2-Introduction to Structure and Bonding in Materials

2-1-Sub-Atomic Structure

Electrons and their interaction with the nucleus of the atom.

The Bohr model is a simplified view of the arrangement of sub-atomic particles.

The atom is made up of THREE types of particles:

1. **Nucleus**: positively charged nucleus surrounded by electrons revolving around it.

2. **Protons**: Positively charged, and with mass

3. **Neutrons**: No charge, but with almost equal mass to the proton.

The number of Protons defines the **ATOMIC NUMBER** of the atom.

The mass of **Protons** plus **Neutrons** defines the **ATOMIC MASS** of the atom **ISOTOPES**.

All chemical bonds involve electrons. Atoms will stay close together if they have a shared interest in one or more electrons. Atoms are at their most stable when they have no partially-filled electron shells. If an atom has only a few electrons in a shell, it will tend to lose them to empty the shell.
The Periodic Table
Columns: similar valence structure

Electropositive elements: readily give up electrons (+ ions)
Electronegative elements: readily accept electrons (- ions)

Electronegativity
• Ranges from 0.7 to 4.0
• Large values: tendency to acquire electrons

smaller electronegativity  larger electronegativity
2-1-1-During bonding

✓ Metals give up outer (valence) electrons to get the inert gas configuration and become Cations.

✓ Non-metals accept electrons to become Anions.

2-2-Atomic Structure

Organization of atoms or molecules. These controls magnetic, electrical, thermal and optical properties, as well as strength and stiffness

2-2-1-Primary Bonding

There are three types of primary bonds

1. Ionic Bonding
2. Covalent Bonding
3. Metal Bonding

Ionic Bonding

Ionic bonding occurs between charged particles. Ionic bonding occurs between metal atoms and nonmetal atoms. Metals usually have 1, 2, or 3 electrons in their outermost shell. Nonmetals have 5, 6, or 7 electrons in their outer shell. Atoms with outer shells that are only partially filled are unstable. To become stable, the metal atom wants to get rid of one or more electrons in its outer shell. Losing electrons will either result in an empty outer shell or get it closer to having an empty outer shell. It would like to have an empty outer shell because the next lower energy shell is a stable shell with eight electrons.
Some Common Features of Materials with Ionic Bonds:

- Strong and high energy bonds
- High melting point
- Nondirectional
- Hard and brittle or cleave rather than deform
- Transparent
- Insulator

Covalent Bonding

Where a compound only contains nonmetal atoms, a covalent bond is formed by atoms sharing two or more electrons. Nonmetals have 4 or more electrons in their outer shells (except boron). With this many electrons in the outer shell, it would require more energy to remove the electrons than would be gained by making new bonds. Therefore, both the atoms involved share a pair of electrons. Each atom gives one of its outer electrons to the electron pair, which then spends some time with each atom. Consequently, both atoms are held near each other since both atoms have a share in the electrons.
Some Common Features of Materials with Covalent Bonds:

1. Often hard
2. Inorganic covalent compounds usually have high melting point
3. Can be strong (Diamond)
4. Can be weak (Bi)
5. Directional

Metallic Bonding

A common characteristic of metallic elements is they contain only one to three electrons in the outer shell. When an element has only one, two or three valence electrons (i.e. electrons in the outer shell), the bond between these electrons and the nucleus is relatively weak.

Some Common Features of Materials with Metallic Bonds:

- Good electrical and thermal conductors due to their free valence electrons
- Opaque
- Relatively ductile
- High packing density
- Non-directional

2-2-2- Secondary Bonding

Van der Waals Bond

The van der Waal bonds occur to some extent in all materials but are particularly important in plastics and polymers.

Hydrogen Bonds
### Summary-Bonding

<table>
<thead>
<tr>
<th>Type</th>
<th>Bond Energy</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionic</td>
<td>Large!</td>
<td>Nondirectional <em>(ceramics)</em></td>
</tr>
<tr>
<td>Covalent</td>
<td>Variable</td>
<td>Directional <em>(semiconductors, ceramics, polymer chains)</em></td>
</tr>
<tr>
<td></td>
<td>large-Diamond small-Bismuth</td>
<td></td>
</tr>
<tr>
<td>Metallic</td>
<td>Variable</td>
<td>Nondirectional <em>(metals)</em></td>
</tr>
<tr>
<td></td>
<td>large-Tungsten small-Mercury</td>
<td></td>
</tr>
<tr>
<td>Secondary</td>
<td>smallest</td>
<td>Directional <em>(polymer)</em></td>
</tr>
<tr>
<td></td>
<td></td>
<td>inter-chain <em>(inter-molecular)</em></td>
</tr>
</tbody>
</table>

**Ceramics** *(Ionic & covalent bonding):* Large bond energy
- large $T_m$
- large $E$
- small $\alpha$

**Metals** *(Metallic bonding):* Variable bond energy
- moderate $T_m$
- moderate $E$
- moderate $\alpha$

**Polymers** *(Covalent & Secondary):* Directional properties
- Secondary dominates
- small $T_m$
- small $E$
- large $\alpha$
2-3-Microscopic Structure

When attempting to classify a material it is useful to know whether it is crystalline (conventional metals and alloys), non-crystalline (glasses) or a mixture of these two types of structure. The critical distinction between the crystalline and non-crystalline states of matter can be made by applying the concept of ordering.

Packing of large groups of atoms, this controls ductility, strength, and toughness

Single and Polycrystalline Materials

- **Single**: atoms pack in periodic, one array
- **Poly**: atoms pack in periodic, 3D arrays
### Metallic Crystal Structures

1. Body-Centered Cubic Structure (BCC)
2. Face-Centered Cubic Structure (FCC)
3. Hexagonal Close Packed Structure (HCP)

<table>
<thead>
<tr>
<th></th>
<th>BCC</th>
<th>FCC</th>
<th>HCP</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1 unit cell</strong></td>
<td>close-packed directions: length = 4R ≈ ( \frac{\sqrt{3}}{2} a )</td>
<td>close-packed directions: length = 4R ≈ ( \frac{\sqrt{2}}{2} a )</td>
<td>-</td>
</tr>
<tr>
<td>Coordination Number = 8</td>
<td>contains 1 + 8 x 1/8 = 2 atoms/unit cell</td>
<td>contains 6 x 1/2 + 8 x 1/8 = 4 atoms/unit cell</td>
<td>-</td>
</tr>
<tr>
<td>atoms/unit cell</td>
<td>( \frac{4}{3} \pi \left( \frac{a}{2} \right)^3 )</td>
<td>( \frac{4}{3} \pi \left( \frac{a}{2} \right)^3 )</td>
<td>-</td>
</tr>
<tr>
<td>APF =</td>
<td>( \frac{2}{3} a^3 )</td>
<td>( \frac{4}{3} \pi \left( \frac{2a}{4} \right)^3 )</td>
<td>-</td>
</tr>
<tr>
<td>CN: 8, APF = 0.68</td>
<td>ABCABC Stacking Sequence.</td>
<td>ABABAB. Stacking Sequence.</td>
<td>-</td>
</tr>
</tbody>
</table>
Theoretical Density

\[ \rho = \frac{n A}{V c N_A} \text{ Atomic weight (g/mol)} \]
\[ \nu \text{ Volume/unit cell (cm}^3/\text{unit cell)} \]
\[ \text{Avogadro's number (6.023 \times 10^{23} \text{ atoms/mol)} } \]

Example: Copper
from Table inside from cover of Callister (see next slide):
\begin{itemize}
  \item crystal structure = FCC \Rightarrow 4 \text{ atoms/unit cell}
  \item atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
  \item Atomic radius \( R = 0.128 \text{ nm (1 nm = 10}^{-7} \text{ cm)} \)
\end{itemize}

\[ V_c = a^3 \text{ for FCC } a = \frac{4R}{\sqrt{2}} \Rightarrow V_c = 4.75 \times 10^{-23} \text{ cm}^3 \]

Result: theoretical \( \rho_{\text{Cu}} = 8.89 \text{ g/cm}^3 \)

actual: 8.94 g/cm³

2-4-Macroscopic Structure

Conditions that can be seen by the naked eye. Surface quality, porosity.