

Materials Science

ME 274

Dr Yehia M. Youssef

From Structure to Properties

- To understand the properties and observable characteristics of engineering materials, it is necessary to understand their structure on an atomic and/or microscopic scale.
- Virtually every major property of the five materials categories outlined will be shown to result directly from mechanisms occurring at either the atomic or the microscopic level.
- There is a special sort of architecture associated with these minute scales.
- Fig. 1.8 illustrates the nature of an atomic-scale architecture for crystalline (regular, repeating) and noncrystalline (irregular, random) arrangements of atoms.

From Structure to Properties

- Fig. 1.14 illustrates the nature of a microscopic-scale architecture, in which the reinforcing glass fibers of a high-strength composite are contrasted against the surrounding matrix of polymer.
- The difference in scale between “atomic” and “microscopic” levels should be appreciated. The structure in Fig. 1.14 represents a magnification of $\sim 1,000$ times, whereas the structure shown in Fig. 1.8 represents a magnification of $\sim 10,000,000$ times.
- A fundamental difference between a ductile Al alloy and a brittle Mg alloy relates directly to their different crystalline structures (see Fig. 1.18).

Crystalline versus Amorphous Structure

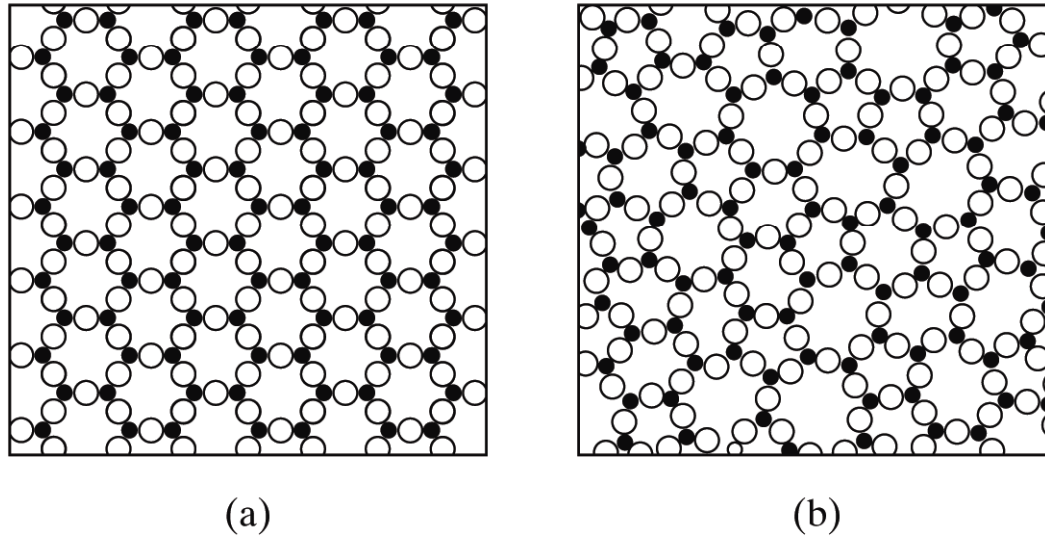


Figure 1.8

Schematic comparison of the atomic-scale structure of (a) a ceramic (crystalline) and (b) a glass (noncrystalline). The open circles represent a nonmetallic atom, and the solid black circles represent a metal atom.

Microscopic Scale Architecture

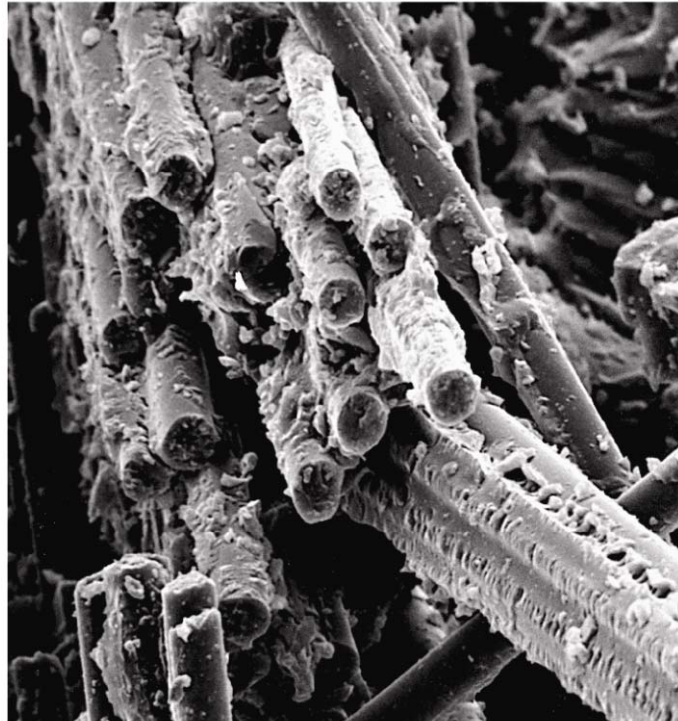


Figure 1.14

Example of a fiberglass composite composed of microscopic-scale reinforcing glass fibers in a polymer matrix. (Courtesy of Owens-Corning Fiberglas Corporation.)

Crystal Structure Comparison

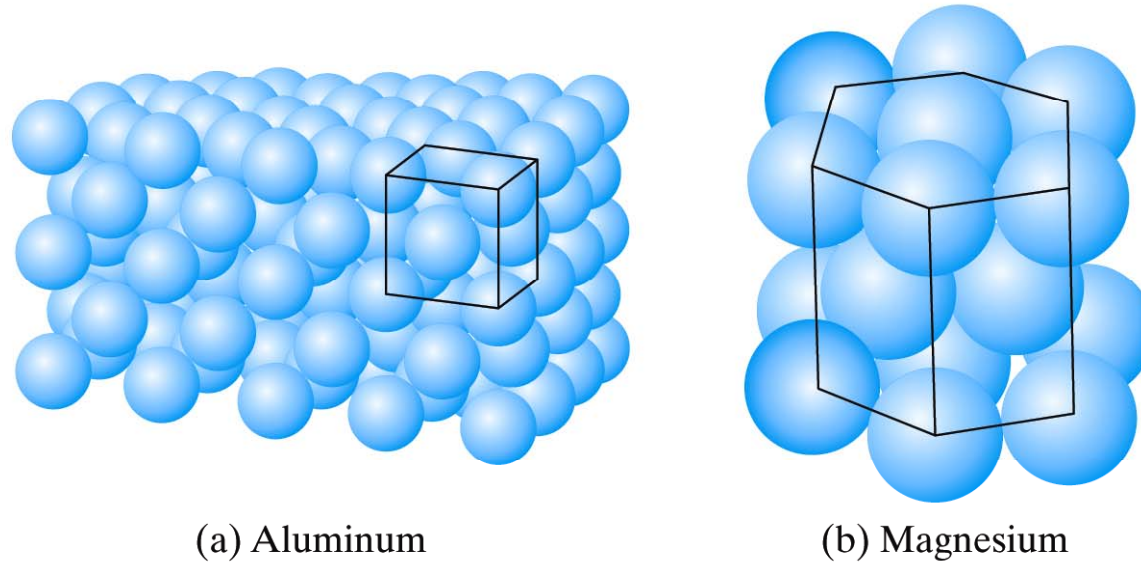


Figure 1.18

Comparison of crystal structures for (a) aluminum and (b) magnesium.

Atomic Bonding in Solids

- The bonding of adjacent atoms is essentially an electronic process.
- Strong **primary bonds** are formed when outer orbital electrons are transferred or shared between atoms.
- Weaker **secondary bonds** result from a more subtle attraction between positive and negative charges with no actual transfer or sharing of electrons.
- The **ionic bond**; it is the result of electron transfer from one atom to another (e.g. NaCl). The transfer of an electron from sodium is favored because it produces a more stable electronic configuration; that is the resulting Na⁺ species has a full outer orbital shell. Similarly chlorine readily accepts the electron producing a stable Cl⁻ species.

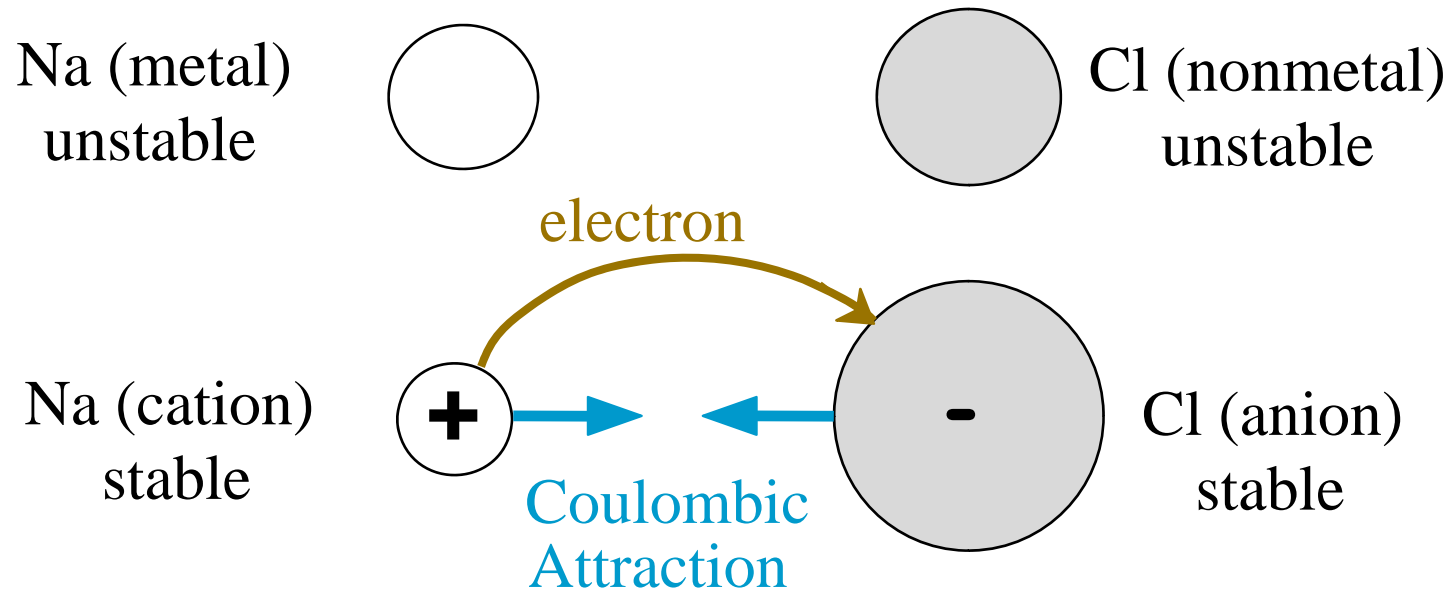
Atomic Bonding in Solids

- The charged species (Na^+ and Cl^-) are termed ions, the positive species (Na^+) is called a cation and the negative species (Cl^-) is called an anion.
- The ionic bond is nondirectional. A positively charged Na^+ will attract adjacent Cl^- equally in all directions.
- The ionic bond is the result of the coulombic attraction between the oppositely charged species.

Atomic Bonding in Solids

Ionic Bonding

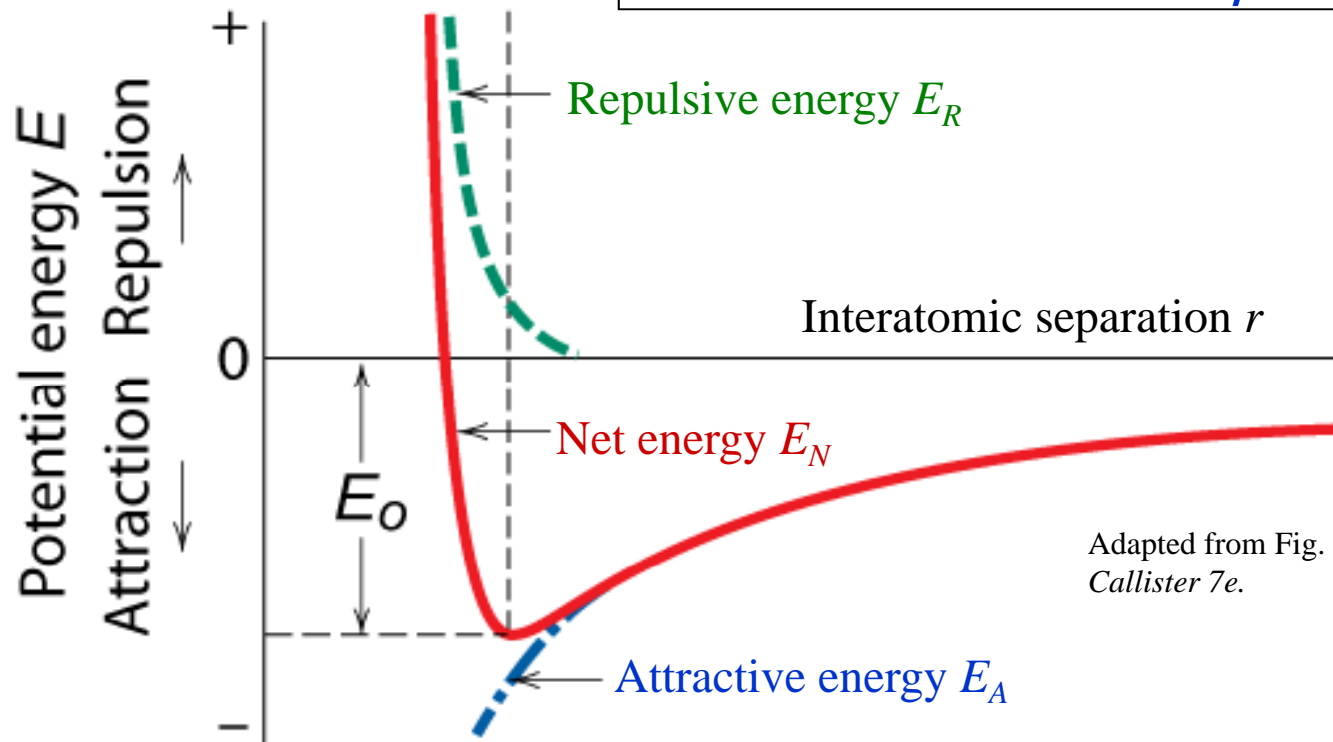
- Occurs between + and - ions.
- Requires **electron transfer**.
- Large difference in electronegativity required.
- Example: NaCl



Atomic Bonding in Solids: Ionic Bonding

- Energy – minimum energy most stable
 - Energy balance of **attractive** and **repulsive** terms

$$E_N = E_A + E_R = -\frac{A}{r} - \frac{B}{r^n}$$



Adapted from Fig. 2.8(b),
Callister 7e.

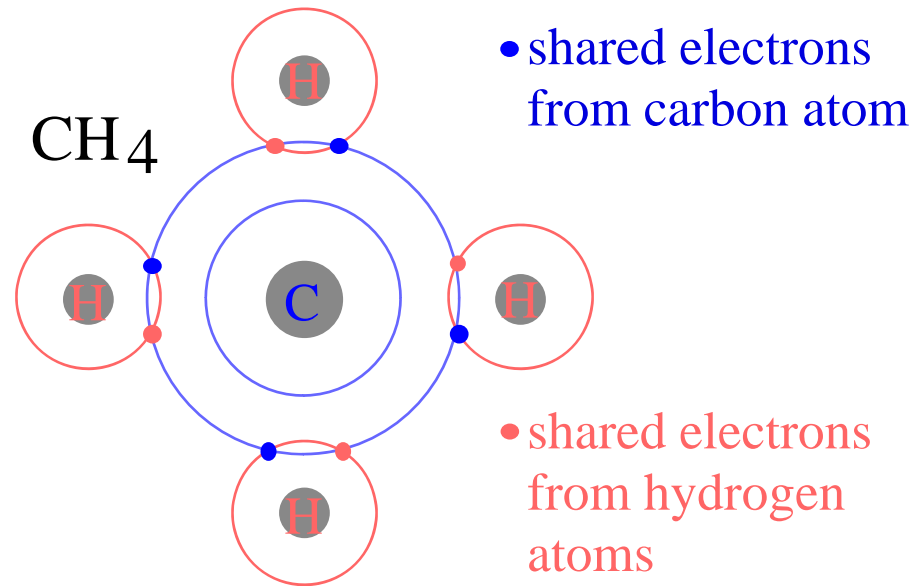
Atomic Bonding in Solids: Covalent Bonding

- similar **electronegativity** \therefore 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*.

Atomic Bonding in Solids: Primary Bonding

- **Metallic Bond** -- delocalized as electron cloud
- **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

Ex: MgO

$$X_{\text{Mg}} = 1.3$$

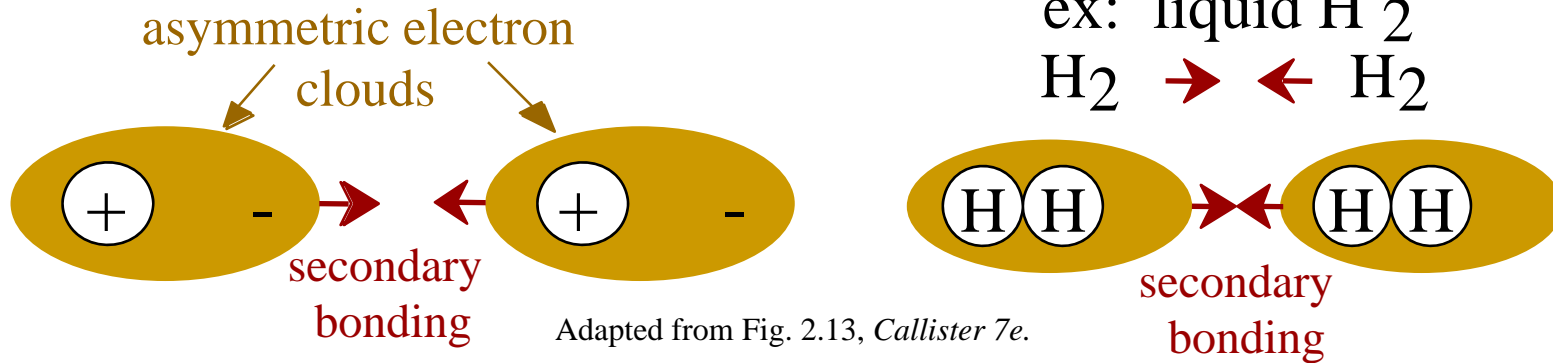
$$X_{\text{O}} = 3.5$$

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

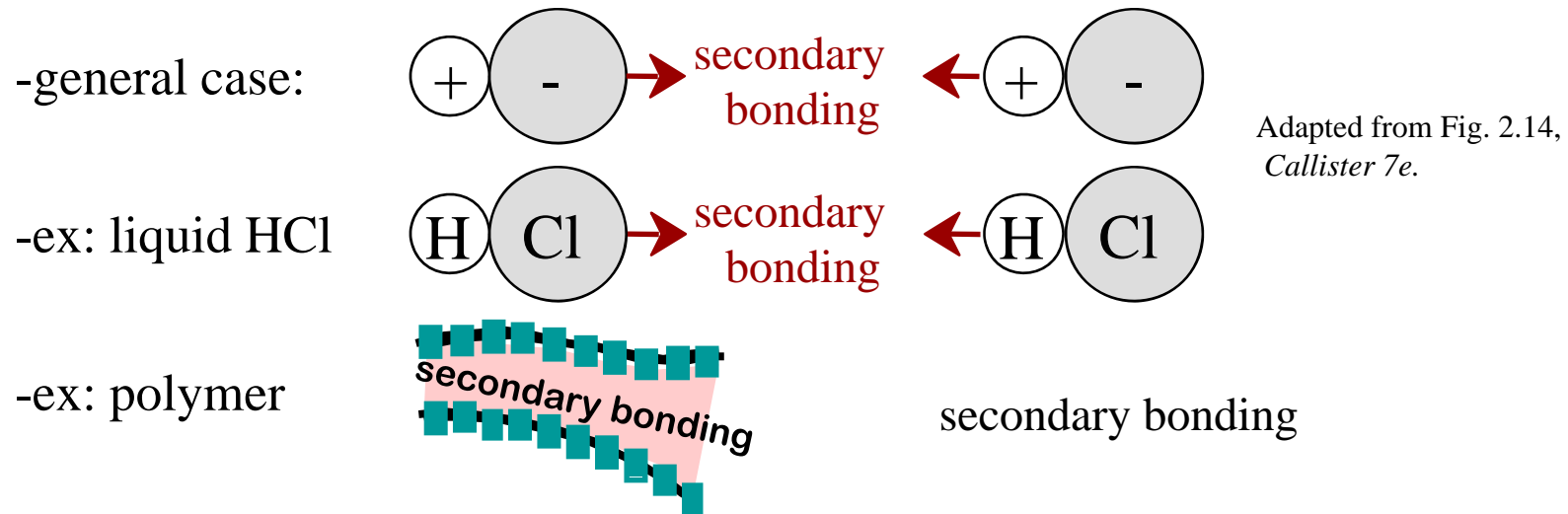
Atomic Bonding in Solids: Secondary Bonding

Arises from interaction between **dipoles**

- Fluctuating **dipoles**



- Permanent **dipoles**-molecule induced



Summary: Atomic Bonding

Type	Bond Energy	Comments
Ionic	Large!	Nondirectional (ceramics)
Covalent	Variable large-Diamond small-Bismuth	Directional (semiconductors , ceramics polymer chains)
Metallic	Variable large-Tungsten small-Mercury	Nondirectional (metals)
Secondary	smallest	Directional inter-chain (polymer) inter-molecular

Comparison Between Materials

Material	Bonding type	Melting point (°C)
NaCl	Ionic	801
C (diamond)	Covalent	~ 3, 550
$-(C_2H_4)_n$	Covalent and secondary	~ 120 ^a
Cu	Metallic	1,084.87
Ar	Secondary (induced dipole)	-189
H ₂ O	Secondary (permanent dipole)	0

^a Because of the irregularity of the polymeric structure of polyethylene, it does not have a precise melting point. Instead, it softens with increasing temperature above 120°C. In this case, the 120°C value is a “service temperature” rather than a true melting point.

Table 2.4

Comparison of Melting Points for Some of the Representative Materials of Chapter 2.