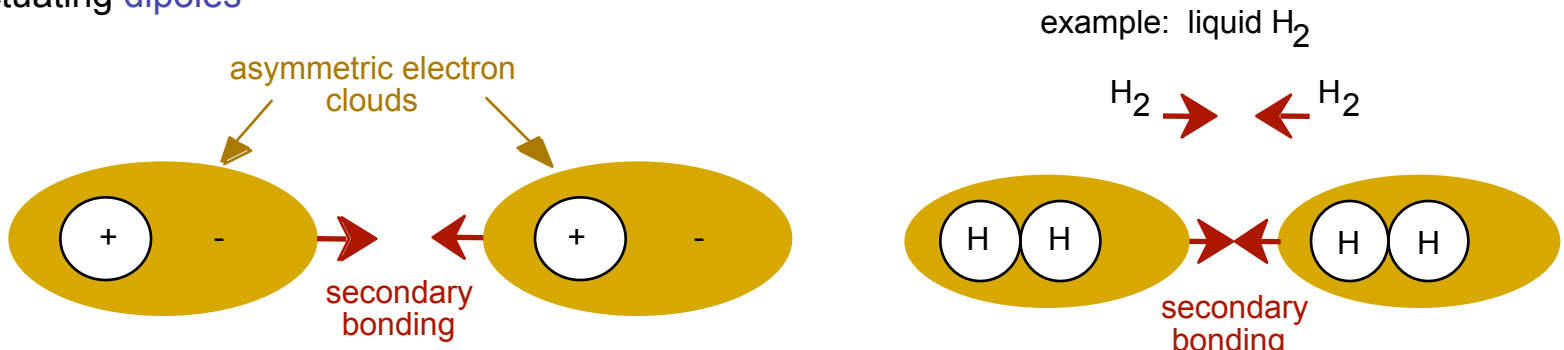
Example: MgO $\quad X_{Mg} = 1.3$, $X_O = 3.5$

$$\% \text{ ionic character} = \left(1 - e^{-\frac{(3.5-1.3)^2}{4}}\right) \times (100\%) = 70.2\% \text{ ionic}$$

# Secondary bonding

Arises from interaction between dipoles

- Fluctuating dipoles

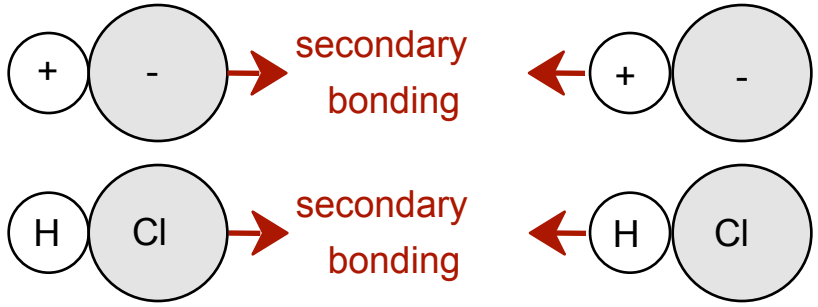



Adapted from Fig. 2.13, *Callister 7e.*

- Permanent dipoles-molecule induced

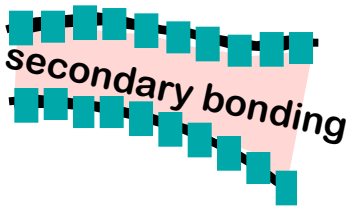
-general case:

-example: liquid HCl




Adapted from Fig. 2.14, *Callister 7e.*

-example: polymer




secondary bonding

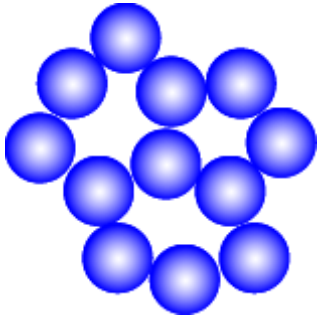
# Summary

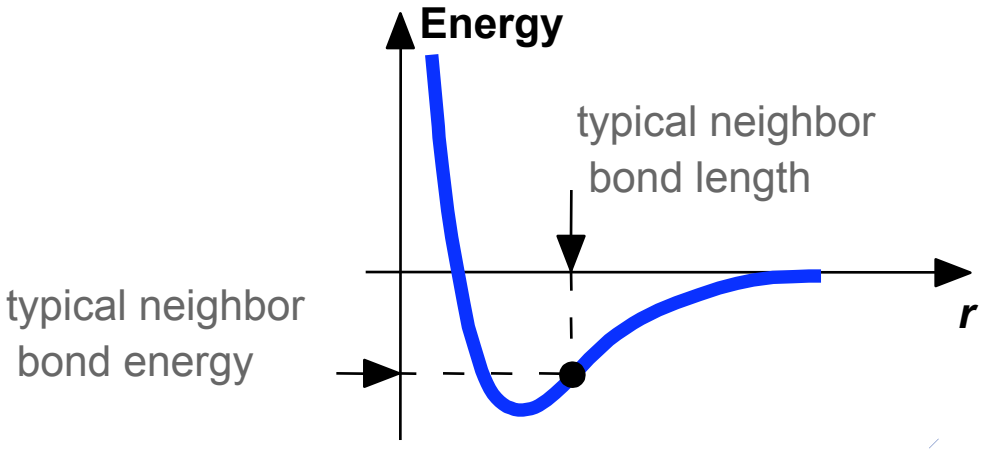
| Type | Bond Energy | Comments |
|---|---|---|
| Ionic | Large! | Non-directional (ceramics) |
| Covalent | Variable<br>Diamond (large)<br>Bismuth (small) | Directional<br>(semiconductors, ceramics, polymer chains) |
| Metallic | Variable<br>Tungsten (large)<br>Mercury (small) | Non-directional (metals) |
| Secondary | Smallest | Directional<br>Interchain (polymer)<br>Intermolecular |

| | |
|---|---|
| Ceramics<br>(Ionic & covalent bonding) | Large bond energy<br>Large $T_m$ and E, small $\alpha$ |
| Metals<br>(Metallic bonding) | Variable bond energy<br>Moderate $T_m$, E, and $\alpha$ |
| Polymers<br>(Covalent & secondary) | Directional properties,<br>Secondary bonding dominates<br>Small $T_m$ and E, large $\alpha$ |

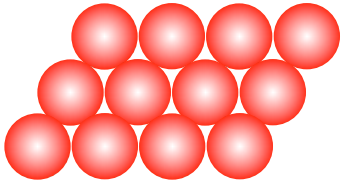
# Energy and packing

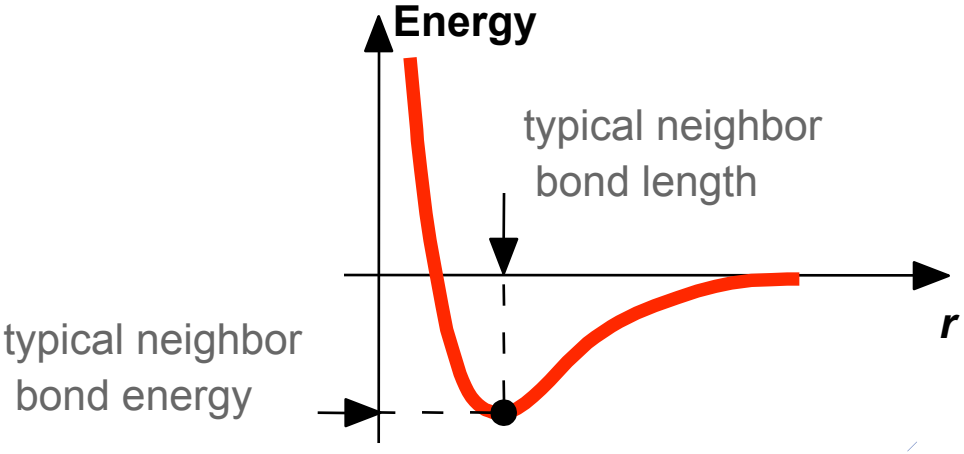
- Non dense, random packing






- Dense, ordered packing



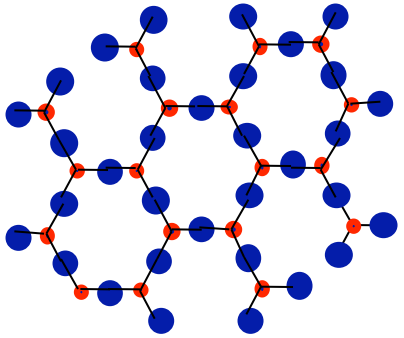



Dense, ordered packed structures tend to have lower energies.

# Materials and packing

Crystalline materials...

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



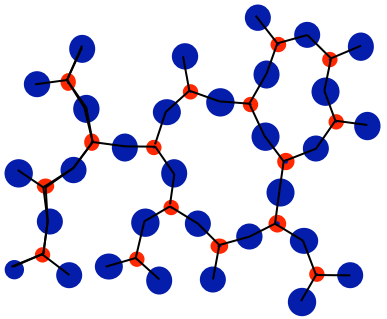
crystalline $SiO_2$

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

● Si ● Oxygen

Noncrystalline materials...

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



noncrystalline $SiO_2$

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

"Amorphous" = Noncrystalline

# Crystals

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

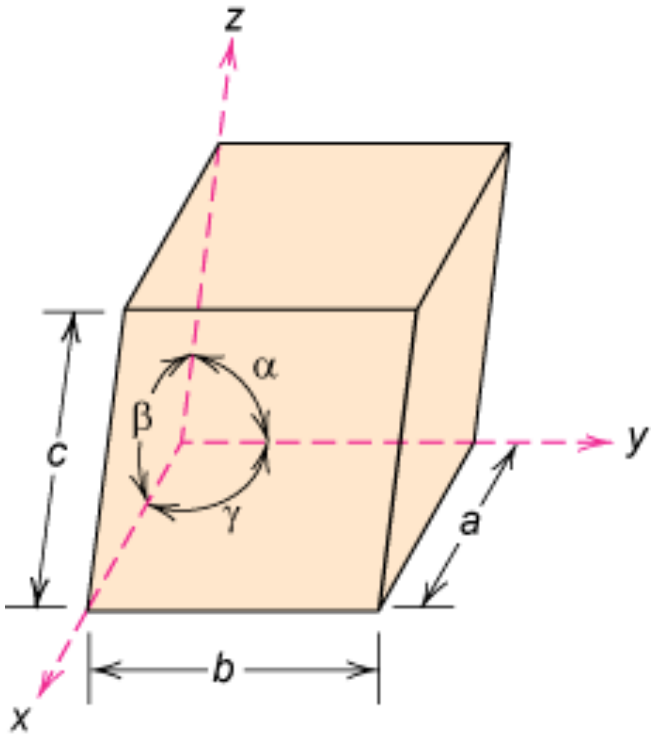



Fig. 3.4, *Callister 7e.*

7 crystal systems

14 crystal lattices

Lattice points: 3D array of points which coincides with atom positions.

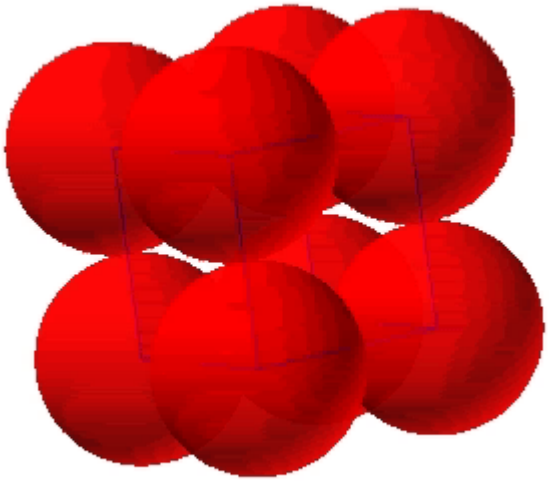
*a, b,* and *c* are the lattice constants

# Simple cubic structure (SC)

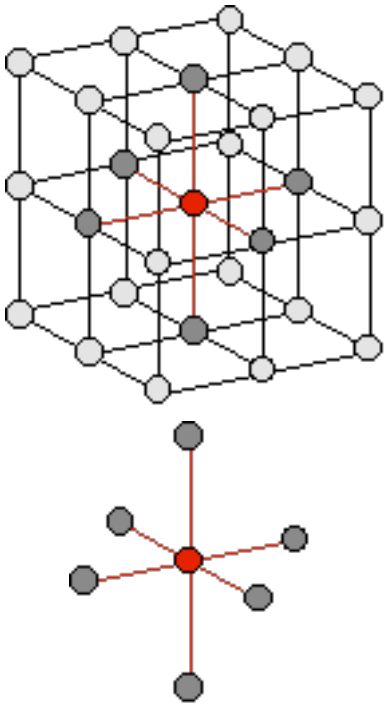
- Rare due to low packing density (only Po has this structure)
- Close-packed directions are cube edges.

- Coordination # = 6
  (# nearest neighbors)

1 atoms/unit cell: 8 corners x 1/8



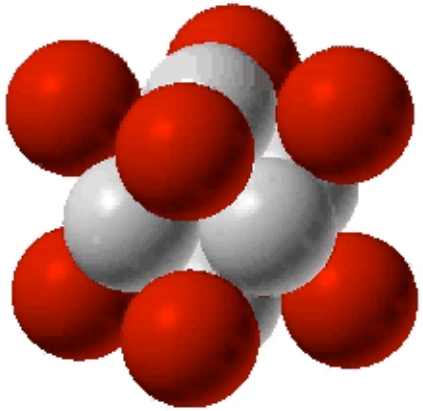
(Courtesy P.M. Anderson)



# Face centered cubic structure (FCC)

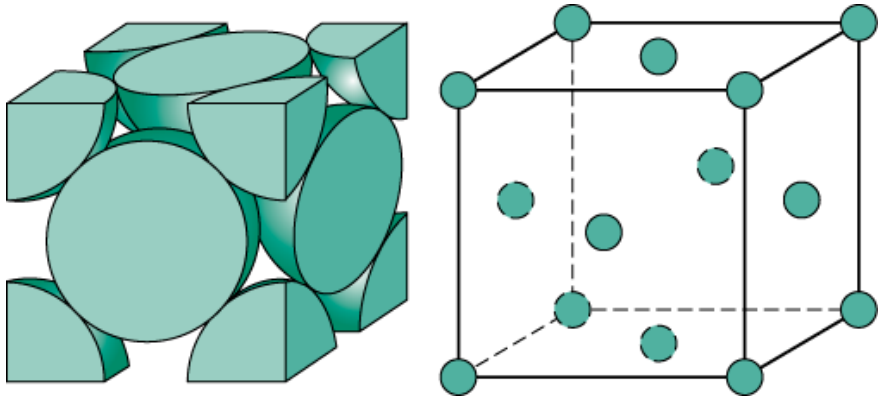
- Atoms touch each other along face diagonals.

  --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

- Coordination # = 12



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

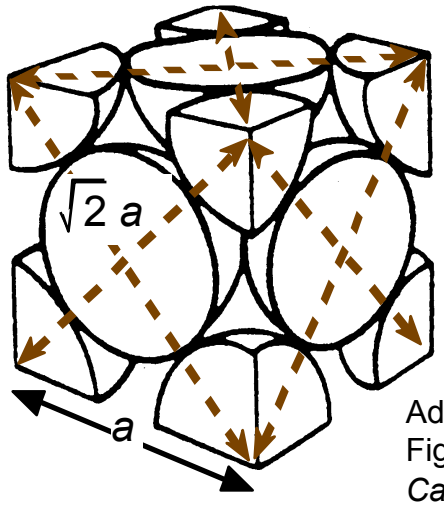
4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

(Courtesy P.M. Anderson)

# Atomic packing factor (APF): FCC

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

*assume hard spheres




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

close-packed directions

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

4 atoms/unit cell

$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} = \frac{4 \cdot \frac{4}{3}\pi R^3}{a^3} \cdot \frac{\text{volume}}{\text{unit cell}}$$

- APF for a FCC structure = 0.74

Maximum achievable APF

# 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
= $6.023 \times 10^{23}$ atoms/mol

Ex: Cu (FCC)

$A$ = 63.54 g/mol

$R$ = 0.128 nm

$n$ = 4

$$\rho = \frac{\dfrac{\text{atoms}}{\text{unit cell}} \cdot 4 \cdot 63.54 \cdot \dfrac{\text{g}}{\text{mol}}}{a^3 \cdot 6.023 \times 10^{23} \cdot \dfrac{\text{volume}}{\text{unit cell}} \cdot \dfrac{\text{atoms}}{\text{mol}}}$$

$a = 2R\sqrt{2}$

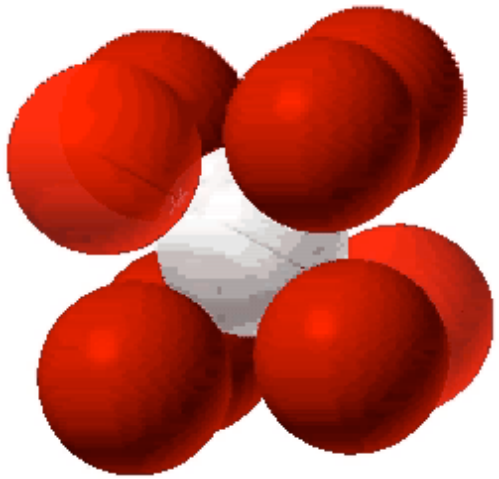
$\rho_{theoretical} = 8.9\ g/cm^3$

$\rho_{actual} = 8.94\ g/cm^3$

# Body centered cubic structure (BCC)

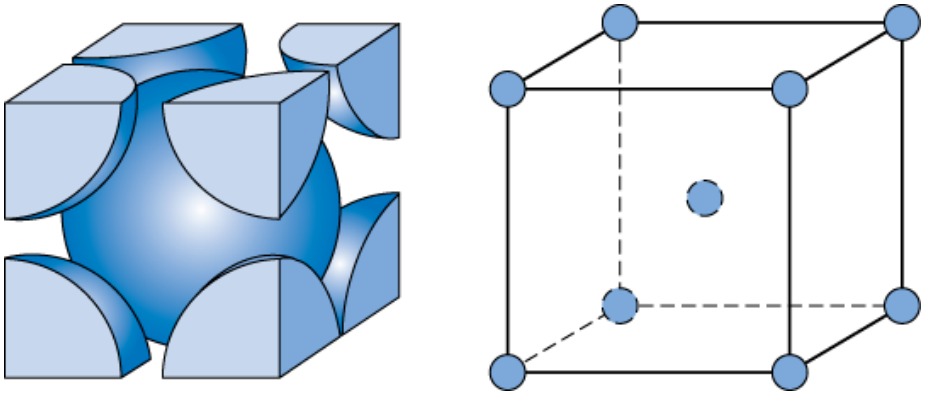
- Atoms touch each other along cube diagonals.

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



(Courtesy P.M. Anderson)

ex: Cr, W, Fe ($\alpha$), Tantalum, Molybdenum

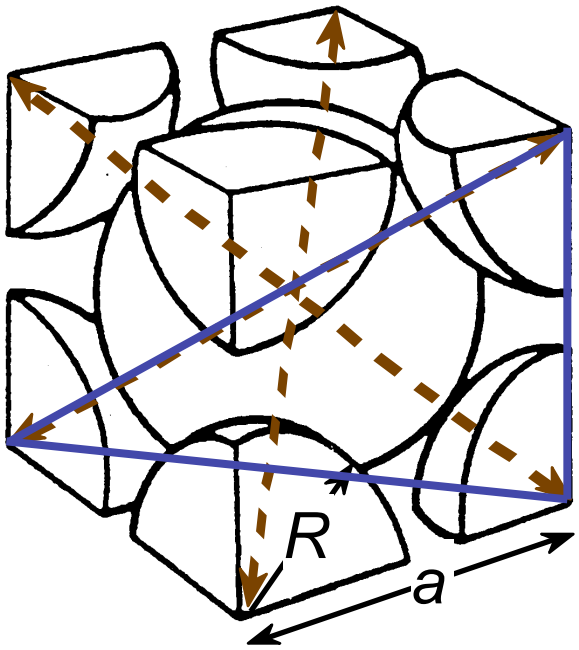


Adapted from Fig. 3.2, *Callister 7e.*

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

- Coordination # = 8

# Atomic packing factor (APF): BCC




$$APF = \frac{\text{atoms}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \Big/ \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{2 \cdot \frac{4}{3}\pi (\sqrt{3}a/4)^3}{a^3}$$

- APF for a FCC structure = 0.68

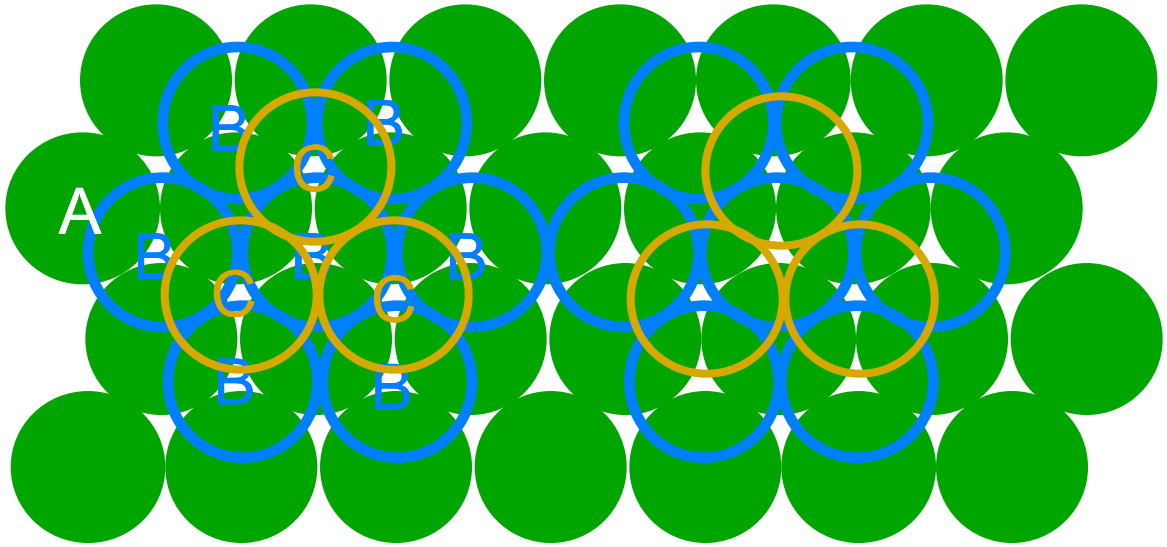
# FCC stacking sequence

- ABCABC... Stacking Sequence
- 2D Projection

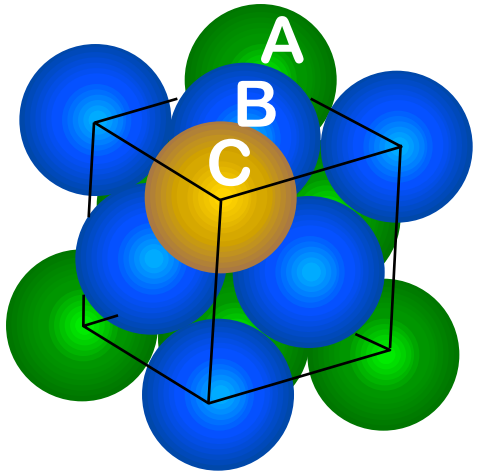
A sites

B sites

C sites



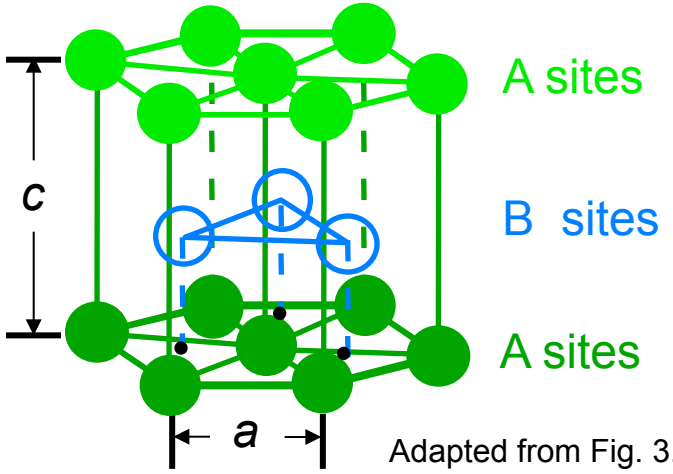

- FCC Unit Cell



# Hexagonal close-packed structure (hcp)

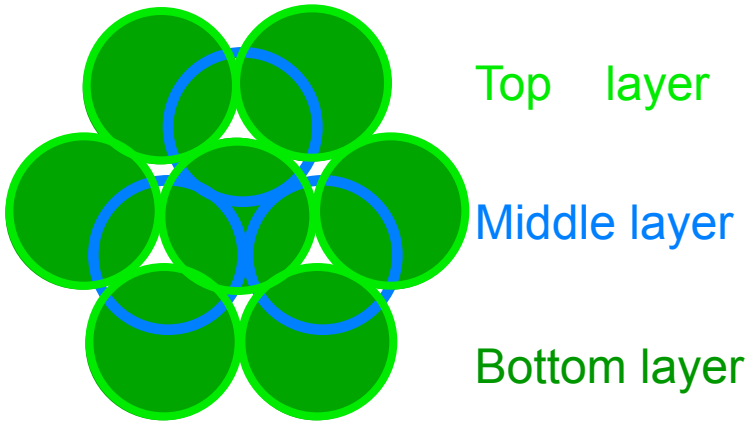
- ABAB... Stacking Sequence

- 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