University of Anbar/ Faculty of Engineering

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Lecturer. Osama Ibrahim

Lecture # 4

INTERATOMIC BONDING

In order to understand the why materials behave like they do and why they differ in properties, it is necessary that one should look at atomic level. The study primarily concentrates on two issues: what made the atoms to cluster together, and how atoms are arranged. As mentioned in earlier chapter, atoms are bound to each other by number of bonds. These inter-atomic bonds are primarily of two kinds: ***Primary bonds and Secondary bonds***. ***Ionic, Covalent and Metallic bonds*** are relatively very strong, and grouped as primary bonds, whereas ***van der Waals and hydrogen bonds*** are relatively weak, and termed as secondary bonds. Metals and Ceramics are entirely held together by primary bonds - the ionic and covalent bonds in ceramics, and the metallic and covalent bonds in metals. Although much weaker than primary bonds, secondary bonds are still very important. They provide the links between polymer molecules in polyethylene (and other polymers) which make them solids. Without them, water would boil at -80˚C, and life as we know it on earth would not exist.

Atomic Bonding

Primary bonds

- ***Ionic, Covalent and Metallic bonds.***
- ***Transfer or sharing of elecrons.***
- ***Stronger.***

Secondary bonds

- ***van der Waals and hydrogen bonds***
- ***There is no elecrons transfered or shared.***
- ***Weak.***

PRIMARY BONDS

Ionic bonding

Ionic bonding occurs between a metal and a non-metal. This bond exists between two atoms when one of the atoms is negative (has an extra electron) and another is positive (has lost an electron). Then there is a strong, direct Coulomb attraction. Basically ionic bond involves electron transfer from electropositive atom to electronegative atom. An example is **NaCl, LiF**.

For **NaCl** molecule, there are more electrons around Cl, forming Cl^- and fewer electrons around Na, forming Na^+. Ionic bonds are the strongest bonds. In real solids, ionic bonding is usually exists along with covalent bonding.

Atomic number (Z) for **Na = 11, $1s^2\ 2s^2\ 2p^6\ 3s^1$**

Atomic number (Z) for **Cl= 17, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$**

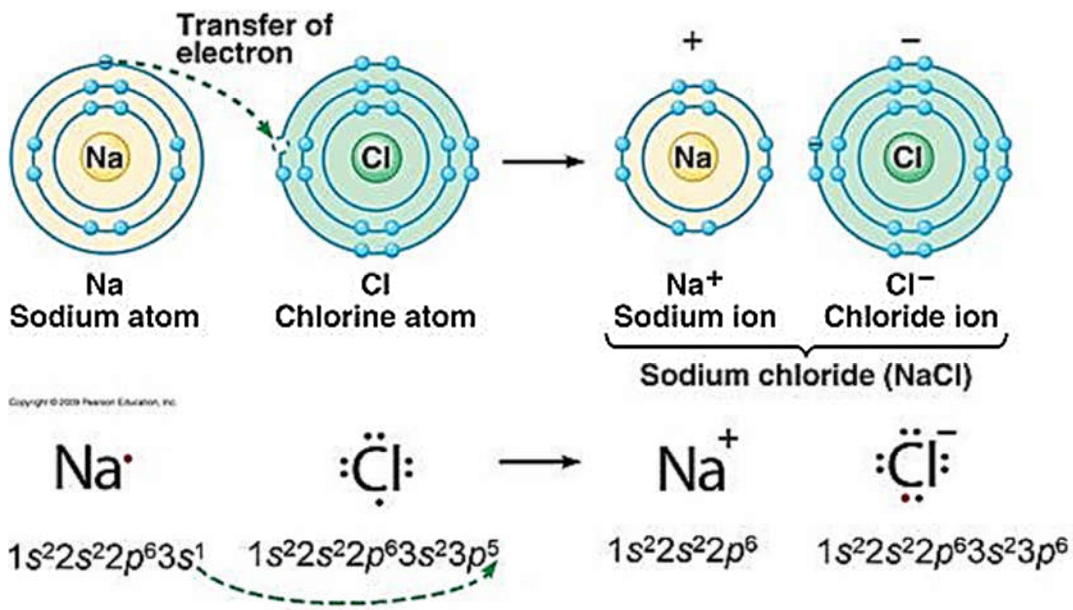

Figure 2.2 Ionic bonding in NaCl.

- Ionic materials very hard and brittle, bad conductor of electricity and heat, they have large bond energy (600-1500KJ/mole).
- Ionic materials have high melting temperature, large modulus of elasticity and small thermal expansion coefficient.
- Ionic bond is non-directional which means the magnitude of the bond is equal in all directions.

Covalent bonding

A covalent bond is formed in compounds that contain only nonmetal atoms by sharing two or more electrons. In covalent bonding, electrons are shared between the atoms, to saturate the valency. The simplest example is the H_2 molecule, where the electrons spend more time in between the nuclei of two atoms than outside, thus producing bonding. In covalent bond, both of atoms will share a pair of electrons. Typically, covalent bonds are very strong, and directional in nature. The hardness of diamond is a result of the fact that each carbon atom is covalently bonded with four neighboring atoms, and each neighbor is bonded with an equal number of atoms to form a rigid three-dimensional structure (***giant lattices***).

Covalent bonding is schematically illustrated in **Figure 2.3** for a molecule of methane (CH_4). The carbon atom has four valence electrons, whereas each of the four hydrogen atoms has a single valence electron.

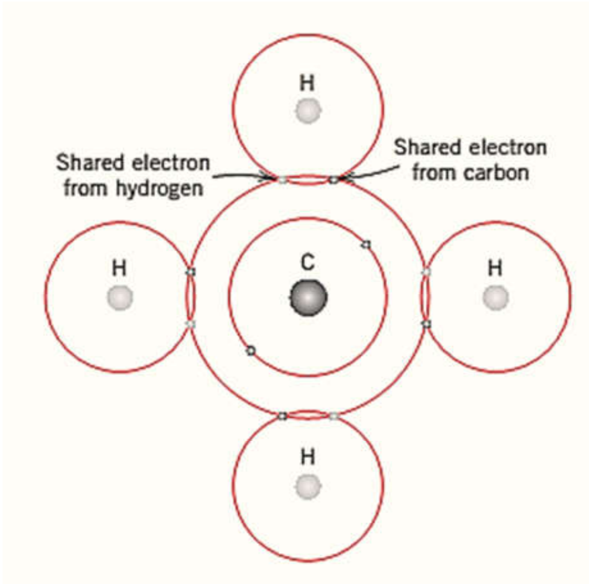

Figure 2.3 Schematic representation of covalent bonding in a molecule of methane (CH_4).

- Examples of covalent bonding are: Cl_2, F_2, SiC, H_2O, CH_4, HF, GaAs.
- Most covalent compounds have low melting and boiling points temperature like Bismuth 270°C. Some, like carbon compounds can be **very large as in diamond** (melting point **3550°C**) in which carbon atoms each share four electrons to form giant lattices.
- Covalent compounds (ceramics, semiconductors, and polymers) are hard, good insulators, transparent, and brittle.

Metallic bonds

Metallic bonds formed when atoms give up their valence electrons 1, 2 or electrons from each atom, which then form sea or cloud of electrons. The positively charged atom cores (ion cores) are bonded by the mutual attraction to negatively charged electrons. The sea or cloud of electrons is responsible for electrical and thermal conductivity, and optical properties luster (shiny). Metallic bonding can be viewed as metal containing a periodic structure of positive ions surrounded by a sea of delocalized electrons.

- Metallic compounds are good electrical and thermal conductors due to their free valence electrons.
- The bond energy is 68KJ/mole for mercury and 850KJ/mole for tungsten.
- non-directional.

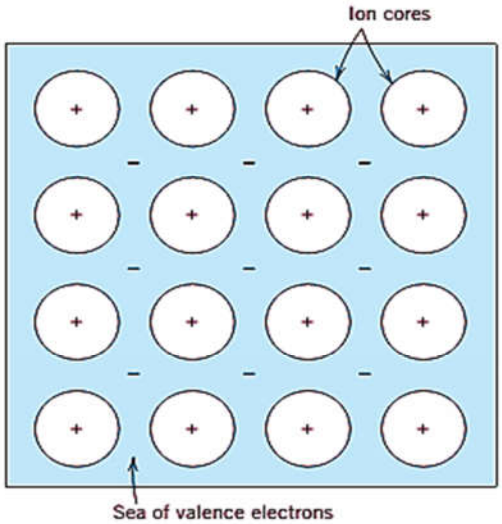

Figure 2.3 Schematic illustration of metallic bonding.

SECONDARY BONDS

Secondary bonds are different from primary bonds in that they involve neither electron transfer nor electron sharing. These are weak bond, bond energy 10KJ/mole arises from atomic or molecular dipole. Examples: HF, H_2O.

Van der Waals bonds

Van der Waals forces include attraction and repulsions between atoms, molecules, and surfaces, as well as other intermolecular forces. They differ from covalent and ionic bonding in that they are caused by correlations in the fluctuating polarizations of nearby particles. Being the weakest of the weakest chemical forces. with a energy between 0.4 and 4kJ/mol.

Since the electrons may be on one side of the atom or the other, a dipole is formed: the + nucleus at the center, and the electron outside. Since the electron moves, the dipole fluctuates. This fluctuation in atom A produces a fluctuating electric field that is felt by the electrons of an adjacent atom, B. Atom B then polarizes so that its outer electrons are on the side of the atom closest to the + side (or opposite to the – side) of the dipole in A.

Hydrogen bonds

Hydrogen bonds keep water liquid at room temperature, and bind polymer chains together to give solid polymers.

Example: a) Give the electronic configurations of the sodium and chlorine atoms (expressed in terms of the s-orbits and p-orbits); and b) repeat this for their ions?

Solution:

a) The electronic configuration of the atoms can be obtained from a standard chemistry handbook. They are:

Na: $1s^2$, $2s^2$, $2p^6$ and $3s^1$

Cl: $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^5$.

(In this configuration, the superscript indicates the number of electrons present in the energy orbits.) Note that both Na and Cl are monovalent.

b) In the ion forms: Na+ : $1s^2$, $2s^2$ and $2p^6$ and Cl- : $1s^2$, 2 s^2, $2p^6$, $3s^2$,$3p^6$

In the ions, both the s- and p-orbits are completely filled. This type of electronic configuration (similar to that of the inert gas) will make the ionic solid relatively stable