ENGINEERING MATERIALS (ME 281)

Atomic Structure and Interatomic Bonding

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Lecture outline

- Atomic Structure
  - Fundamental concepts
  - Electrons in atoms
- Atomic Bonding in Solids
  - Bonding energies and forces
- Primary Bonding
  - Ionic, covalent and metallic
- Secondary Bonding
  - Types of dipole-dipole bonds

Learning Objectives

After this chapter, you should be able to do the following:

- Explain the concept of atomic structure.
- Describe Bohr atomic model in relation to quantum mechanics.
- Identify the principal quantum numbers and their energy levels.
- State the Pauli Exclusion Principle
- List the electron configuration of some elements.
- Explain the types of primary bonding in solids
- Define van der Waals or secondary bonding

Atomic Structure

Fundamental concepts

- Atoms are composed of electrons, protons, and neutrons.

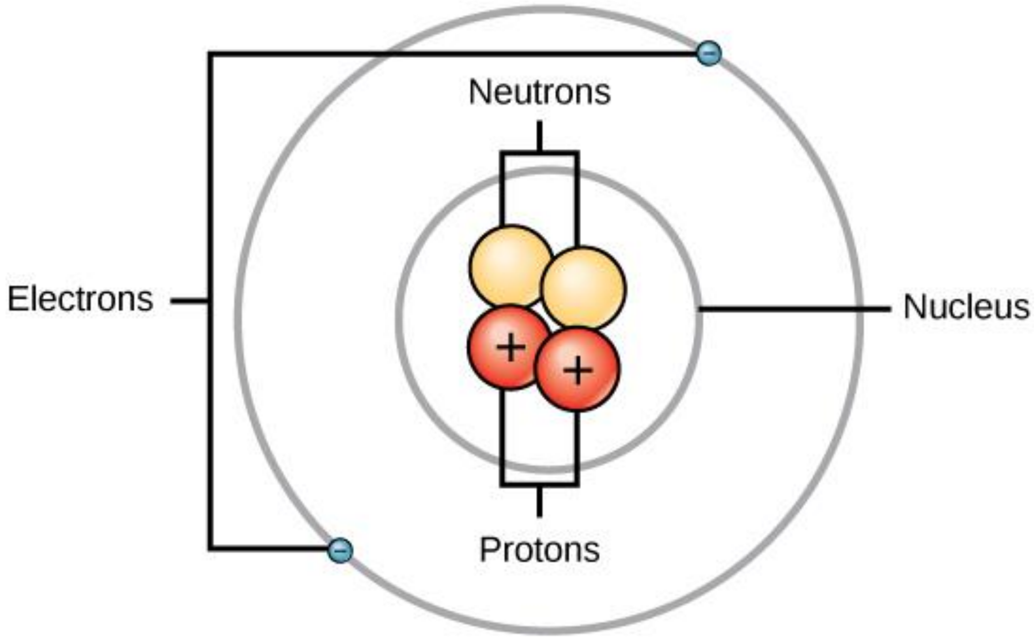
Atoms = nucleus (protons and neutrons) + electrons

- Electrons and protons are negative and positive charged particles respectively.
- The magnitude of each charged particle in an atom is 1.6×10^{-19} Coulombs.
- ***The mass of the electron is negligible compared to the proton and neutron, which form the nucleus of the atom.***
- Protons and Neutrons have the same mass, 1.67×10^{-27} kg
- Mass of an electron is much smaller, 9.11×10^{-31} kg and can be neglected in calculation of atomic mass.

Atomic Structure Contd.

Fundamental concepts

- **Atomic mass (A)** = mass of protons + mass of neutrons
- **Atomic number (Z)** = number of protons
- Protons gives chemical identification of the element.
- Neutrons defines isotope number



Atomic Structure Contd.

- The **atomic mass unit (amu)** is often used to express atomic weight. 1 amu is defined as 1/12 of the atomic mass of the most common isotope of carbon atom, carbon 12 (^{12}C).
- $M_{proton} \approx M_{neutron} = 1.66 \text{ x } 10^{-24}$ g = 1 amu.
- The atomic mass of the ^{12}C atom is 12 amu.
- The **atomic weight of an element** = weighted average of the atomic masses of the atoms naturally occurring isotopes.
- Atomic weight of carbon is 12.011 amu.
- The atomic weight is often specified in mass per mole.
- A **mole (mol)** is the amount of matter that has a mass in grams equal to the atomic mass in amu of the atoms (A mole of carbon has a mass of 12 grams).
- The number of atoms in a mole is called the Avogadro number, $N_{av} = 6.023 \times 10^{23}$. **Note that N_{av} = 1 gram/1 amu.**

Atomic Structure Contd.

- The number of atoms per cm^3 of a material of density δ (g/cm^3) is calculated by using:

$$n = N_{av}\frac{\delta}{M}$$

- *M* is the atomic mass in *amu* (*grams* per *mol*).

- For Graphite (carbon): $\delta = 2.3\ g/cm^3$, $M = 12\ g/mol$

  $n = 6\times10^{23}$ atoms/mol $\times\ 2.3\ g/cm^3\ /\ 12\ g/mol$

  $= 11.5 \times 10^{22}$ atoms/cm^3

- For Water (H_2O) $\delta = 1\ g/cm^3$, $M = 18\ g/mol$

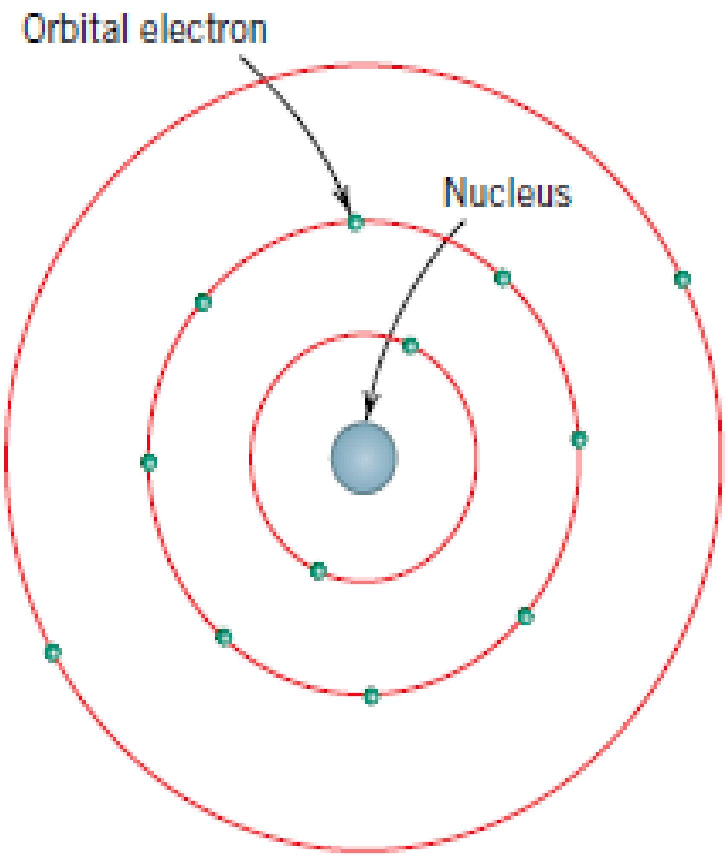
  $n = 6\times10^{23}$ molecules/mol $\times\ 1\ g/cm^3\ /\ 18\ g/mol$

  $= 3.3 \times 10^{22}$ molecules/cm^3

Electrons in Atoms

Bohr atomic model (quantum mechanics)

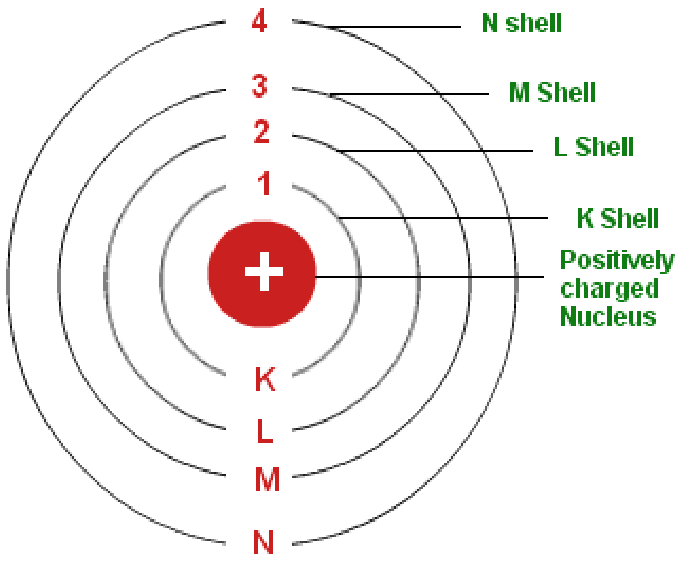
- Electrons revolve around the atomic nucleus in discrete orbitals.
- The position of any particular electron is more or less well defined in terms of its orbital.
- Energies of electrons are quantized; thus, electrons are permitted to have only specific values of energy.



The allowed electron energies are associated with energy levels or states. The states do not vary continuously with energy.

Electrons in Atoms

- Every electron in an atom is characterized by four parameters called **quantum numbers**.
- Quantum numbers dictate the number of states within each subshell.
- Shells are specified by a principal quantum number n, which may take on integral values beginning with unity



- ***Shells are designated by the letters K, L, M, N, O, etc., which correspond, respectively, to principal quantum numbers, n = 1, 2, 3, 4, 5, ... (See Table 2.1)***
- ***The quantum number, is related to the distance of an electron from the nucleus, or its position.***

Electrons in Atoms

Table 2.1The number of available states in electron shells & subshells

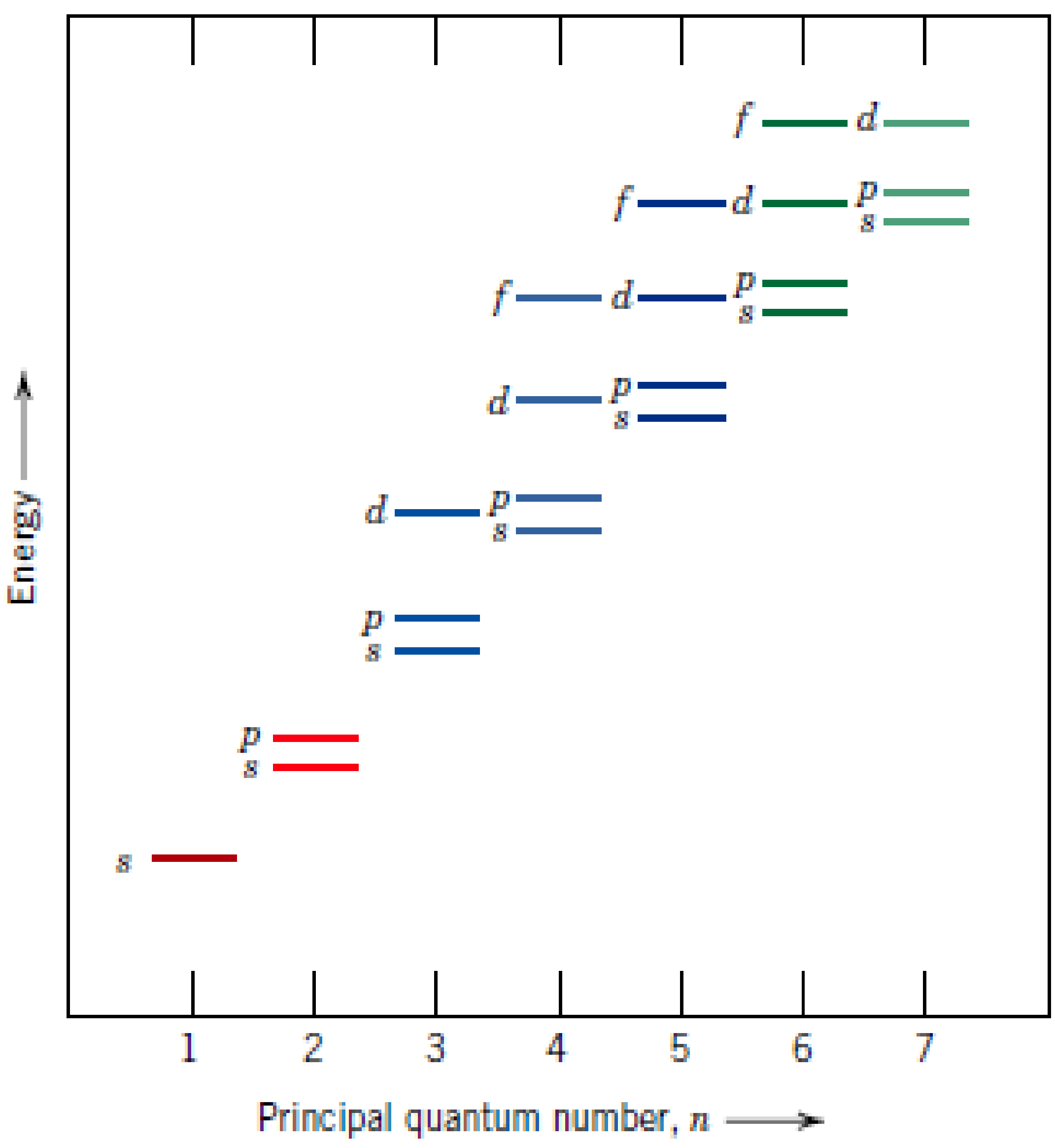
Principal Quantum Number n	*Shell Designation*	*Subshells*	*Number of States*	*Number of Electrons* Per Subshell	*Number of Electrons* Per Shell
1	*K*	*s*	1	2	2
2	*L*	*s*	1	2	8
		p	3	6	
3	*M*	*s*	1	2	18
		p	3	6	
		d	5	10	
4	*N*	*s*	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

- ***The most inner K-shell can accommodate only two electrons, called s-electrons; the next L-shell two s-electrons and six p-electrons; the M-shell can host two s-electrons, six p-electrons, and ten d-electrons; and so on…***

Electron configuration

Pauli exclusion principle

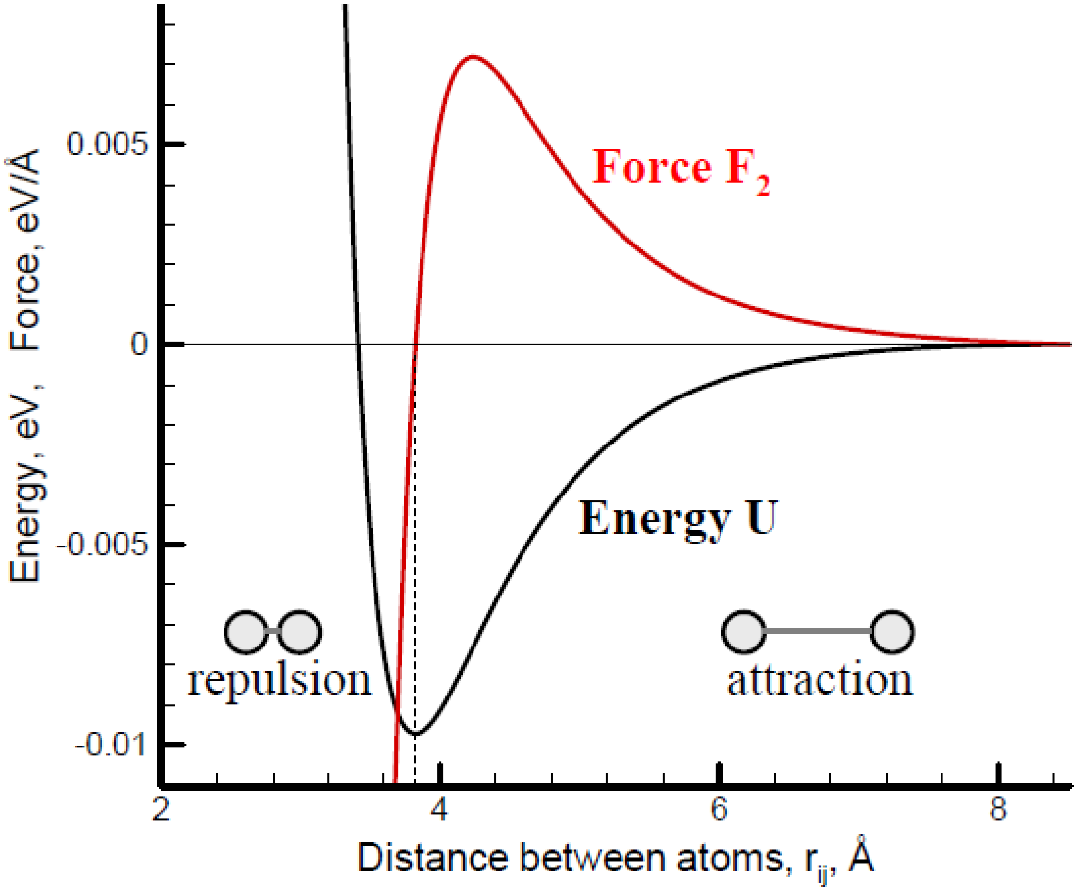
- ***Each electron state can hold at most two electrons, which must have opposite spins.***
- Thus, *s*, *p*, *d*, and *f* subshells may each accommodate, resp ectively, a total of 2, 6, 10, an d 14 electrons.
- Electrons that occupy the outermost filled shell (valence electrons) are responsible for bonding.
- Electrons fill quantum levels in order of increasing energy.
- Eg. Na, Z =11:$1s^2 2s^2 2p^6 3s^1$
- Ar, Z = 18: $1s^2 2s^2 2p^6 3s^2 3p^6$



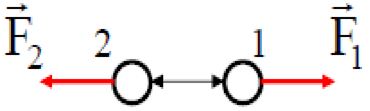
Atomic Bonding in Solids

Bond energy and forces

- Forces can be calculated from the potential energy of interatomic interaction.
- For a system of two atoms (e.g. a diatomic molecule), the potential energy depends only on the distance between the two atoms.
- The electron volt (eV) is the energy unit convenient for de scription of atomic bonding.
- ***Electron volt is the energy lost/ gained by an electron when it is taken through a potential diff. of 1volt.***
- ***1 eV = 1.6 x 10^{-19} J***



$$\vec{F}_1 = -\vec{F}_2 = -\frac{dU(r_{12})}{dr_{12}}$$

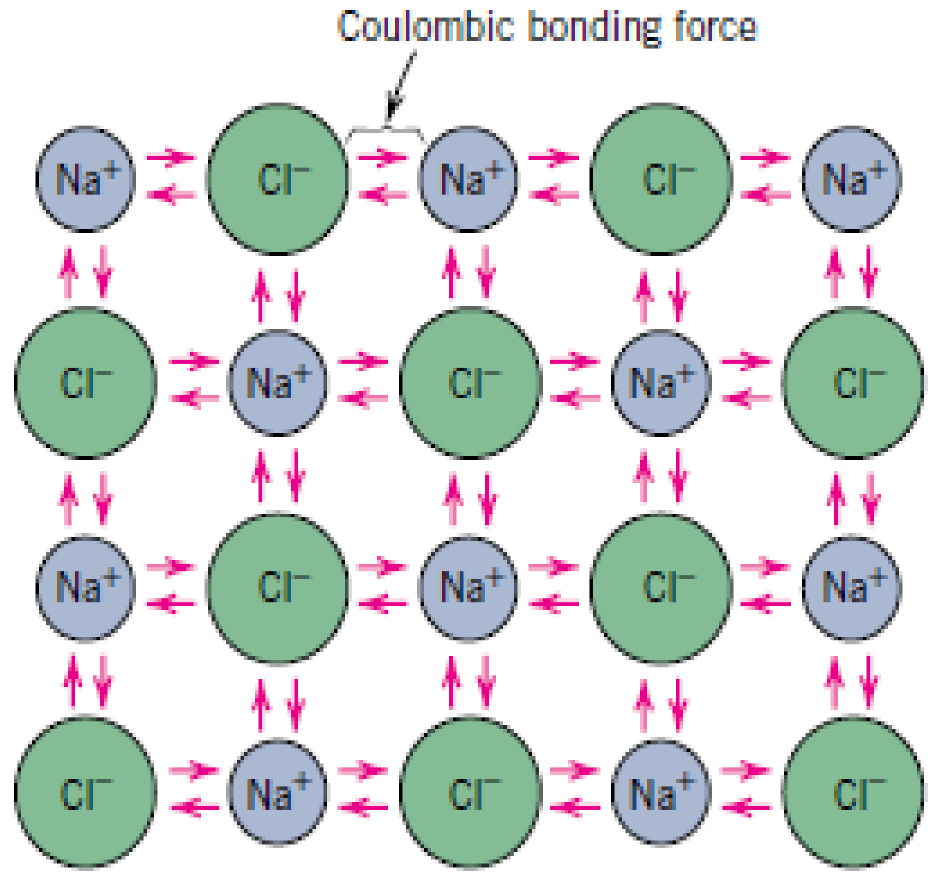


$$r_{12} = |\vec{r}_1 - \vec{r}_2|$$

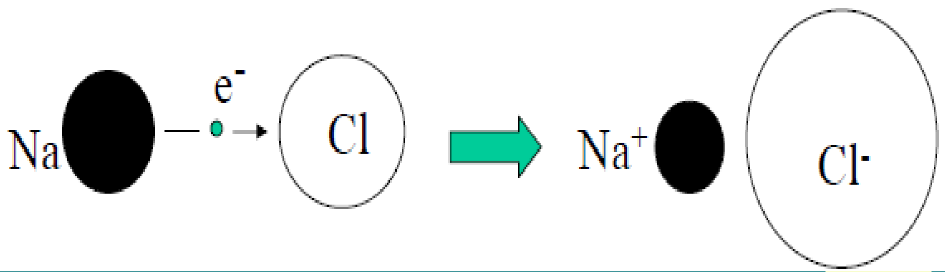
Primary Bonding in Solids

Ionic Bonding

- It involves the transfer of valence electrons between two atoms to form ions.
- Ionic bond is the force of attraction that holds negative and positive ions together.
- The attractive bonding forces are coulombic.
- It forms when atoms of a metallic element donate electrons to atoms of non-metallic element.



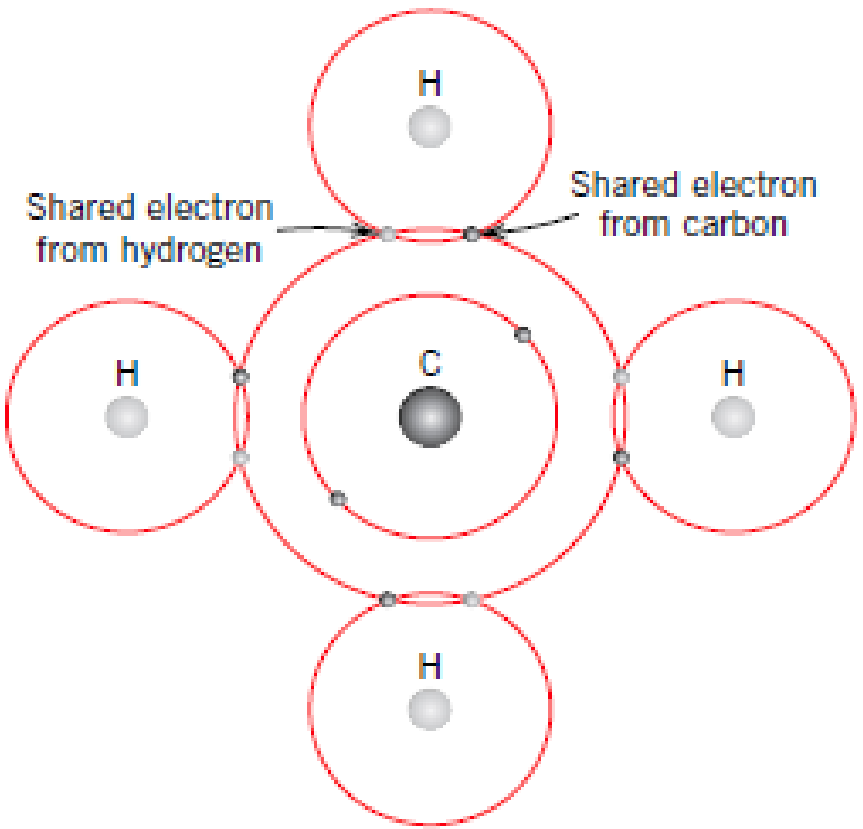
- Ionic bonds are the strongest bonds.
- Non-directional (magnitude of the bond is equal in all directions around an ion)



Primary Bonding in Solids Contd.

Covalent Bonding

- Involves the sharing of electron pairs between atoms.
- Stable balance of attractive and repulsive forces between the atoms, when they share electrons, is known as covalent bonding.
- Two covalently bonded atoms will each contribute at least one electron to the bond.
- Shared electrons may be considered to belong to both atoms.

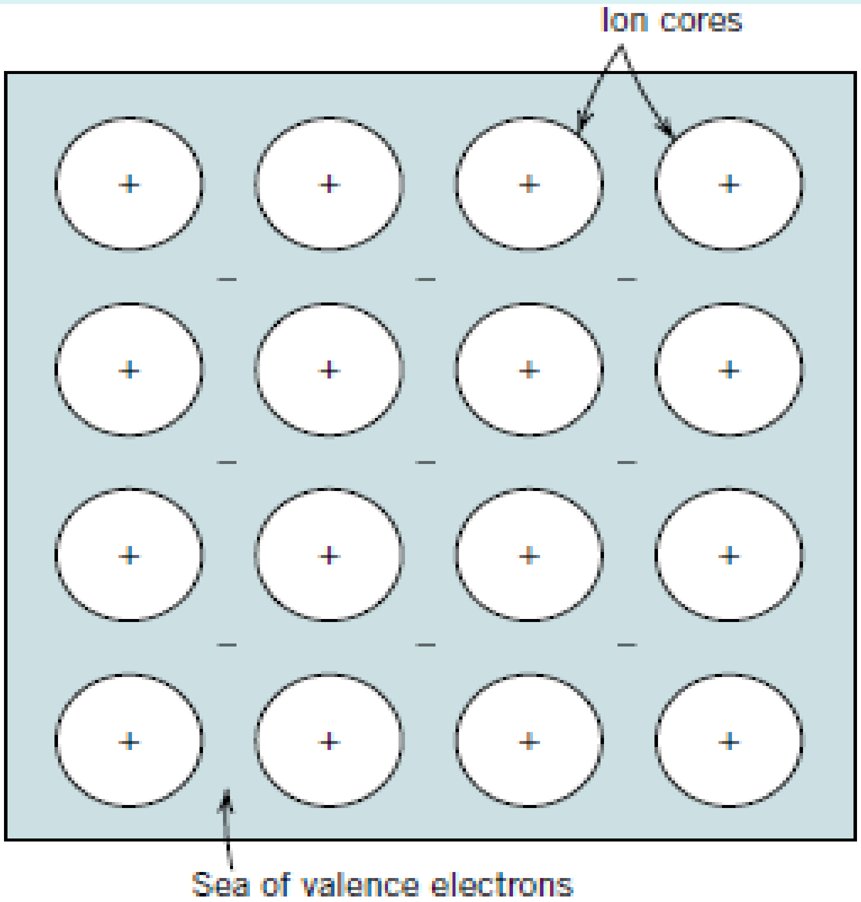


- Covalent bonds are very strong.
- Directional in nature; thus, it is between specific atoms and may exist only in the direction between one atom and another that participates in the electron sharing.

Primary Bonding in Solids Contd.

Metallic Bonding

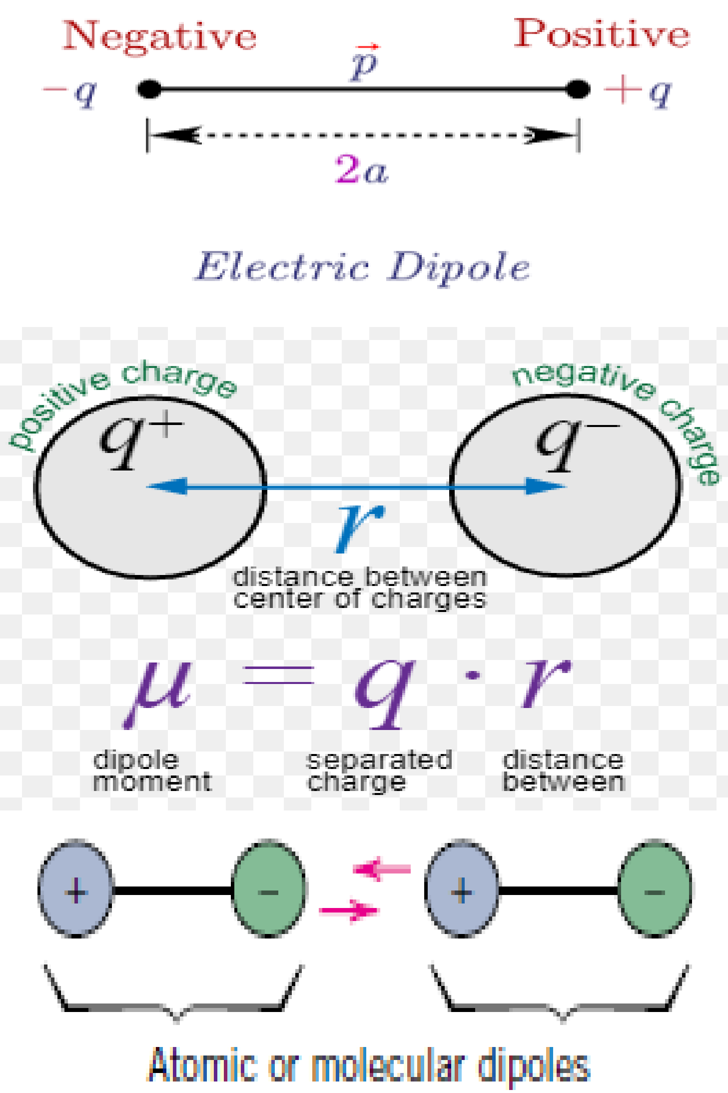
- Valence electrons are detached from atoms (delocalized), and spread in an ' electron sea' that binds the positively charged metal ions together.
- It accounts for the physical properties of metals, such as strength, ductility, conductivity, etc.
- Metallic bond is non-directional (bonds form in any direction) → atoms closely packed.
- Bonds do not break when atoms are rearranged.



- The free electrons shield the positively charged ion cores from mutually repulsive electrostatic forces, which they would otherwise exert upon one another.
- Examples: Cu, Al, Ag, etc. Transition metals (Fe, Ni, etc.)

Secondary Bonding in Solids

- These bonds are caused by permanent or temporary **dipoles** within the atom or molecule.
- Electric dipole exists whenever there is some separation of positive and negative portions of an atom or molecule.
- Smaller bond energies not involving the transfer or sharing of electrons.
- Weaker in nature (~0.1 eV/atom or ~10 kJ /mol.)
- Broadly classified into Van der Waal's and hydrogen bonds.
- Coulombic attraction between the (+) end of one dipole and the (-) region of an adjacent dipole.

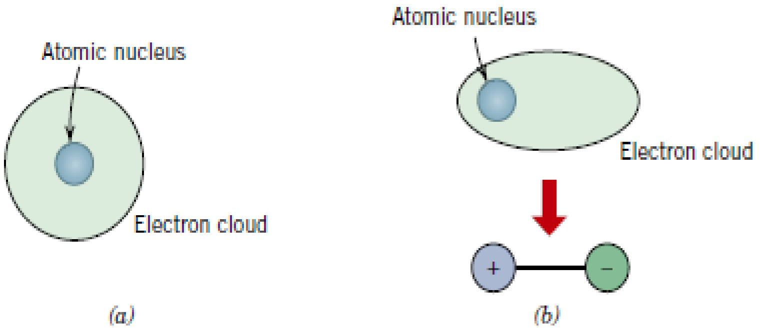


Secondary Bonding in Solids

- Dipole interactions occur between induced dipoles, induced dipoles and polar molecules and polar molecules.
- An **induced dipole** is when interactions between two molecules cause one or both of them to have separation of charges.
- In a **polar molecule**, one end of the molecule has a positive charge while the other end has a negative charge. Eg. H_2O, NH_3, H_2S, SO_2, etc.

- **Fluctuating induced dipole bonds (Van der Waals bond)**
- A dipole induced in an atom or molecule that is normally electrically symmetric.
- Nucleus (+) and outside electron cloud form a dipole due to constant vibrational motion of the atoms. As the electron moves, the dipole fluctuates.

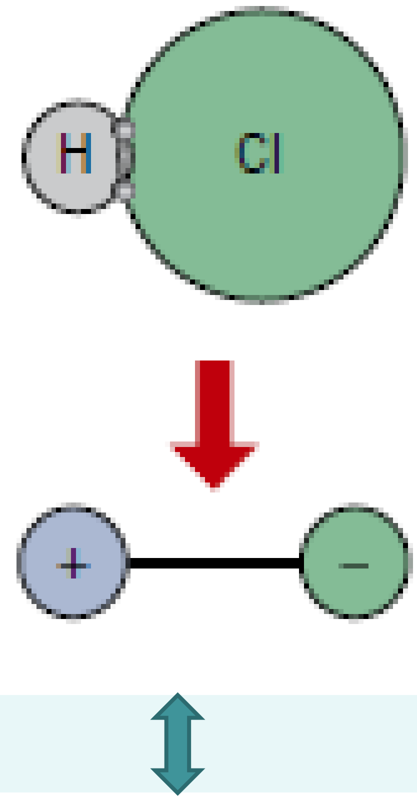
- Fluctuation in one atom (X), produces a fluctuating electric field that is felt by the electrons of an adjacent atom (Y).
- Atom Y then polarizes (its outer electrons are on the side of the atom closest to the (+) side of dipole in X). Eg. H_2, Cl_2, inert gases.



Secondary Bonding in Solids

Polar molecule-induced dipole bonds

- Permanent dipole moments exist in some molecules (called polar molecules) due to the asymmetrical arrangement of positively and negatively regions (HCl, H_2O).
- Bonds between adjacent polar molecules (permanent dipole bonds) are the strongest among secondary bonds.
- Polar molecules can induce dipoles in adjacent non-polar molecules and a bond will form as a result of attractive forces between the two molecules (permanent and induced dipoles)
- Magnitude of this bond is greater than fluctuating induced dipoles.



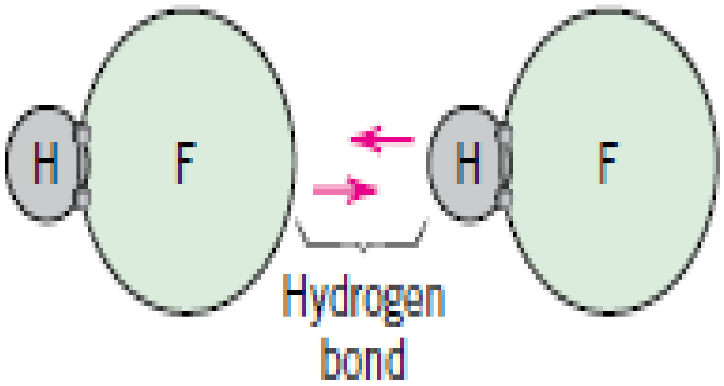
Permanent dipole moment from net (+) and (-) charge associated with the H and Cl ends of the HCl molecule.

Secondary Bonding in Solids

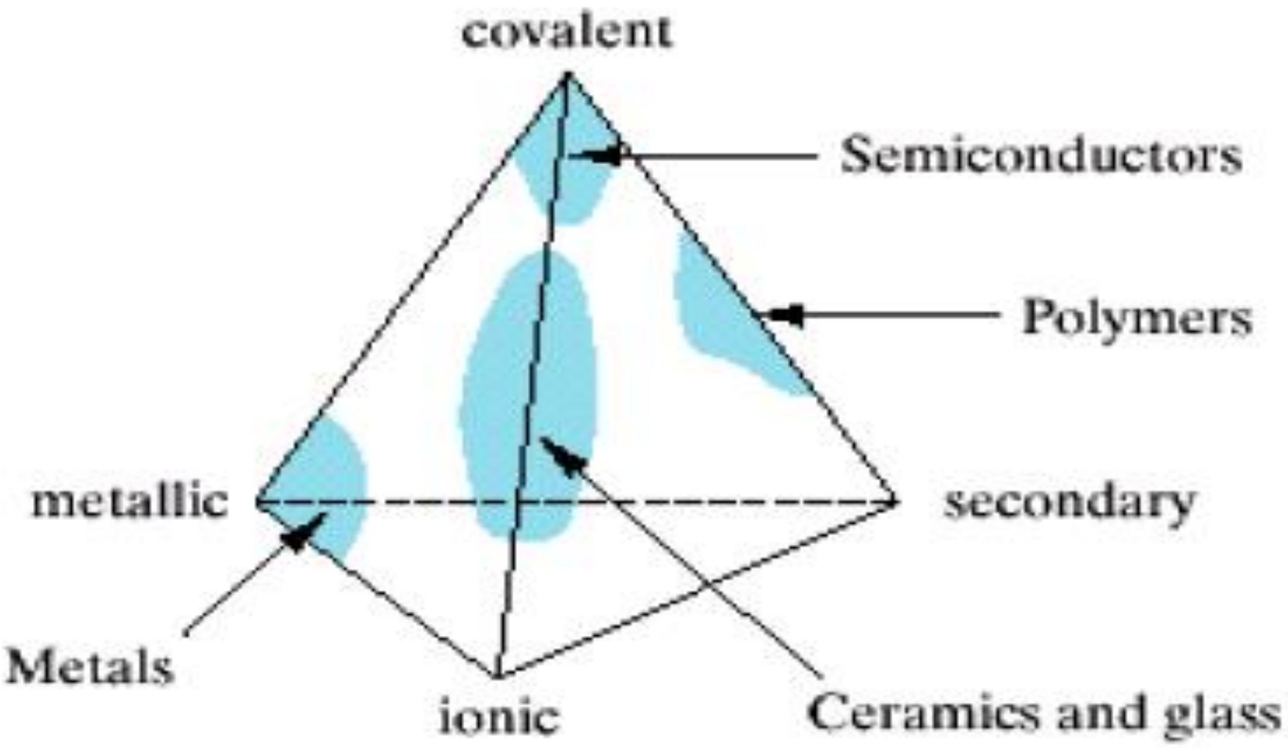
Permanent dipole bonds (Hydrogen bonding)

- Interaction involving a hydrogen atom located between a pair of other atoms having a high affinity for electrons.
- **Permanent dipole:** partial charge separation within a molecule along the bond that forms between two different atoms.
- Hydrogen bond is weaker than ionic or covalent bond but stronger than van der Waals forces. Its magnitude may be as high as 51 kJ/mol (0.52 eV/molecule).
- Melting and boiling temperatures for HF and H_2O are abnormally high in light of their low molecular weights, as a consequence of hydrogen bonding.

- ***Hydrogen bond is a special case of polar molecule bonding***
- Highly positively charged end of the molecule is capable of strong attractive force with the negative end of an adjacent molecule, as illustrated for HF.



Types of Bonding in Materials



- Metals: Metallic bonds
- Ceramics: Ionic/Covalent bonds
- Polymers: Covalent and Secondary bonds
- Semiconductors: Covalent or Covalent/Ionic bonds

Lecture Ends