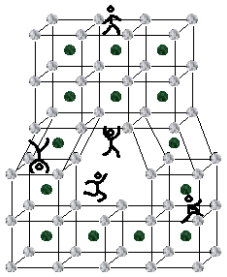
The Structure of Solids
Atoms



- The Relationship Between Structure and Properties
- Atomic (Electronic)Structure
- Bonding
  - Ionic
  - Covalent
  - Metallic

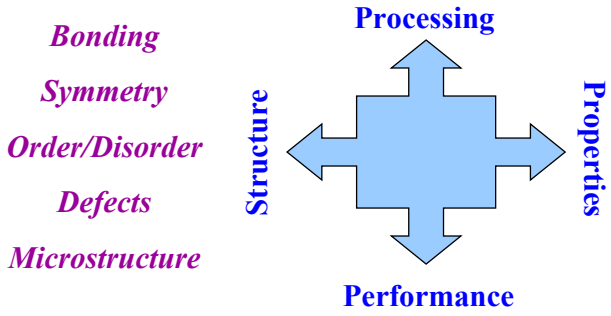
Monday
Aug. 25, 2003

MATS275: INTRODUCTION TO MATERIALS SCIENCE

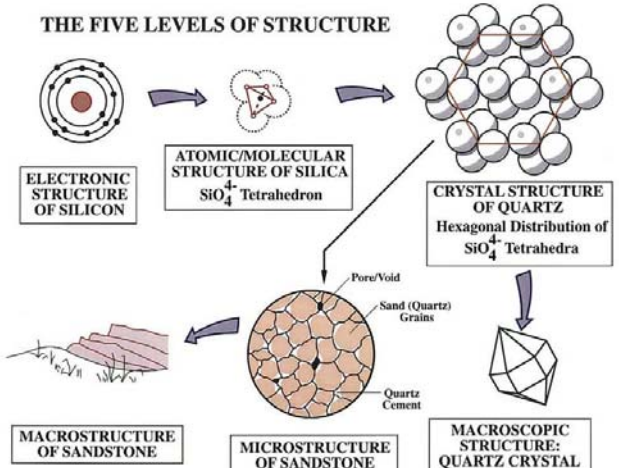
- ***HW #1 - Due 9/1***

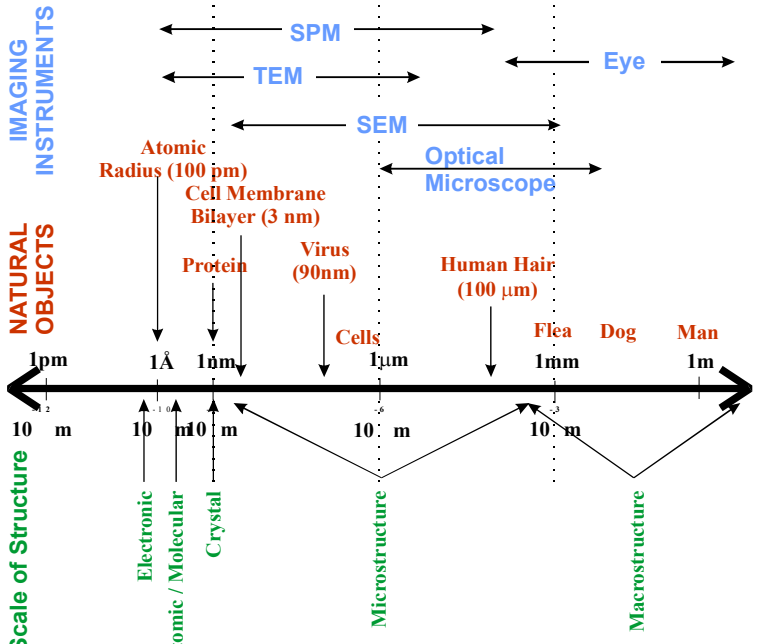
What is Materials Science?

- **How the microscopic structure of a material relates to it macroscopic properties**



Five Levels of Structure





Ionic Bonding
Two Forces

- The Li^+ and F^- are attracted by the Coulomb force...

$$F = \frac{|Z_1 Z_2| q^2}{4\pi\varepsilon_0 x^2} \quad \left(\varepsilon_0 = 8.85\times10^{-12}\ \frac{C^2}{N\cdot m^2}\right)$$

- But repelled when they get too close (Pauli again)...

$$F_r = \frac{K}{x^m}$$

Ionic Bonding
Force to Energy

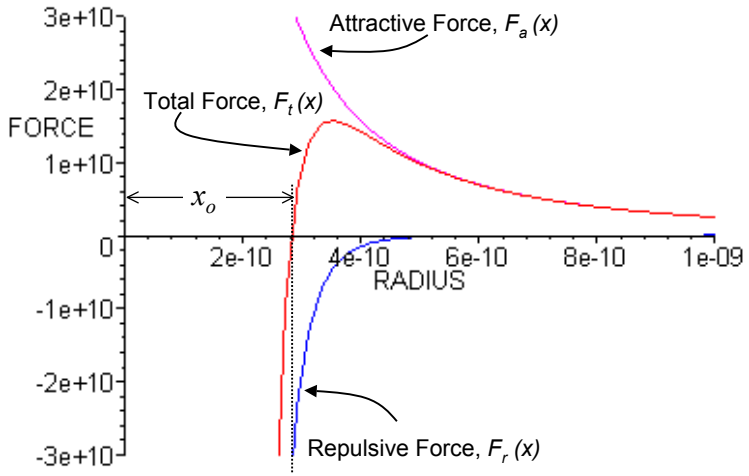
- The potential energy stored is the integral of the force...

$$U = \int_x^\infty F\,dx = \int_x^\infty \left(\frac{A}{x^2} - \frac{K}{x^m}\right)dx$$

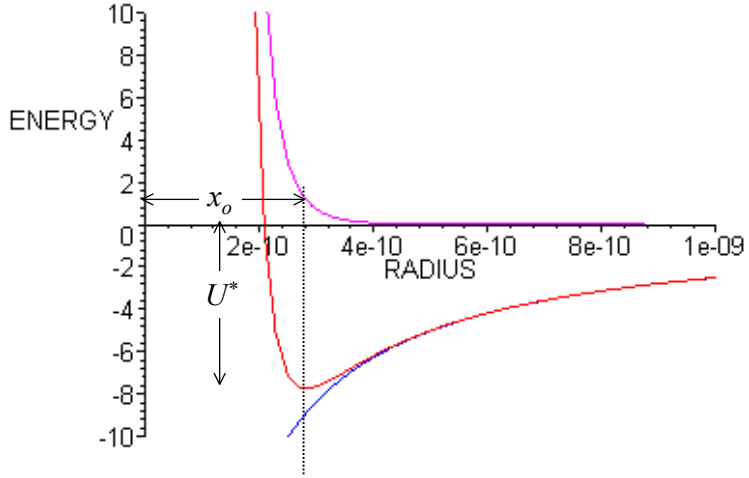
$$= U_\infty - \frac{B}{x} + \frac{C}{x^n}$$

dU/dx = 0 at equilibrium (F=0)

Bonding Forces



Potential Energy Curve



Ionic Bonding

- Scales with difference in EN...

	Bond (kJ/mol)	T_m	ΔEN
LiCl	829	613ºC	1.9
NaCl	766	801ºC	1.9
MgO	3932	2800ºC	2.2

Note transfer of 2 electrons

Covalent Bonding Typical Values

C-C	370 kJ/mol
C=C	680 kJ/mol
C≡C	890 kJ/mol
C-H	435 kJ/mol
C-N	305 kJ/mol
C-O	360 kJ/mol
C=O	535 kJ/mol

Bonding A Comparison

- Ionic 600 - 1600 kJ/mol
- Covalent 500 - 1250 kJ/mol
- Metallic 100 - 800 kJ/mol
- Van der Waals 2 - 30 kJ/mol
- Hydrogen ~10 kJ/mol

Arrhenius Processes

- Rate of process goes as *exp(-Q/kT)*

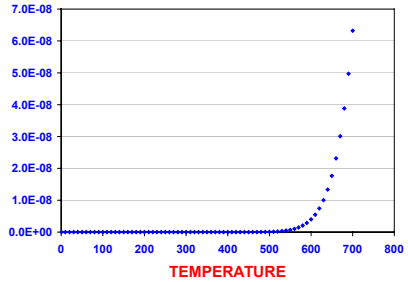
$$R = R_0 e^{-\frac{Q}{kT}} \qquad R = R_0 e^{-\frac{Q}{RT}}$$

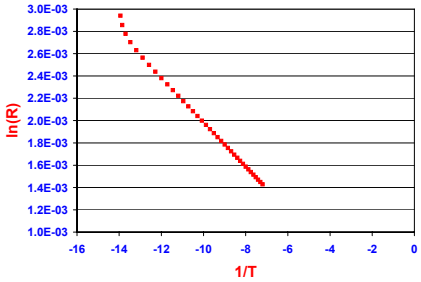
$$\frac{1}{k} = 11308 \frac{K}{eV} \qquad R = 8.314 \frac{J}{mol \cdot K}$$

$$\ln R = \ln R_0 - \frac{Q}{kT}$$

$$\ln R = -\frac{Q}{k}\left(\frac{1}{T}\right) + \ln R_0$$

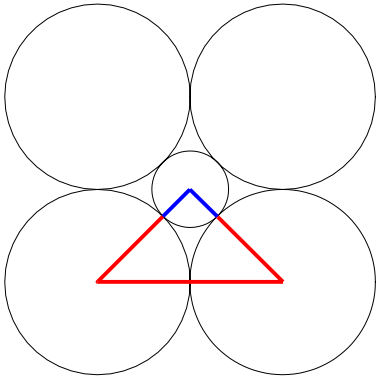
Arrhenius Relations





Get slope to find Q

Planar Close Packing



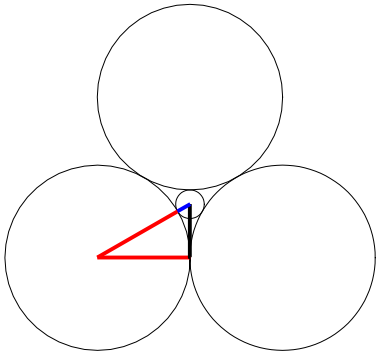
$$(R+R)^2=(R+r)^2+(R+r)^2$$

$$4R^2=2(R+r)^2$$

$$\sqrt{2}R=R+r$$

$$\frac{r}{R}=\sqrt{2}-1=0.414$$

Planar Close Packing



$$\frac{R}{R+r}=cos\,30^\circ=\frac{\sqrt{3}}{2}$$

$$R=\frac{\sqrt{3}}{2}R+\frac{\sqrt{3}}{2}r$$

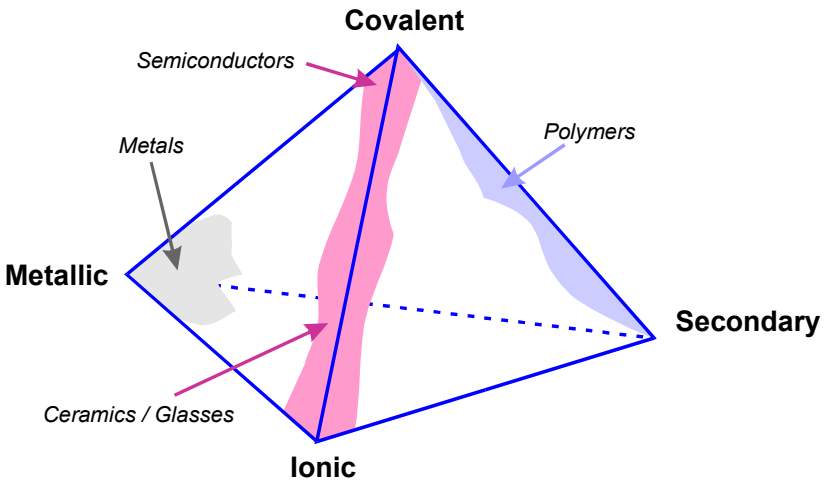
$$\frac{2-\sqrt{3}}{\sqrt{3}}=\frac{r}{R}=0.155$$

Summary of Bonding

Bond Type	*Character*	*Bond Strength*	*Materials*	*Ductility*
Covalent	Primary, Directional	Strong / Very Strong	Ceramics / Polymers	Poor (ceramics)
Ionic	Primary, Non-directional	Strong	Ceramics	Poor
Metallic	Primary, Non-directional	Moderate	Metals	Excellent (mostly)
Hydrogen	Secondary, Directional	Weak	Polymers* (biological molecules like DNA)	_____
Van der Waals	Secondary, Non-directional	Very weak	Polymers*	_____

* Polymers normally contain both primary and secondary bonds, and can be either ductile or brittle

The Bonding Tetrahedron



Summary of Primary Bonded Materials

Properties:	*Structural*	*Mechanical*	*Thermal*	*Electrical*	*Examples*
Ionic Solids (Ceramics)	Non-directional bonding.	Strong bonding. High strength and hardness. Brittle	Fairly high melting point. Low thermal conductivity	Insulators	NaCl, MgO, Al_2O_3
Covalent Solids (Ceramics or Semiconductors)	Bonds are directional and numerically limited per atom.	Strong bonding. High strength and hardness	High melting point. Low thermal conductivity.	Insulators or semiconductors	C (diamond), Si, Ge, SiC
Metallic Solids (Metals)	Non-directional bonding yielding close packing. Metals have high densities	Strength and hardness are low to moderate	Low to high melting point. High thermal conductivity	Conductors	Au, Fe, Ni, Brass, Bronze

Summary of Secondary Bonded Materials

Properties:	*Structural*	*Mechanical*	*Thermal*	*Electrical*	*Examples*
Atomic / Molecular Solids	Structurally similar to metals	Very weak bonding. Very low strength and hardness	Very low melting point. Low thermal conductivity	Insulators	He, Ne, Cl_2, CO_2, CH_4
Hydrogen Bonded Solids	Directional Bonding (not too many exist)	Weak bonding. Low strength and hardness	Low melting point. Thermal insulators	Insulators	H_2O, HF
Macromolecular Solids (Polymers)	Directional Bonding (intramolecular). Intermolecular bonding either directional or non-directional	Strong intramolecular bonding.Weak to strong intermolecular bonding. Low strength.	Low melting point for weak intermolecular bonding.	Mostly Insulators	Polyethylene, PVC, Epoxy