Elementary Materials Science Concepts - Interatomic Bonding

- Atomic Bonding in Solids

Atomic Bonding in Solids

A basic force model:

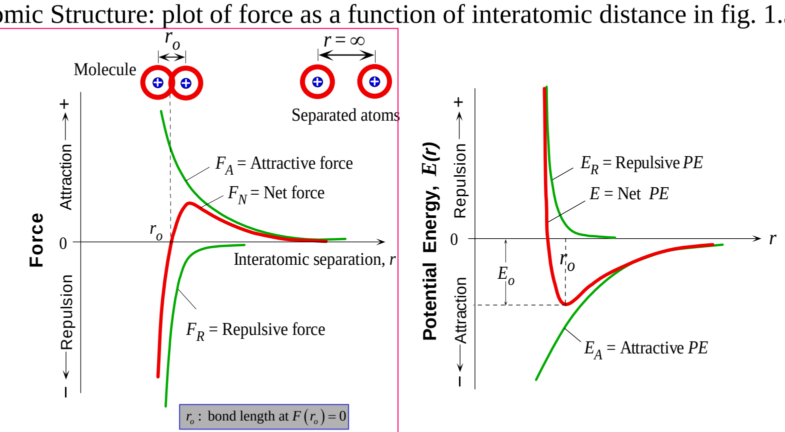
- As 2 atoms are brought together, the atoms exert forces (perturb) on one another.
- The forces are:
  1) Attractive Force (F_A): This force is primarily a coulombic attraction.
  2. Repulsive Force (F_R): as the outer e^- orbitals of each atom begin to overlap, their is a repulsion between these e^-'s.

NET FORCE: $F_N = F_A + F_R$

Additional Information:
See: Chapter 2
Materials Science and Engineering – An Introduction, William D. Callister, Jr. 6th Ed or 7th Ed (Wiley, 2003)

Interatomic Bonding

- Atomic Structure: plot of force as a function of interatomic distance in fig. 1.3a



(a) Force vs r (b) Potential energy vs r

Fig. 1.3: (a) Force vs interatomic separation and (b) Potential energy vs interatomic separation.

From *Principles of Electronic Materials and Devices, Second Edition*, S.O. Kasap (© McGraw-Hill, 2002) http://Materials.Usask.Ca

Interatomic Bonding

- Atomic Bonding in Solids

· At $\sum F = 0$, molecular equilibrium exists.

· At $r \to \infty$, $F_A \to 0$ & $F_R \to 0$ $\therefore$ $F_N \to 0$

Relationship between Force, Distance & Energy

$E = \int F\,dr$ OR $\frac{dE}{dr} = F$

Similar to ~~Poissons~~ Poissons Eqn:

$E = eV$

$-\frac{d^2V}{dx^2} = \frac{dE}{dx} = \frac{\rho}{\epsilon\epsilon_o} = \frac{qN}{\epsilon_r\epsilon_o}$

For our system (atomic system)

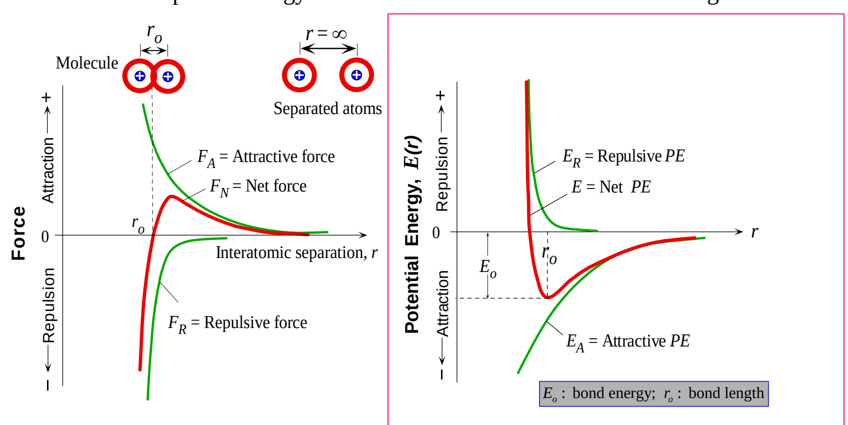
$E_N = \int_\infty^r F_N\,dr$

$= \int_\infty^r F_A\,dr + \int_\infty^r F_R\,dr$

$= E_A + E_R$

Interatomic Bonding

- Atomic Structure: plot of energy as a function of interatomic distance in fig. 1.3a



(a) Force vs r (b) Potential energy vs r

Question: at a given $E=f(r)$, how would one find $E(r_o)$ which is E_o?

Fig. 1.3: (a) Force vs interatomic separation and (b) Potential energy vs interatomic separation.

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Interatomic Bonding

❑ Atomic Bonding in Solids

Answer:

Step 1: We know that E_N-vs-r has a minima @ $r = r_0$.

Step 2: Thus, we can take the derivative of E and set this to zero.

$$\left.\frac{dE}{dr}\right|_{r_0} = 0 \quad (\text{slope} = 0$$ )

Step 3: Solve for r which is actually r_0

Step 4: Substitute r_0 into E_N and this gives $E_N(r_0)$.

In essence, you are finding at what r_0 is $\Sigma F = 0$. That is, molecular equilibrium.

Question:

How could one ensure that r_0 occurred at a minimum and not a maximum?

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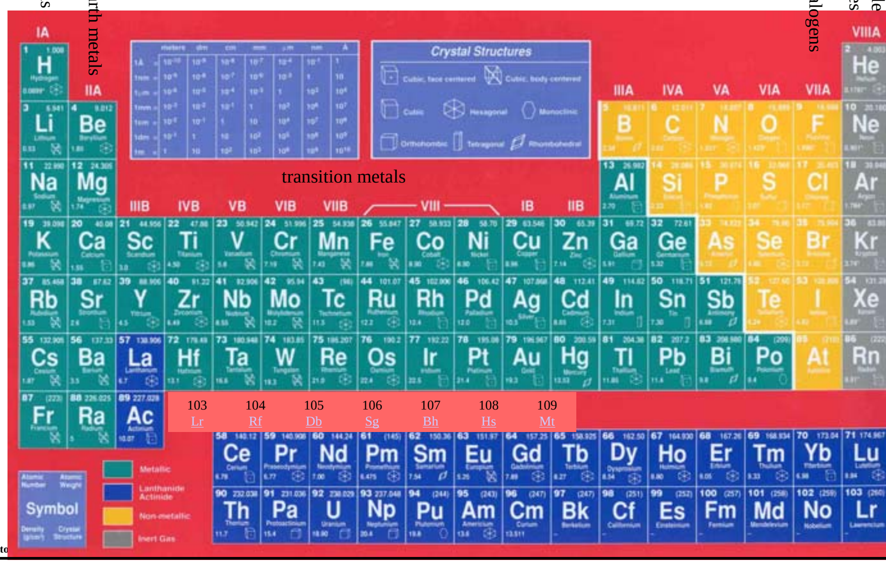
Interatomic Bonding

❑ Primary Interatomic Bonding
- ✓ Ionic
- ✓ Covalent
- ✓ Metallic
- ✓ Van der Waals (London dispersion forces)

❑ Electronegativity:
- ✓ The ability of an atom in a molecule to attract shared electrons to itself.
- ✓ High electronegativity: F = 4
- ✓ Low Electronegativity: Cs = 0.7

Atomic Structure and Interatomic Bonding

- Atomic Structure – Periodic Table



Atomic Structure and Interatomic Bonding

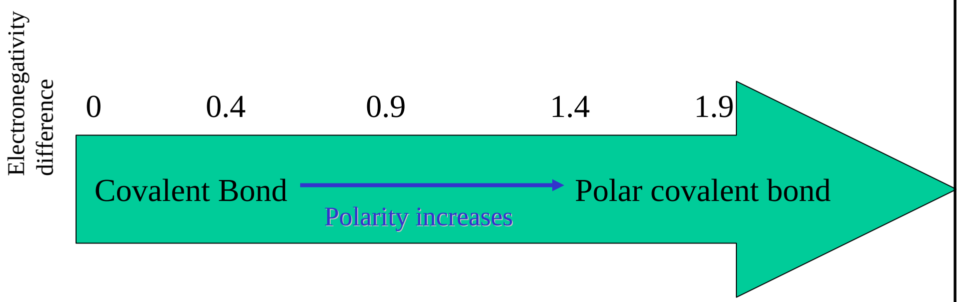
- Relationship between Electronegativity and Bond Type

Electronegatibity Difference In the Bonding Atoms	Bond Type
zero	covalent
intermediate	Polar covalent
large	ionic

Covelent character decreases; Ionic character increases

Atomic Structure and Interatomic Bonding

❑ Relationship between Electronegativity and Bond Type



Atomic Structure and Interatomic Bonding

❑ Primary Interatomic Bonding

- ✓ Ionic Bonding:
  - o Electronegativity difference is greater than ~ 2.
  - o Anion steals an electron from the cation.
  - o Anion typically is a nonmetal.
  - o Cation is typically a metal.
  - o Very little sharing of the valence electrons, so the bonds are nondirectional (i.e., delocalized).
  - o Thus, nearest neighbors are of opposite charge.
  - o Bond energies are between 3 – 8 eV/atom.
  - o Thus, melting temperatures are relatively high.
  - o Other properties:
    - Brittle
    - Hard
    - Insulative
      - » Thermally
      - » electrically

Atomic Structure and Interatomic Bonding

- Primary Interatomic Bonding
  - ✓ Covalent Bonding
    - o Electronegativity difference is less than ~ 2.
    - o Electron stealing does not occur.
    - o Electron sharing rather than stealing of the valence electrons, so the bonds are very directional (i.e., delocalized).
    - o Occurs primarily between Group III through Group VII.
    - o Directional because of p-orbital interaction.
    - o Number of covalent bonds possible:
      - N = number of valence electrons
      - An atom can have at most: 8 – N
      - C: 4 bonds
      - B: 5 bonds
    - o Polar Covalent: unequal sharing of electrons. That is, there is an electronegativity difference.

Atomic Structure and Interatomic Bonding

- Primary Interatomic Bonding
  - ✓ Metallic Bonding
    - o The resulting mixture of elemental metals is called an *alloy*.
    - o In an alloy, the electronegativity difference is very little.
    - o The valence electrons in transition metals are in d-orbitals.
    - o Although a specific d-orbital is very directional, there 10 of them that an average over space gives a somewhat spherical spatial distribution.
    - o Hence, the bonds are quite nondirectional or delocalized.
    - o Since the electronegativity difference is small and the valence electron orbitals are spherical, electron sharing is minimal.
    - o Thus, valence electron sharing is averaged over many metal atoms rather than just two atoms. This creates a "*sea*" of electrons.
    - o The metal atoms are ionic in nature since their valence electrons are shared over many atoms.
    - o The "*sea*" of electrons shield the ion cores from each other which reduces the repulsive electrostatic forces between ions.
    - o Bond Energy: 0.7 to 8.8 eV/atom

Atomic Structure and Interatomic Bonding

- Primary Interatomic Bonding
  - ✓ Van der Waals Bonding
    - o A.K.A.
      - Secondary bonding
      - Dipole-dipole
      - Special cases: *Hydrogen bonding* & *London dispersion forces*
    - o Dipole-dipole interaction between molecules
    - o London dispersion forces:
      - dipole-dipole interaction between non-polar molecules such as O_2.
      - Dipole is caused by the fluctuating electron distribution over time.
      - This induces a dipole in a neighboring atom and a bond occurs.
    - o Polar molecules have positively and negatively charged ends and will interact with each other accordingly and cause dipole-dipole bonding.
    - o A polar molecule with hydrogen as a constituent, such as water, will bond due to dipole-dipole interaction. This is called *hydrogen bonding*.
    - o Bond Energy: 0.1 eV/atom.