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Lecture # 3

CHAPTER TWO/ ATOMIC STRUCTURE, INTERATOMIC BONDING

Introduction

Some of the important properties of solid materials depend on geometrical atomic arrangements, and also the interactions that exist among constituent atoms or molecules. This chapter, by way of preparation for subsequent discussions, considers several fundamental and important concepts—namely, atomic structure, electron configurations in atoms and the periodic table, and the various types of primary and secondary interatomic bonds that hold together the atoms that compose a solid.

ATOMIC STRUCTURE

Fundamental Concepts

Elements are assumed to be made of atoms. Each atom consists of a very small nucleus composed of protons and neutrons, which is encircled by moving electrons. Both electrons and protons are electrically charged, the same charge magnitude being 1.602×10^{-19} Coulombs, which is negative in sign for electrons and positive for protons; neutrons are electrically neutral. Masses for these subatomic particles are infinitesimally small; protons and neutrons have approximately the same mass, (m_n=m_p) 1.67 $\times 10^{-27}$ kg, which is significantly larger than that of an electron m_e, 9.11$\times 10^{-31}$ kg.

- **Atomic number (Z)** = is the number of protons in the nucleus, Each chemical element is characterized by (Z).
- **The atomic mass (A)** of a specific atom may be expressed as the sum of the masses of protons and neutrons within the nucleus.
- Although the number of protons is the same for all atoms of a given element, the number of neutrons (N) may be variable. Thus atoms of some elements have two or more different atomic masses, which are called **isotopes**, (**Isotopes** - atoms with same atomic number but different atomic masses).
- **The atomic weight** of an element is specified in mass per mole.
- **Mole** is the amount of matter that has a mass in grams or the amount of material that corresponds to atomic weight.
- The **atomic mass unit** (**amu**) may be used to compute atomic weight. The atomic mass unit is equal to 1.67 $\times 10^{-27}$ kg, and is defined as 1/12 the mass of carbon atom (1 amu = 1/12) that has Z=6, and N=6, where Z is the number of neutrons, (A=Z+N= 12).
- The number of atoms in a mole is defined as **Avogadro's number (N_{av}),** equal to **6.022×10^{23} atoms/mole**, (i.e. the atomic mass (A) of carbon =12; 1 mole of carbon =1×12=12gram).

The atomic weight of an element or the molecular weight of a compound may be specified on the basis of amu/atom (molecule) or mass/mole of material.

1 amu/atom (or molecule) = 1 g/mol

For **example**, the atomic weight of iron is 55.85 amu/atom, or 55.85 g/mol.

The number of atoms per cm^3 (**n**) in a piece of material of density ρ (g/cm^3) can be calculated as:

$$\mathbf{n = N_{av} \times \rho / M}$$

where; M is atomic mass in amu (g/mol), N_{av} is avogadro's number (6.022×10^{23} atoms/mol)

Example: Graphite (carbon) has a density of $1.8 g/cm^3$ and atomic weight of 12 grams per mol, calculate the atomic density?

Solution:

$$\mathbf{n = N_{av} \times \rho / M}$$

$\mathbf{N_{av}} = 6.022\times10^{23}$ atoms/mol

$\boldsymbol{\rho} = 1.8 g/cm^3$

M = 12 g/mol

Atomic density is defined as (n) the number of atoms per cm^3.

$$\mathbf{n} = \mathbf{(}6.022\times10^{23} \text{ atoms/mol} \times 1.8 \text{g/cm}^3\mathbf{)} / \mathbf{(}12 \text{ g/mol})$$

$$\mathbf{n = 9.33 \times 10^{22} \text{ atoms/ cm}^3}$$

Example: Ice has density of $1 g/cm^3$, calculate the number of atoms?

Solution:

$$\mathbf{n = N_{av} \times \rho / M}$$

$\mathbf{N_{av}} = 6.022\times10^{23}$ atoms/mol

$\boldsymbol{\rho} = 1 g/cm^3$

M (H_2O) = [(2×1)+(1×16)] g/mol = 18 g/mol

$$\mathbf{n} = \mathbf{(}6.022\times10^{23} \text{ atoms/mol} \times 1 \text{g/cm}^3\mathbf{)} / 18 \text{ g/mol}$$

$$\mathbf{n = 3.3 \times 10^{22} \; H_2O \text{ molecules/ cm}^3}$$

Since H_2O molecule contain 3 atoms, so;

$$\mathbf{n = 9.9 \times 10^{22} \text{ atoms/ cm}^3}$$

Example: Calculate the number of copper atoms present in a cylinder that has a diameter and a height both equal to 1 µm. The mass density of copper is 8.93 x 10^3 kg/m^3 and its atomic mass is 63.55 g/mol?

Solution: to calculate no. of atoms present in specific volume as follow;

a) The volume of the copper cylinder is given by:

$$\mathbf{V = \Pi \times r^2 \times h}$$

$$= 3.14 \times (0.5 \times 10^{-6})^2 \times 1 \times 10^{-6}\ m^3 = 0.78 \times 10^{-18}\ m^3$$

b) Its mass is:

$$\mathbf{Mass = \rho \times V}$$

$$8.93 \times 10^3\ kg/m^3 \times 0.78 \times 10^{-18}\ m^3 = 7.96 \times 10^{-15}\ kg = 7.96 \times 10^{-12}\ g;$$

c) The number of copper atoms present is:

$$\mathbf{n = Mass \times Nav / M}$$

$$\mathbf{n} = (7.96 \times 10^{-12}\ g \times 6.02 \times 10^{23}\ atoms/mol) / 63.55\ g/mol$$

$$= 6.6 \times 10^{10}\ atoms.$$

- **Valence**: The number of electrons in atoms that participate in bonding or chemical reaction.
- **Cation**: a positively charged ion, **i.e.,** the element that lost an electron.
- **Anion**: a negatively charged ion, **i.e.,** the element that attract an electron.
- **Electropositive element:** is an element whose atoms want to participate in chemical reactions by donating the electrons (*lose electrons and form positive ion*).
- **Electronegative element:** is an element whose atoms want to participate in chemical reactions by accepting the electrons (*accept electrons and form negative ion*).

H.W.(1): The mass density of copper is 8930 kg/m^3 and its atomic mass is 63.55 amu/atom. Calculate the number of copper atoms?

Electrons in Atoms

One early outgrowth of quantum mechanics was the simplified ***Bohr atomic model***, in which electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital. This model of the atom is represented in Figure 2.1.

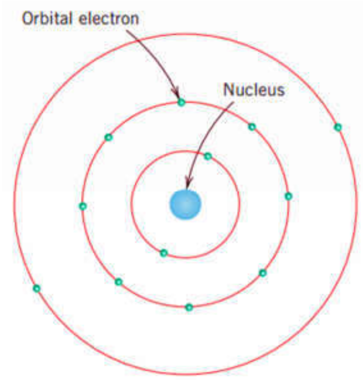


Figure 2.1 Schematic representation of the Bohr atom.

Every electron in an atom is characterized by four parameters called quantum numbers.

a) ***a principal quantum number n***, which may take on integral values beginning with unity; sometimes these shells are designated by the letters K, L, M, N, O, and so on, which correspond, respectively, to n = 1, 2, 3, 4, 5, . . . , as indicated in Table 2.1. Note also that this quantum number, and it only, is also associated with the Bohr model. This quantum number is related to the distance of an electron from the nucleus, or its position.
b) ***The second quantum number, angular momentum number, l***, signifies the subshell, which is denoted by a lowercase letter—an s, p, d, or f; it is related to the shape of the electron subshell. In addition, the number of these subshells is restricted by the magnitude of n. Allowable subshells for the several n values are also presented in Table 2.1.
   l, is quantized (***l*** = 0, 1, 2, 3……..n-1)
   at n = 1 (k shell) , l = 0 (s subshell)
c) The number of energy states for each subshell is determined by the third quantum number ***magnetic quantum number***, **ml**. For an s subshell, there is a single energy state, whereas for p, d, and f subshells, three, five, and seven states exist, respectively (**Table 2.1**). In the absence of an external magnetic

field, the states within each subshell are identical. However, when a magnetic field is applied, these subshell states split, with each state assuming a slightly different energy.

ml = (-l……..0…….+l)

d) Associated with each electron is a spin moment, which must be oriented either up or down. Related to this ***spin moment number*** is the ***fourth quantum number***, ms, for which two values are possible (+1/2 and -1/2), one for each of the spin orientations.

Pauli exclusion principle is used to determine the structure of the atom. The number of electrons in each shell is **($2n^2$)**, and the number of electrons in each sub shell is **2(2 l+1)** as shown in Table 2.1. Electron configurations for some of the more common elements are listed in Table 2.2.

Table 2.1 The Number of Available Electron States in Some of the Electron Shells and Subshells

Principal Quantum Number n	*Shell Designation*	*Subshells*	*Number of States*	*Number of Electrons*	
				Per Subshell	*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	

Table 2.2 A Listing of the Expected Electron Configurations for Some of the Common Elements[a]

Element	*Symbol*	*Atomic Number*	*Electron Configuration*
Hydrogen	H	1	$1s^1$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s^1$
Beryllium	Be	4	$1s^2 2s^2$
Boron	B	5	$1s^2 2s^2 2p^1$
Carbon	C	6	$1s^2 2s^2 2p^2$
Nitrogen	N	7	$1s^2 2s^2 2p^3$
Oxygen	O	8	$1s^2 2s^2 2p^4$
Fluorine	F	9	$1s^2 2s^2 2p^5$
Neon	Ne	10	$1s^2 2s^2 2p^6$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	Mg	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	Al	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus	P	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur	S	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine	Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon	Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
Potassium	K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium	Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium	Sc	21	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
Titanium	Ti	22	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Vanadium	V	23	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
Chromium	Cr	24	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Manganese	Mn	25	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$
Iron	Fe	26	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
Cobalt	Co	27	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
Nickel	Ni	28	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
Copper	Cu	29	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
Zinc	Zn	30	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
Arsenic	As	33	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$
Selenium	Se	34	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$
Bromine	Br	35	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$
Krypton	Kr	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

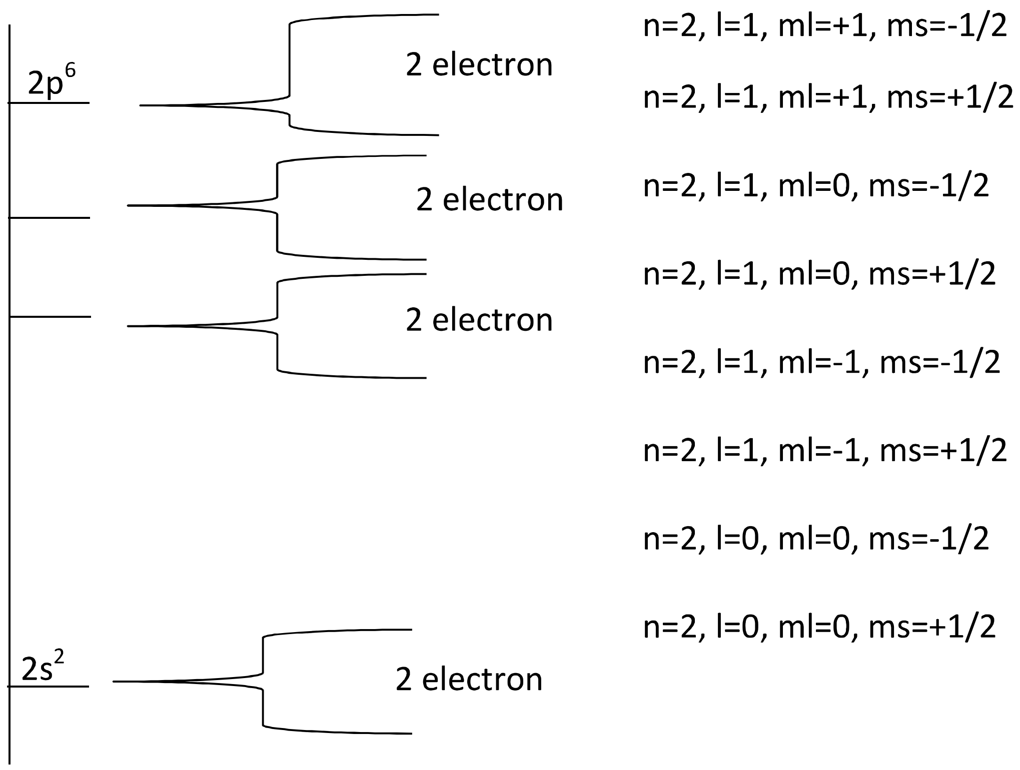
Example: Write the electron configuration for L shell?

Solution:

For L shell, quantum numbers are:

a) n = 2 (for L shell)
b) l = 0, 1, 2, 3 …………… (n-1) = 0, 1
c) ml = -l…….0…….+l = -1, 0, +1
d) ms = -1/2, +1/2

- The number of electrons in each shell is **($2n^2$)** = ($2 \times (2)^2$) = 8
- The number of electrons in each sub shell is **2(2 l+1),** l = 0, 1
  at l = 0, no. of electrons in each sub shell = 2, ***s level***
  at l = 1, no. of electrons in each sub shell = 6, ***p level***



H.W.(2): Write the electron configuration for K shell?

H.W.(3): Write the four quantum number for M and N shell?