MSE 170: Introduction to Materials Science and Engineering

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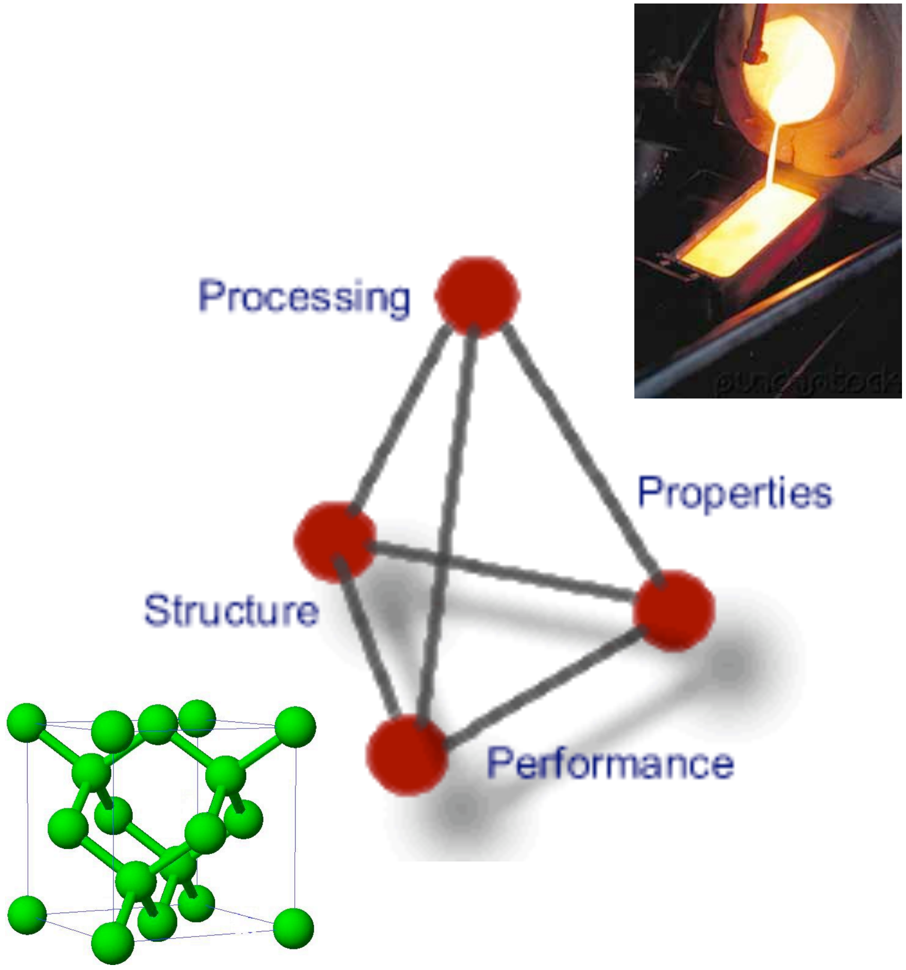
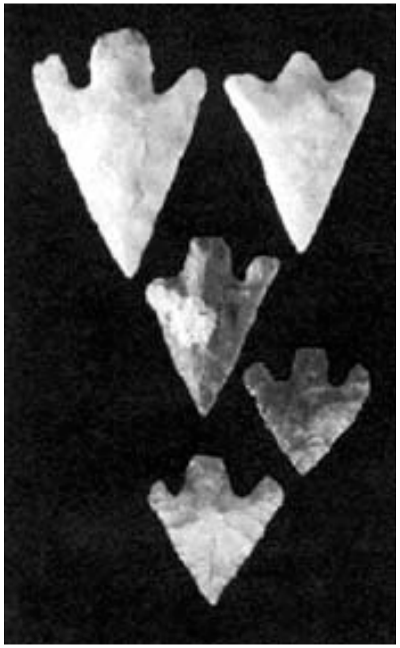
What is Materials Science and Engineering?

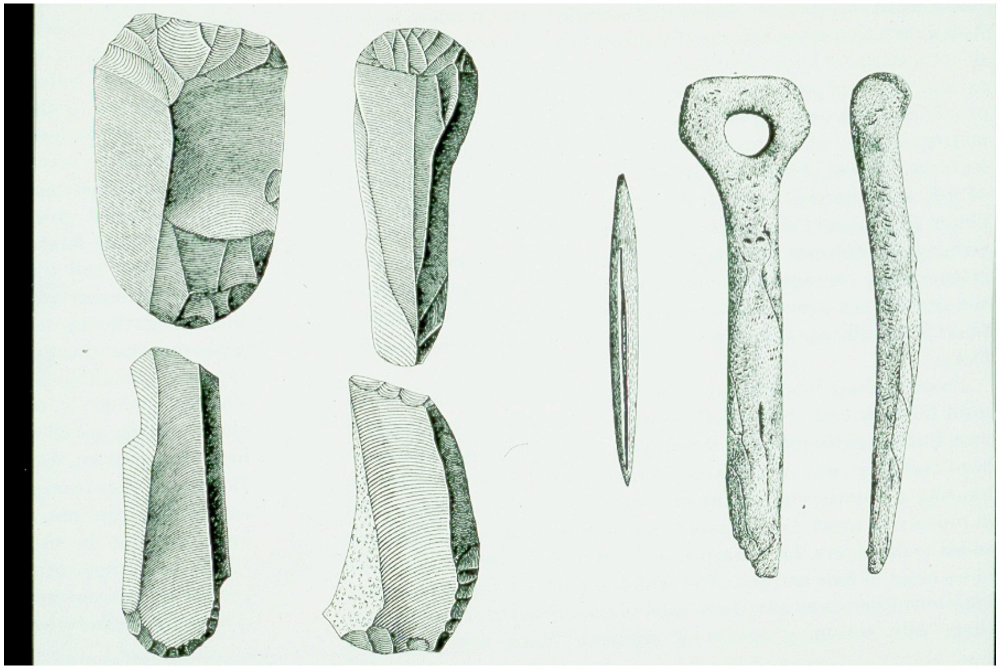


An interdisciplinary field that addresses the fundamental relationships between the Processing, Structure and Properties of materials and develops them for the desired technological application (Performance).

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

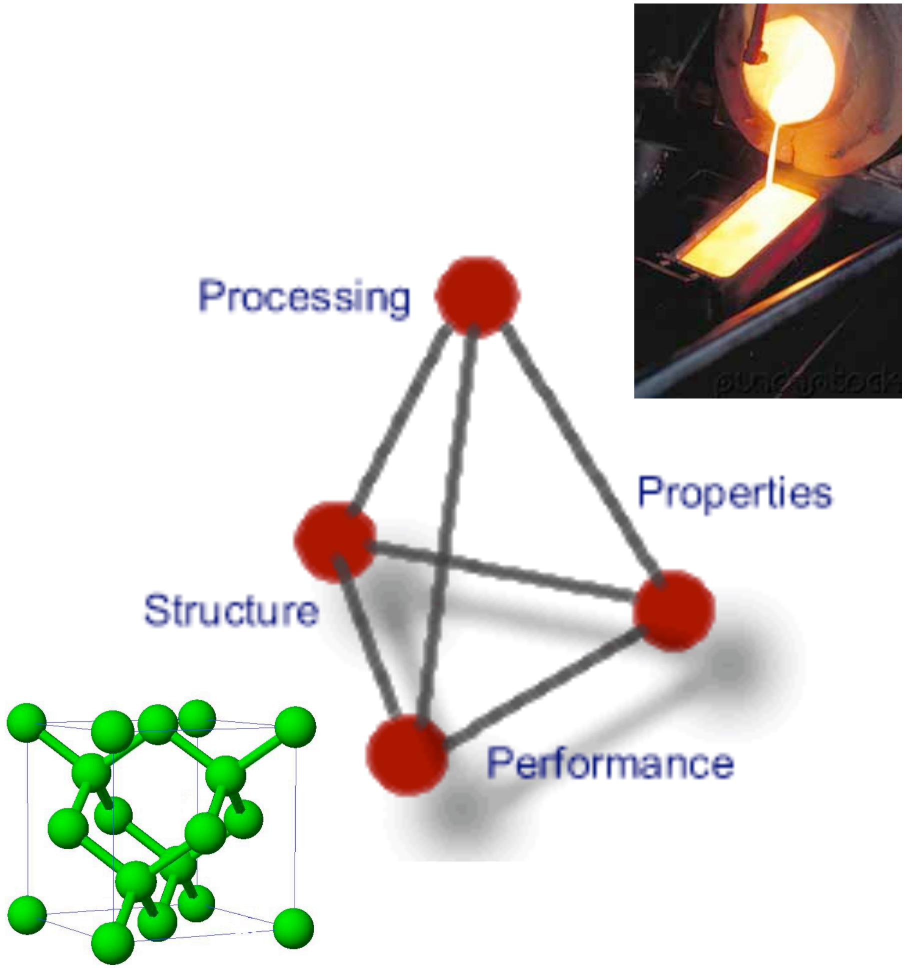
1. **Nanotechnology**
   - Synthesis and characterizations of nanomaterials and nanostructure

2. **Biotechnology**
   - biomimetics and biomaterials

3. **Energy/Environmental**
   - Next generation energy conversion

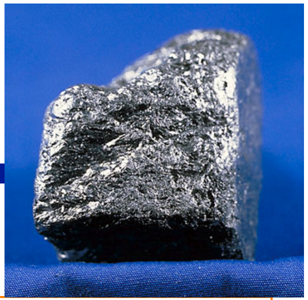
4. **Information Technology**
   - Materials informatics

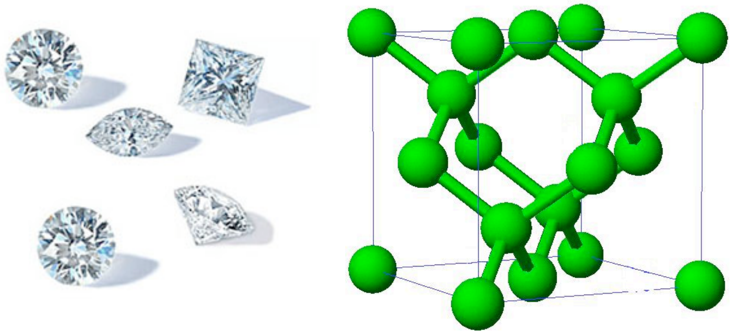
What is Materials Science and Engineering?



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).

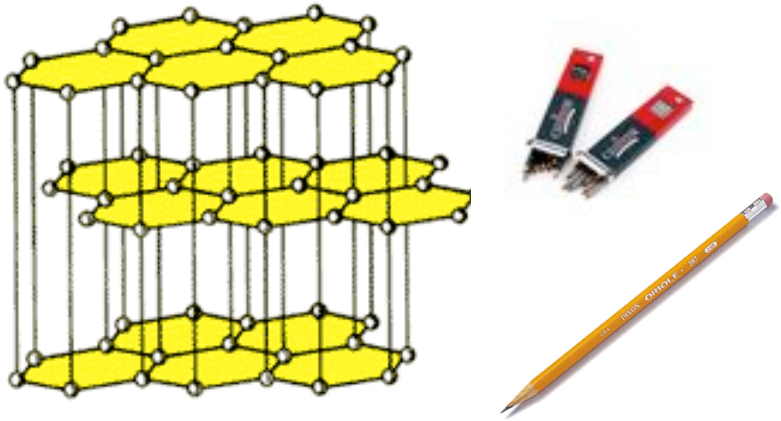
Two Forms of Carbon





Diamond

vs.

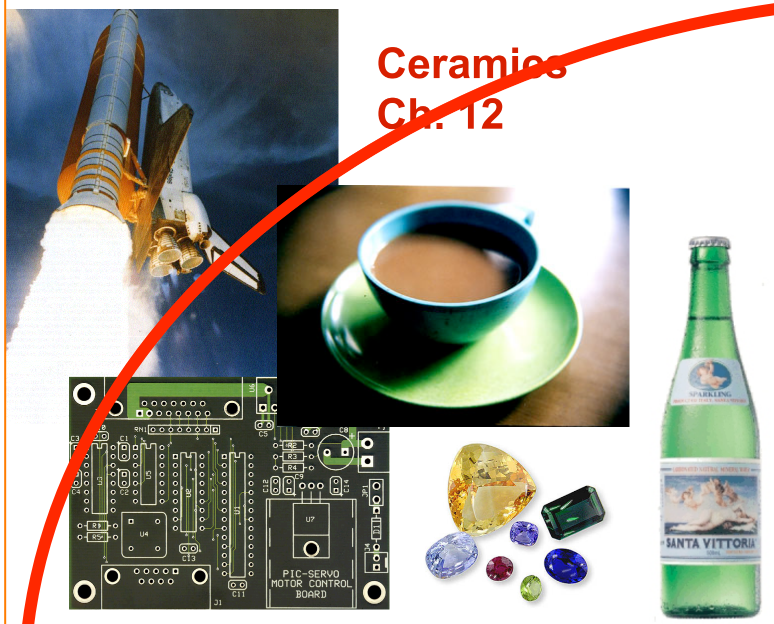


Graphite

- 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



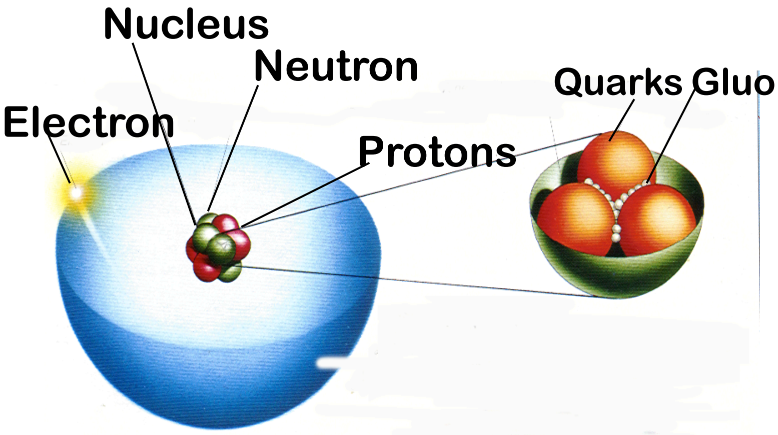
Ceramics
Ch. 12

Polymers
Ch.14 and 15

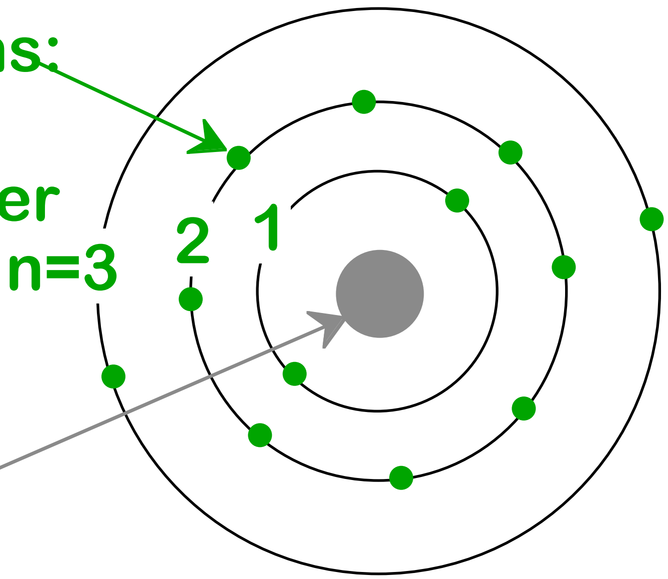
Metals
Ch. 11

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

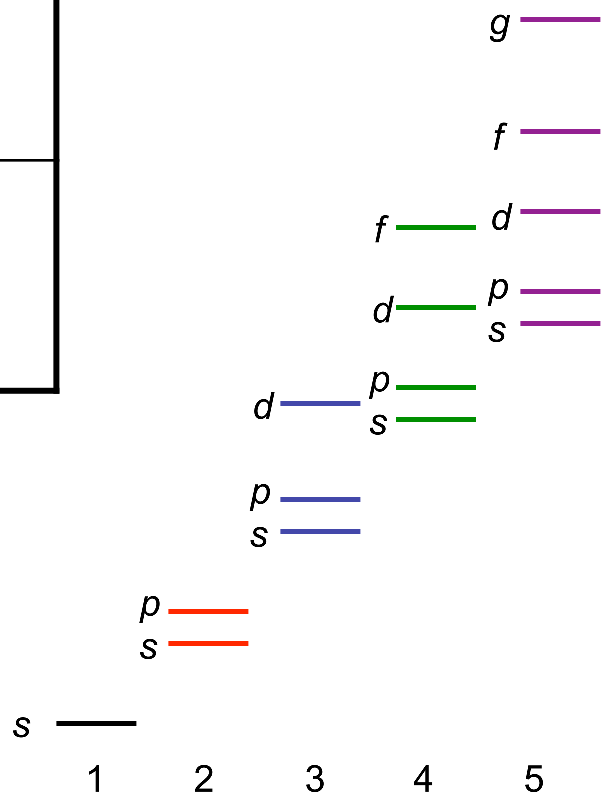
Electrons have wavelike and particulate properties.

- 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

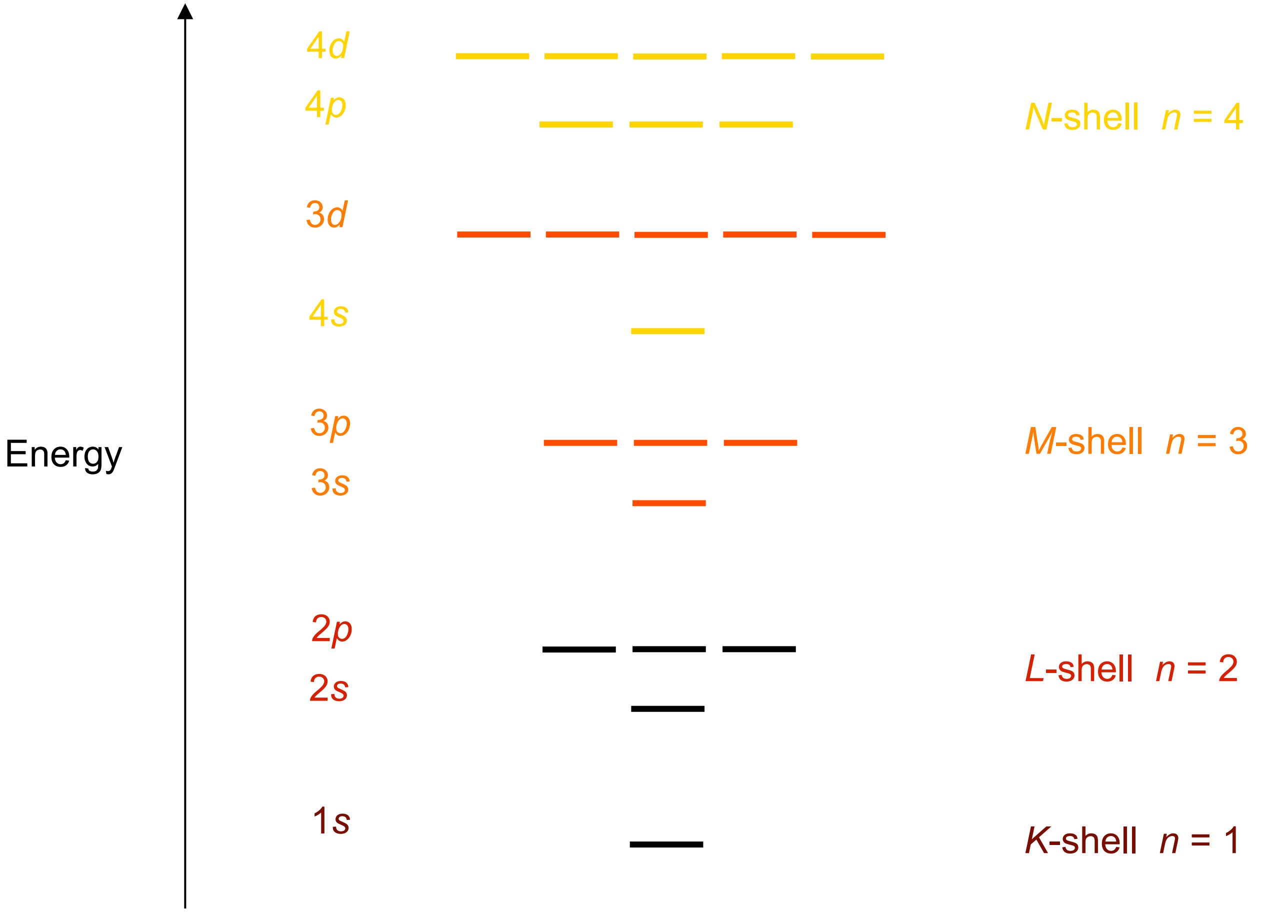
Principal quantum no.	Shell designation	Subshells	No. of states	Number of electrons	
				Per subshell	Per shell
1	*K*	*s*	1	2	2
2	*L*	*s*	1	2	8
		p	3	6	
3	*M*	*s*	1	2	18
		p	3	6	
		d	5	10	
4	*N*	*s*	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	



Electron energy states

Electrons...

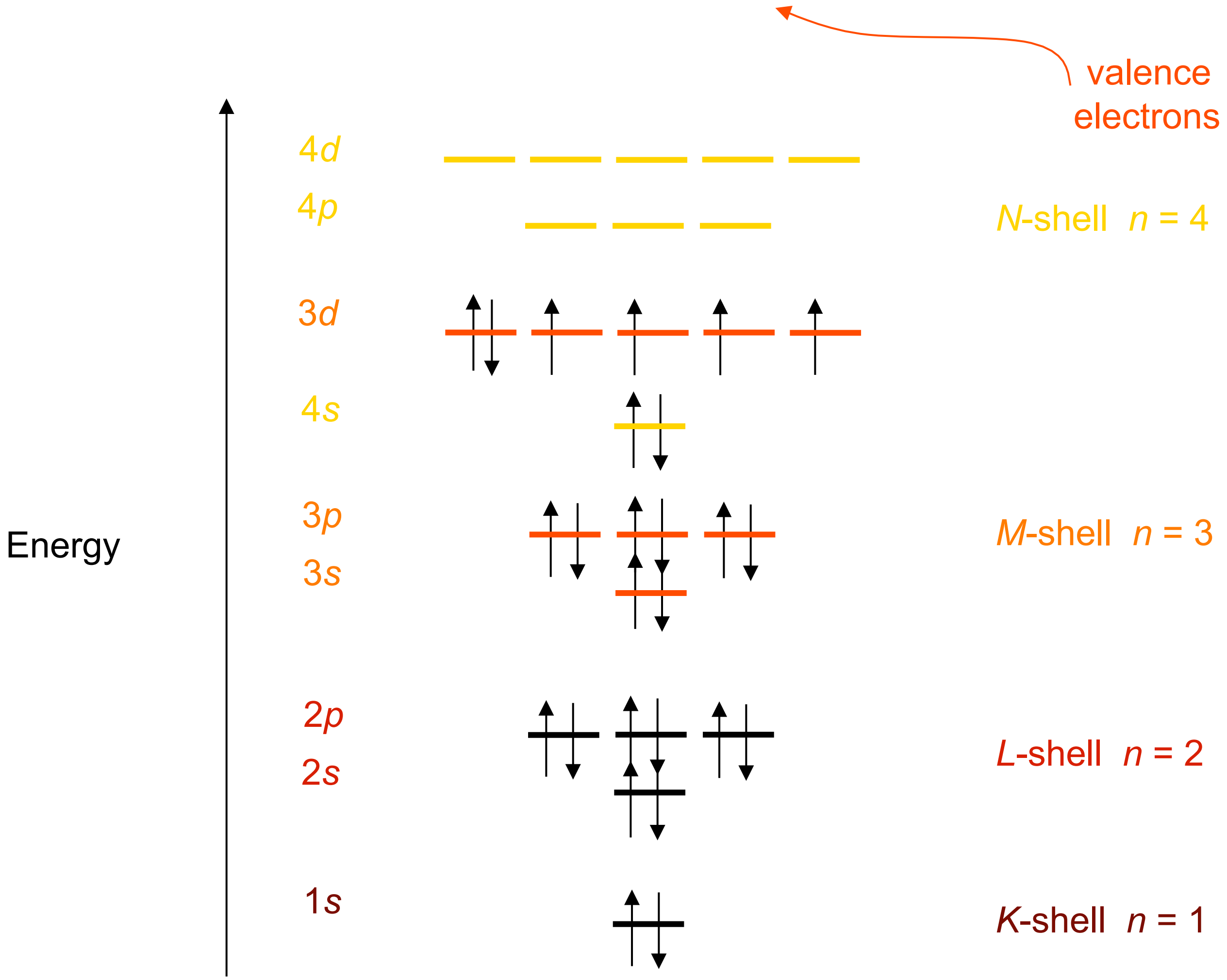
- have discrete energy states
- tend to occupy lowest available energy state.



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

Electronic configuration

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



valence electrons

Energy

4*d*

4*p*

N-shell *n* = 4

3*d*

4*s*

3*p*

3*s*

M-shell *n* = 3

2*p*

2*s*

L-shell *n* = 2

1*s*

K-shell *n* = 1

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

Survey of elements

- Most elements: Electron configuration not stable.

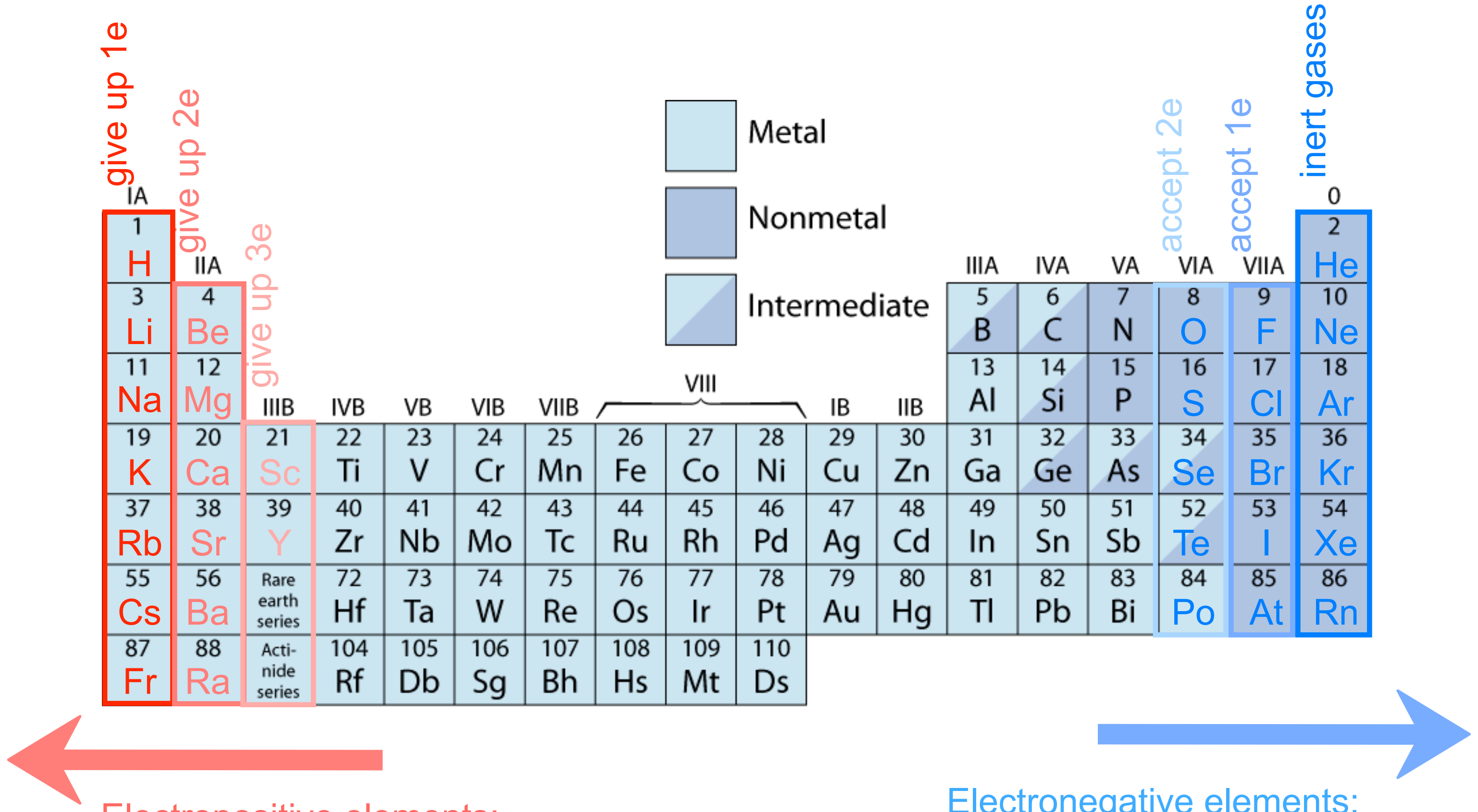
Element	Atomic #	Electron configuration
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...		...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
...		...
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



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	Rare earth series	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	Acti-nide series	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds								

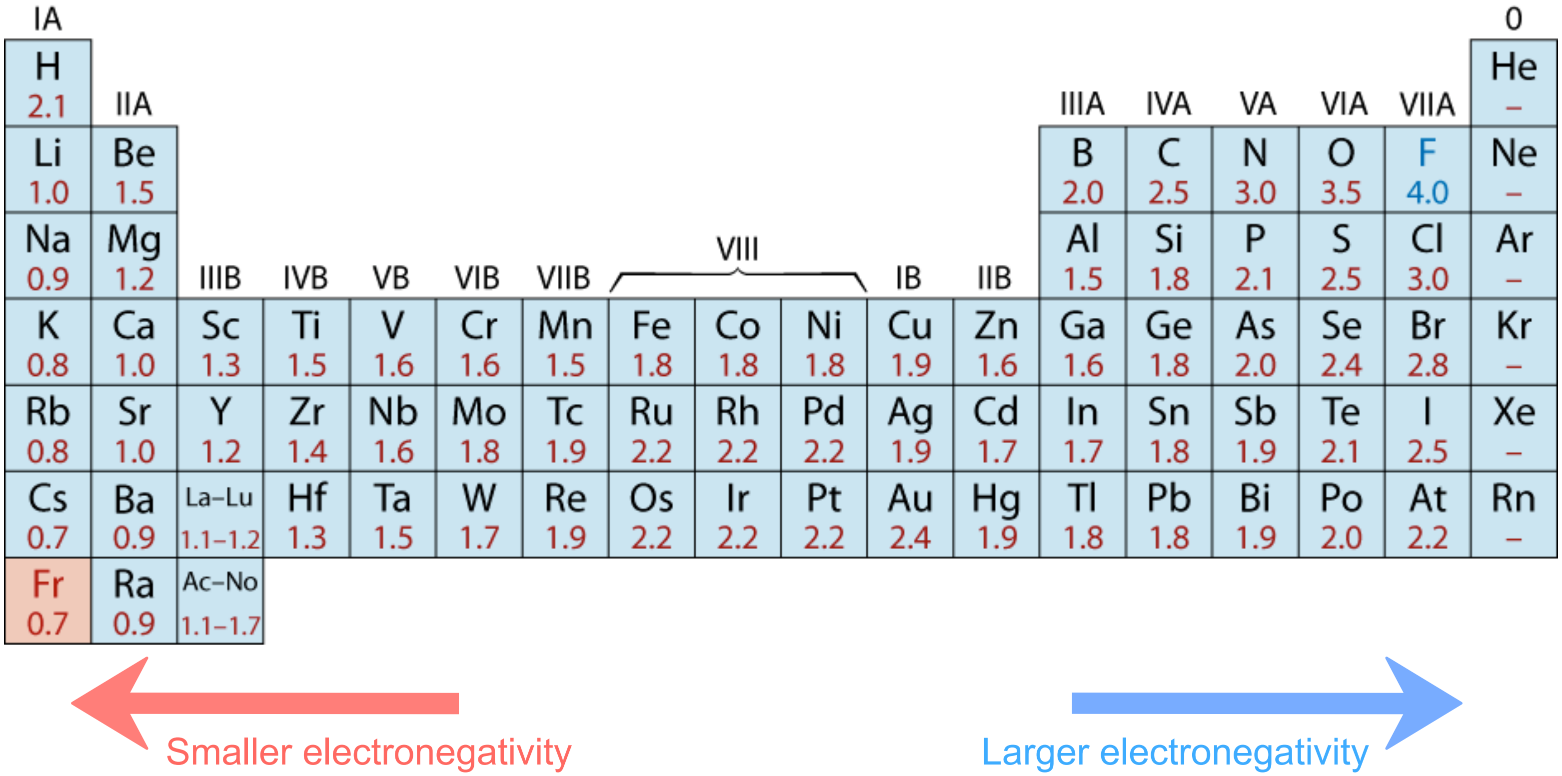
Electropositive elements:
Readily give up electrons
to become + ions.

Electronegative elements:
Readily acquire electrons
to become - ions.

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

Electronegativity

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



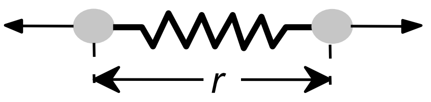
IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Smaller electronegativity

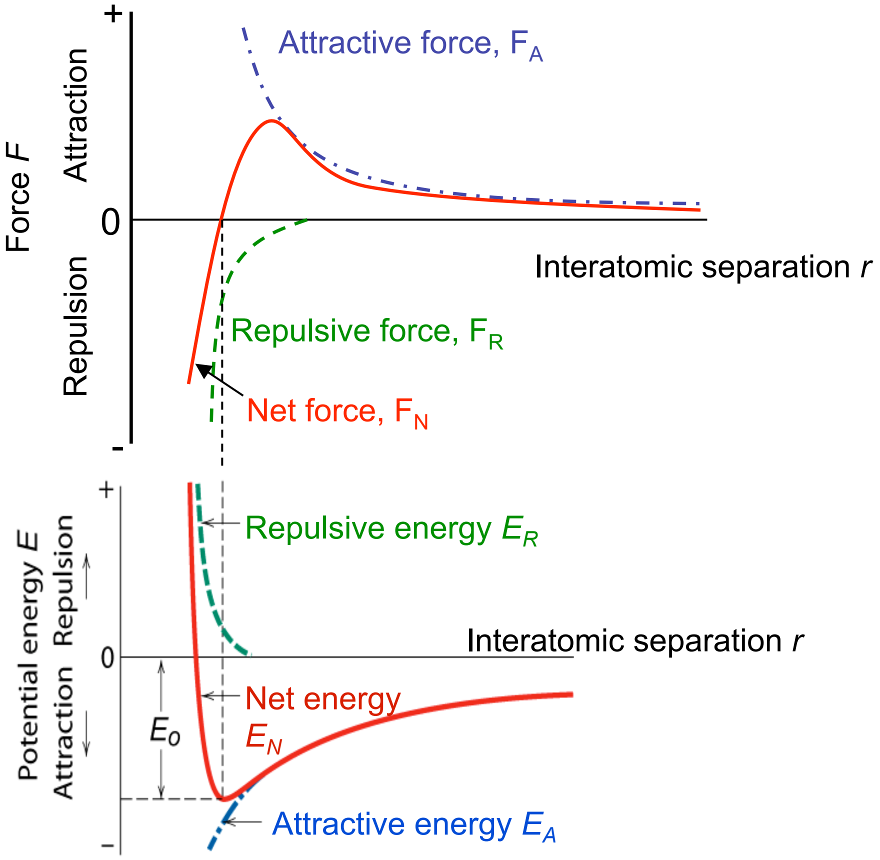
Larger electronegativity

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



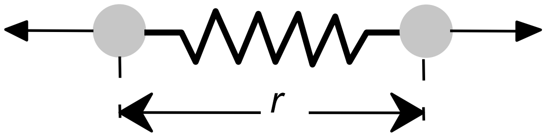
$$E = \int F dr$$

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

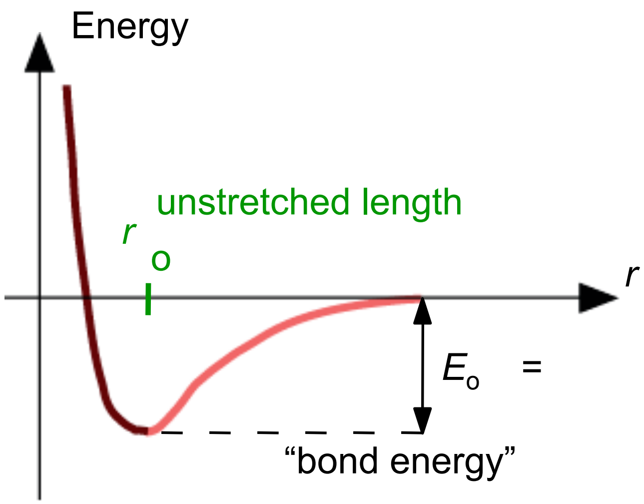
$$= E_A + E_R$$

Properties from bonding

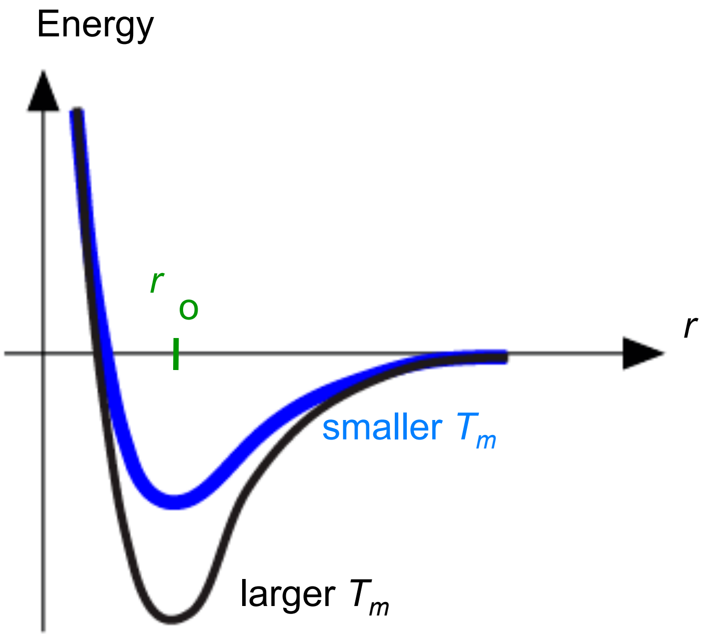
- Bond length, r



- Bond energy, E_o



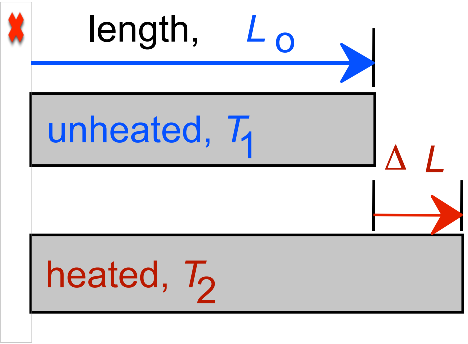
- Melting Temperature, T_m



T_m is larger if E_o is larger.

Properties from bonding: thermal expansion coefficient

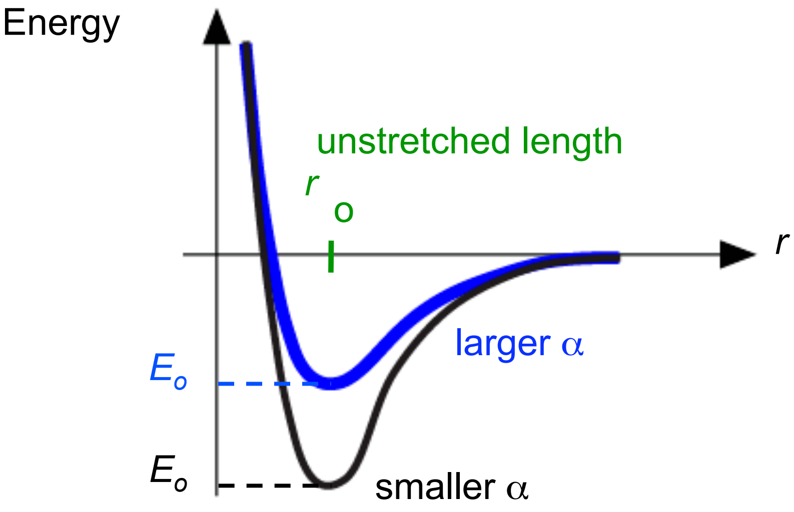
- Coefficient of thermal expansion, α



coeff. thermal expansion

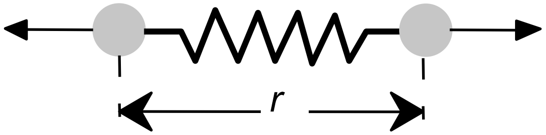
$$\frac{\Delta L}{L_o} = \alpha (T_2 - T_1)$$

- α ~ symmetry at r_o

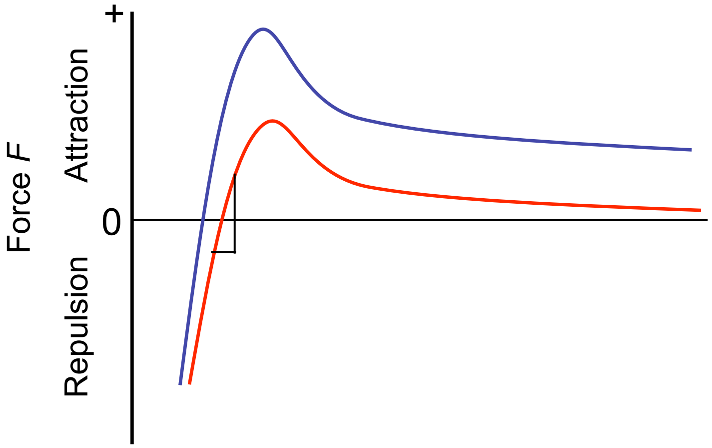


α is larger if E_o is smaller.

Properties from bonding: modulus *E*

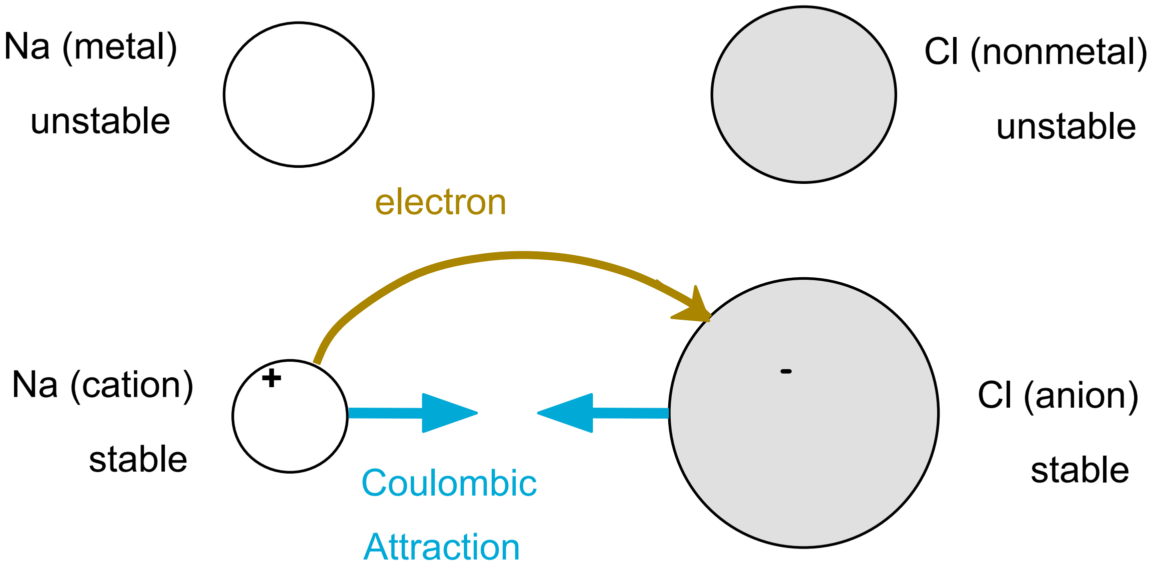


F = kx



Types of bonding: ionic

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



Na (metal)

unstable

Cl (nonmetal)

unstable

electron

Na (cation)

stable

+

-

Cl (anion)

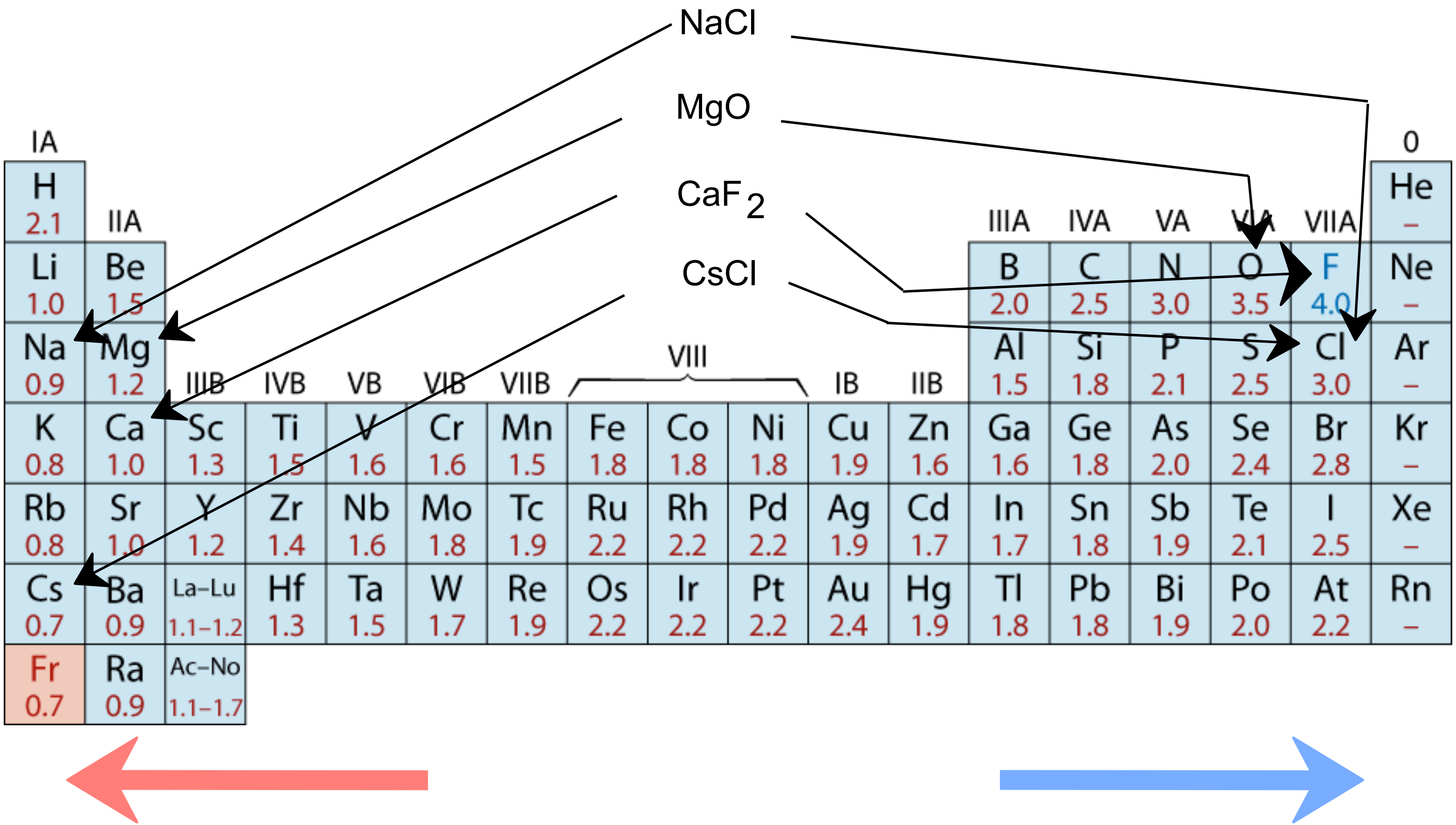
stable

Coulombic

Attraction

Examples of ionic bonding

- Predominant bonding in Ceramics



NaCl

MgO

CaF_2

CsCl

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	La–Lu 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9	Ac–No 1.1–1.7															

Give up electrons

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.

Covalent bonding

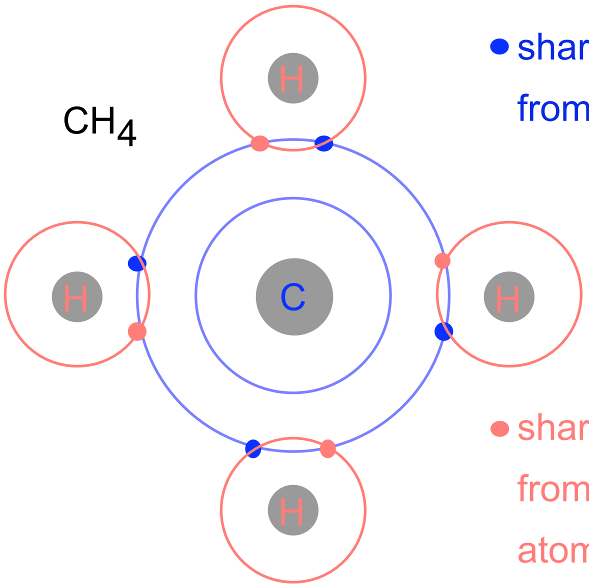
- similar electronegativity ∴ share electrons
- bonds determined by valence – *s* & *p* orbitals dominate bonding

- Example: CH_4

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

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

Electronegativities
are comparable.



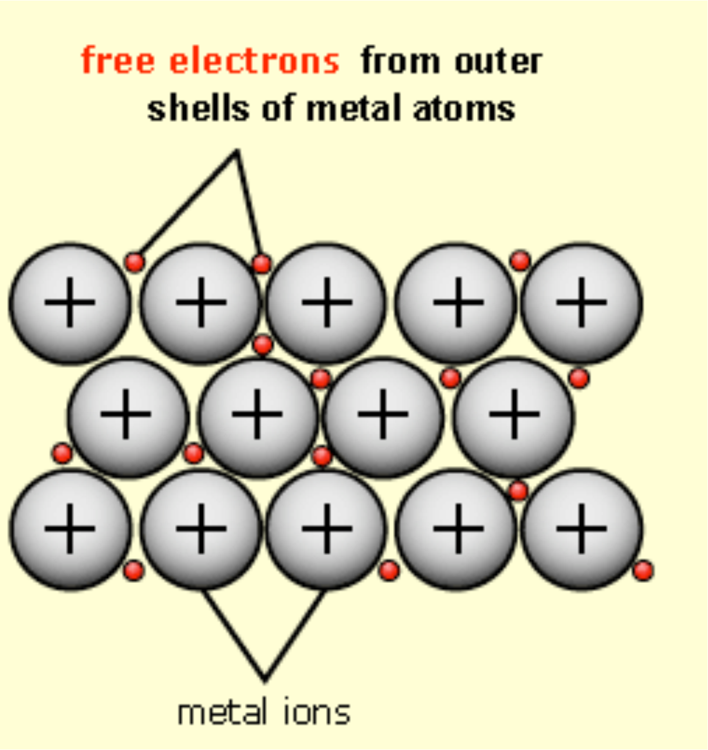
● shared electrons from carbon atom

● shared electrons from hydrogen atoms

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

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

where X_A & X_B are Pauling electronegativities

Example: MgO

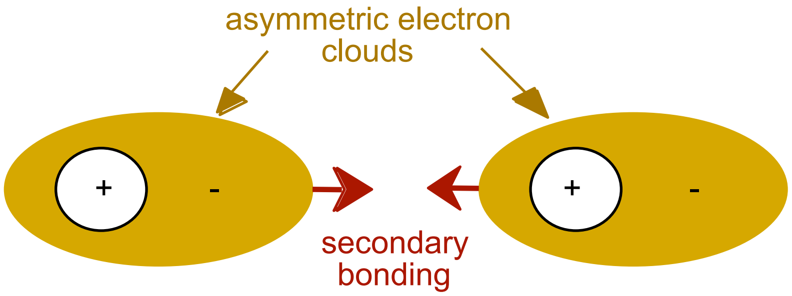
$X_{Mg} = 1.3$
$X_O = 3.5$

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

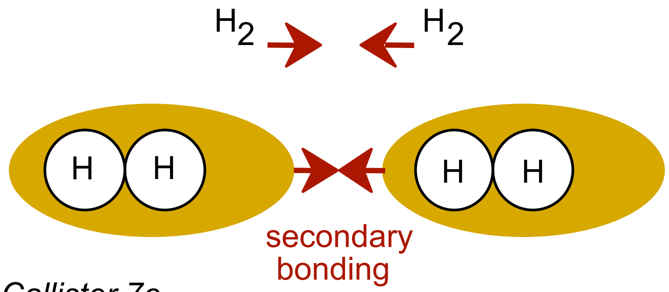
Secondary bonding

Arises from interaction between dipoles

- Fluctuating dipoles



example: liquid H_2

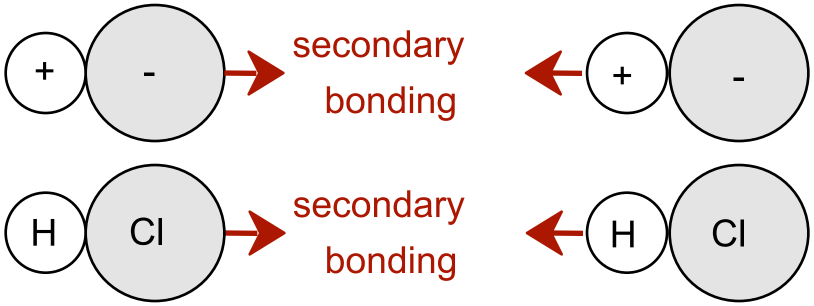


Adapted from Fig. 2.13, *Callister 7e.*

- Permanent dipoles-molecule induced

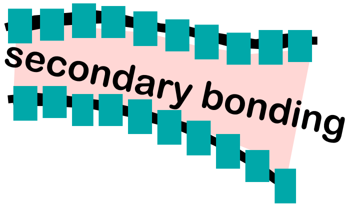
-general case:

-example: liquid HCl



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

-example: polymer



secondary bonding

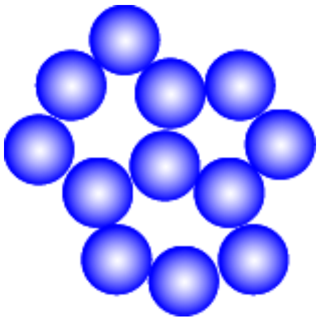
Summary

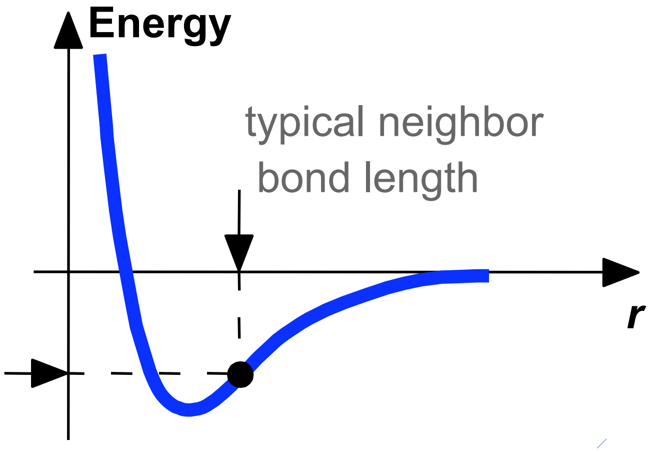
Type	**Bond Energy**	**Comments**
Ionic	Large!	Non-directional (ceramics)
Covalent	Variable Diamond (large) Bismuth (small)	Directional (semiconductors, ceramics, polymer chains)
Metallic	Variable Tungsten (large) Mercury (small)	Non-directional (metals)
Secondary	Smallest	Directional Interchain (polymer)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

Ceramics (Ionic & covalent bonding)	Large bond energy Large T_m and E, small α
Metals (Metallic bonding)	Variable bond energy Moderate T_m, E, and α
Polymers (Covalent & secondary)	Directional properties, Secondary bonding dominates Small T_m and E, large α

Energy and packing

- Non dense, random packing

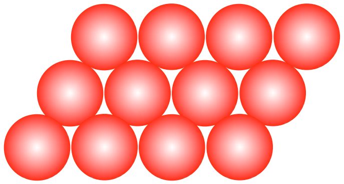


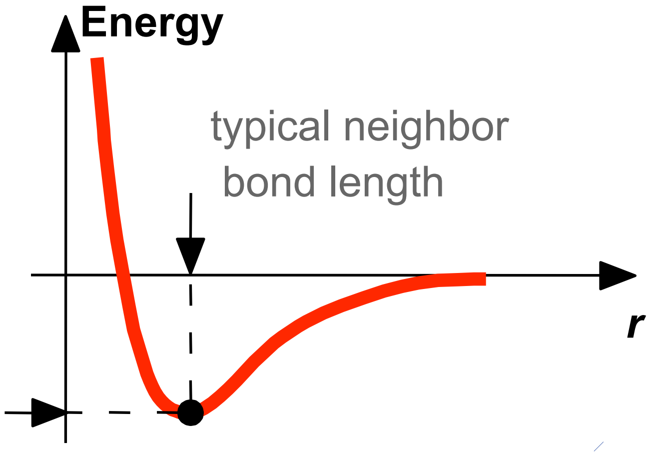


typical neighbor bond length

typical neighbor bond energy

- Dense, ordered packing





typical neighbor bond length

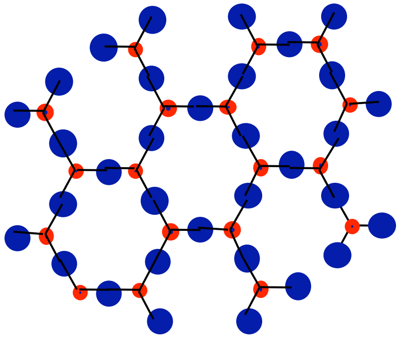
typical neighbor bond energy

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



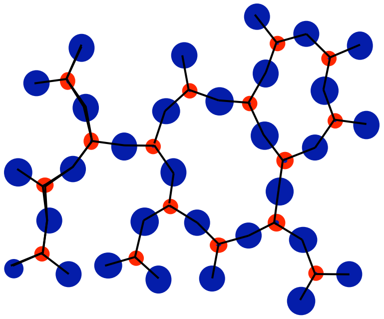
crystalline SiO_2

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.

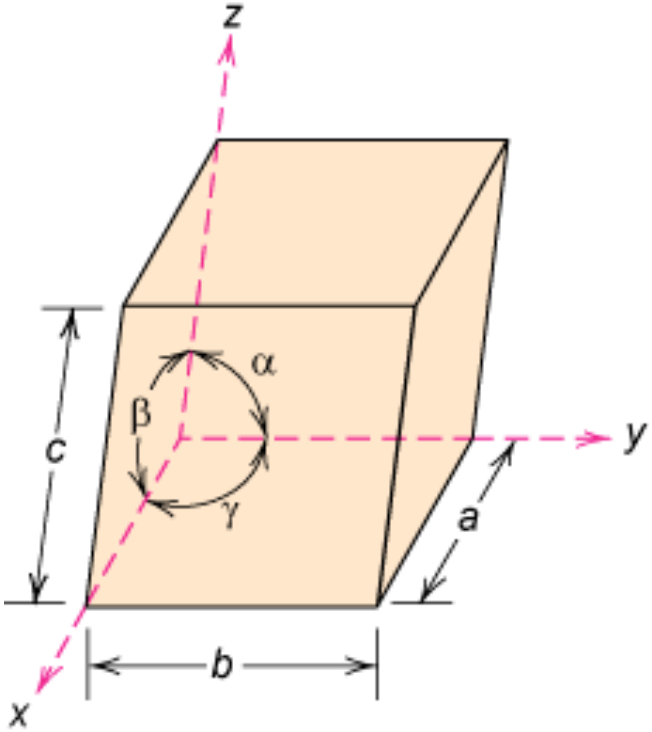


Fig. 3.4, *Callister 7e.*

7 crystal systems

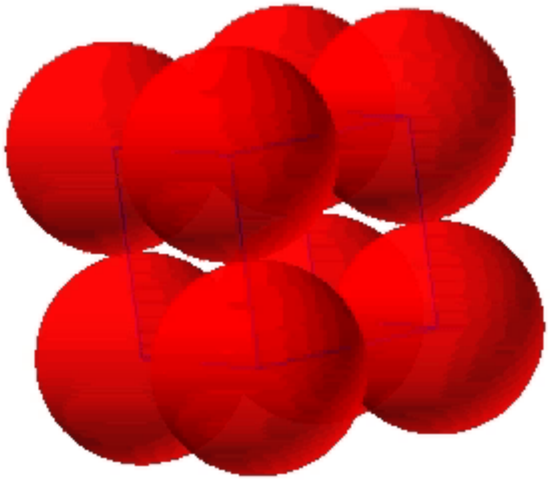
14 crystal lattices

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

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

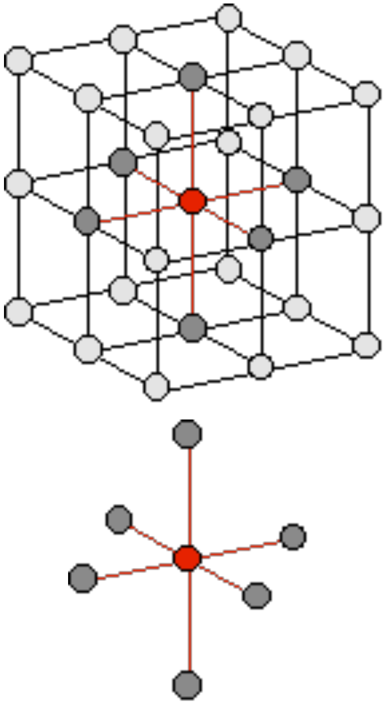
Simple cubic structure (SC)

- 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



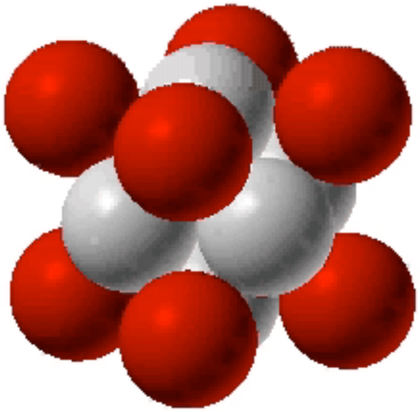
(Courtesy P.M. Anderson)

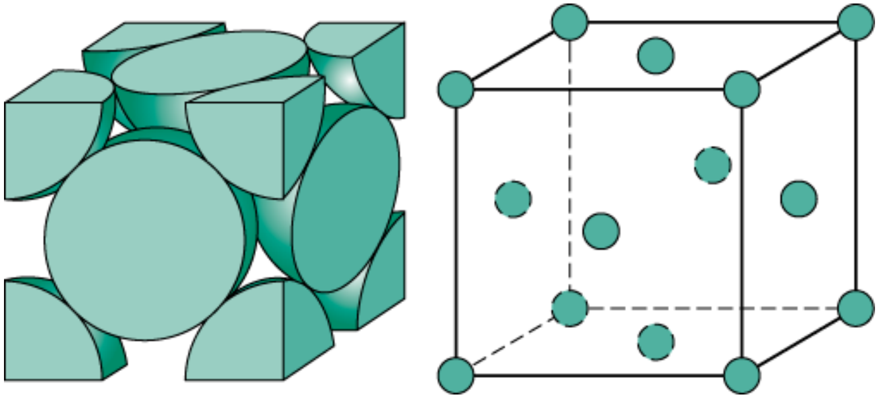
Face centered cubic structure (FCC)

- 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.*

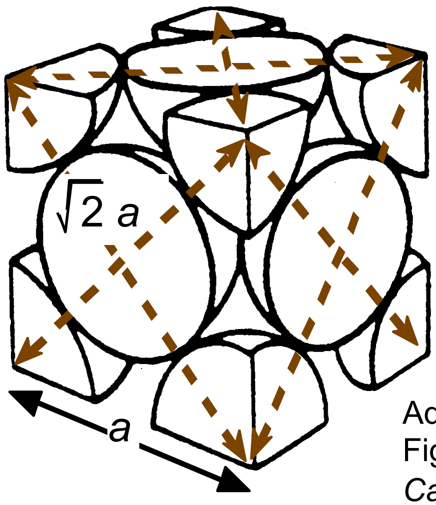
4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8

(Courtesy P.M. Anderson)

Atomic packing factor (APF): FCC

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

*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

$$\text{APF} = \frac{\overbrace{4}^{\frac{\text{atoms}}{\text{unit cell}}}\;\overbrace{\frac{4}{3}\pi R^3}^{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}}$$

- APF for a FCC structure = 0.74

Maximum achievable APF

Theoretical density, ρ

$$\text{Density} = \rho = \frac{\text{Mass of atoms in unit cell}}{\text{Total volume of unit cell}}$$

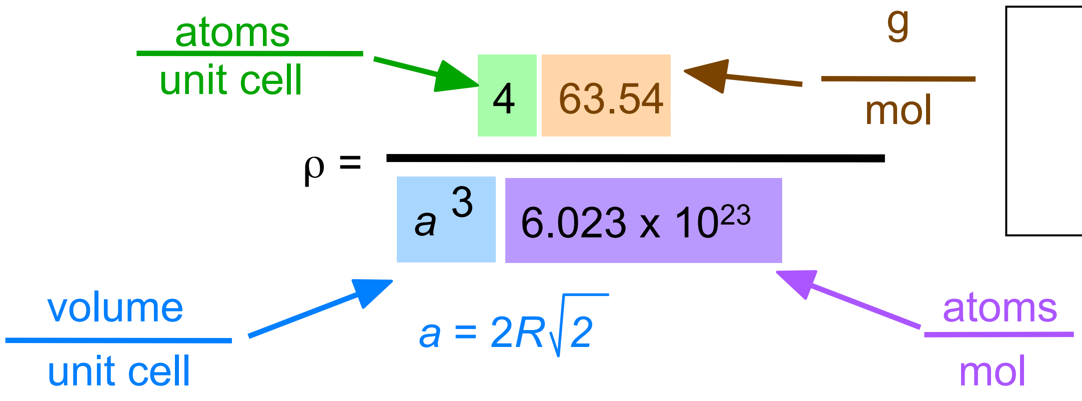
$$\rho = \frac{n\,A}{V_C\,N_A}$$

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
= 6.023×10^{23} atoms/mol

Ex: Cu (FCC)

A = 63.54 g/mol
R = 0.128 nm
n = 4



$$\rho = \frac{4 \quad 63.54}{a^3 \quad 6.023 \times 10^{23}}$$

$\frac{\text{atoms}}{\text{unit cell}}$

$\frac{\text{g}}{\text{mol}}$

$\frac{\text{volume}}{\text{unit cell}}$

$a = 2R\sqrt{2}$

$\frac{\text{atoms}}{\text{mol}}$

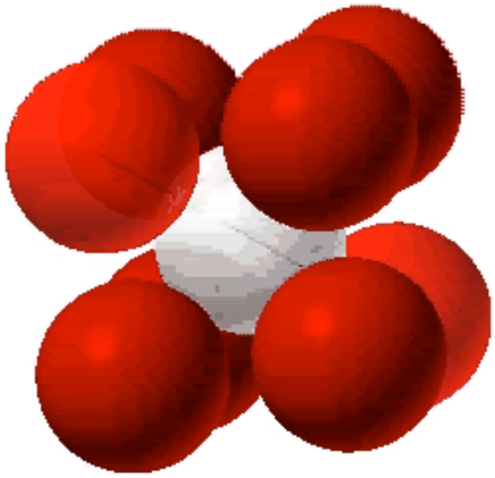
$\rho_{\text{theoretical}}$ = 8.9 g/cm^3

ρ_{actual} = 8.94 g/cm^3

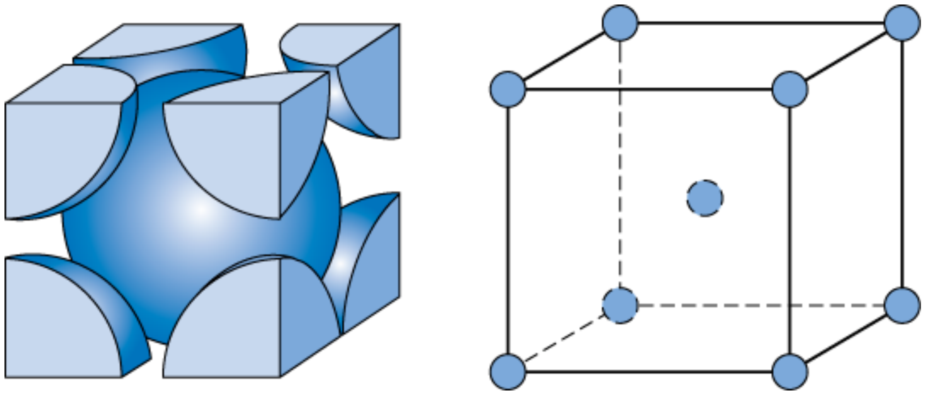
Body centered cubic structure (BCC)

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

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



(Courtesy P.M. Anderson)

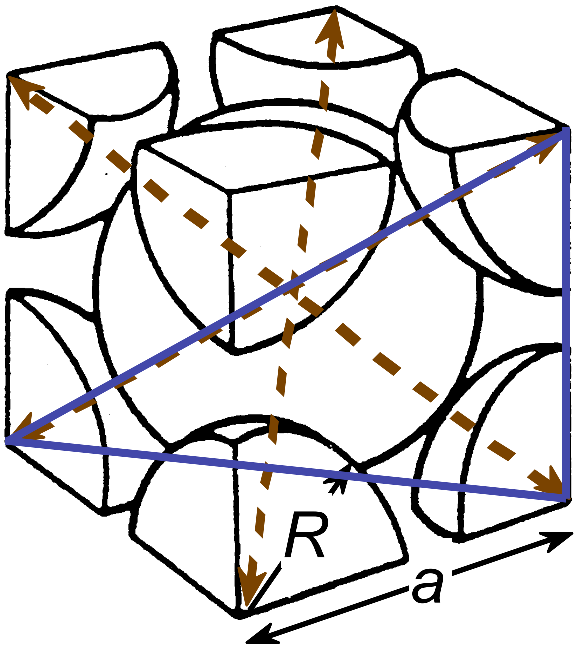


Adapted from Fig. 3.2, *Callister 7e.*

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

- Coordination # = 8

Atomic packing factor (APF): BCC

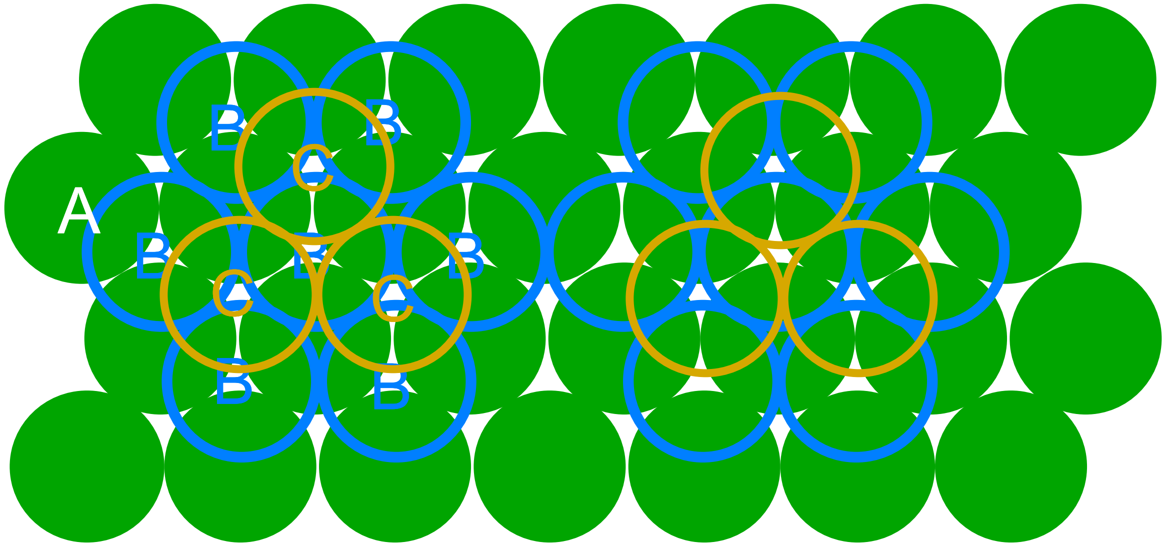


$$\text{APF} = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{2}\;\overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi\,(\sqrt{3}a/4)^{3}}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^{3}}}$$

- APF for a FCC structure = 0.68

FCC stacking sequence

- ABCABC... Stacking Sequence
- 2D Projection

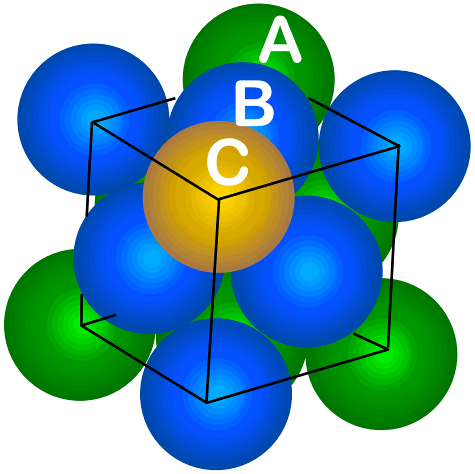


A sites

B sites

C sites

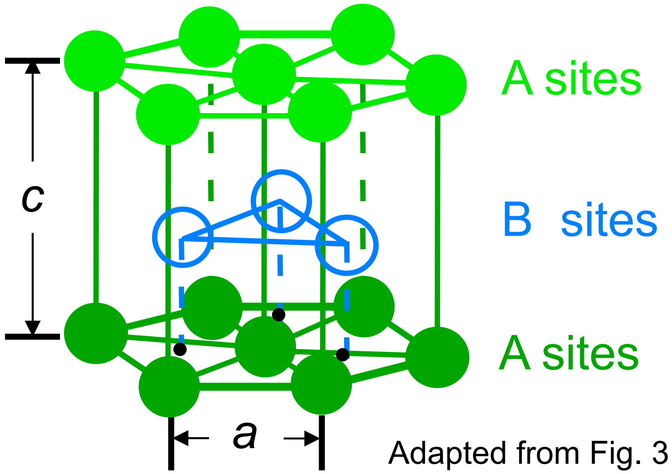
- FCC Unit Cell



Hexagonal close-packed structure (hcp)

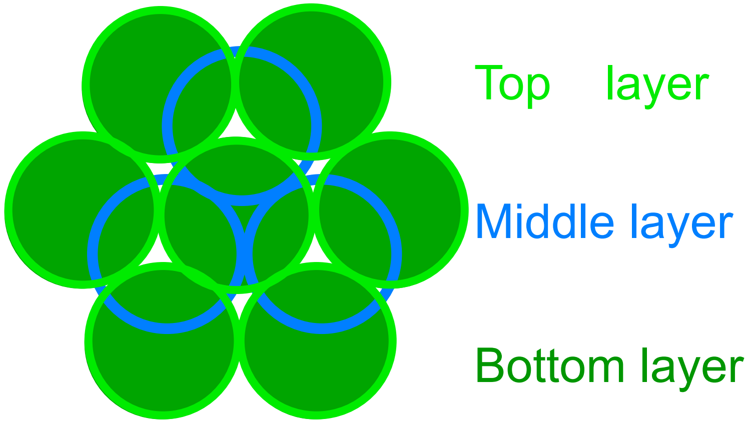
- ABAB... Stacking Sequence

- 3D Projection



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

- 2D Projection



- Coordination # = 12

6 atoms/unit cell

- APF = 0.74

ex: Cd, Mg, Ti, Zn

- $c/a = 1.633$