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Atomic Structure and Bonding: A Review

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Abstract: All materials are built up from atoms and molecules, so there is a close relationship between the atomic basis of a material and its properties. Therefore, it is important to understand the atomic structure and the way atoms combine to form solid materials in order to understand the properties of materials.

Keywords: *Atomic Structure, Bonding.*

Atomic structure:

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, which is negative in sign for electrons and positive for protons; neutrons are electrically neutral (1).

Fundamental concepts

Atomic number:

Each chemical element is characterized by the number of protons in the nucleus, or the **atomic number (*Z*)**. For an electrically neutral or complete atom, the atomic number also equals the number of electrons. This atomic number ranges in integral units from 1 for hydrogen to 92 for uranium (1).

Atomic mass:

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** (1).

Significance of Isotopes:

The chemical properties of different isotopes are nearly identical because they have the same number of electrons. However, the physical properties of isotopes such as mass, melting or boiling point, density, and freezing point are all different. The physical properties of any isotope are primarily determined by its atomic mass.

The existence of mass differences leads to the dependence of phonon spectrum and phonon related effects on the isotope distribution in the material. Also, the unit-cell volume is isotope-dependent. Several properties such as thermal conductivity, superconductivity, adsorption, and diffusion are isotopic dependent (2). The **atomic weight** of an element corresponds to the weighted average of the atomic masses of the atom's naturally occurring isotopes (1).

Atomic models:

Classical physics, the collection of theories that existed before the advent of quantum mechanics, describes many aspects of nature at an ordinary (macroscopic) scale, but is not sufficient for describing them at small (atomic and subatomic) scales. On the other hand, **Quantum mechanics** is a fundamental theory in physics that provides a description of the physical properties of nature at the scale of atoms and subatomic particles (1).

Bohr atomic model:

It is a 2D model which is an early outgrowth of quantum mechanics, in which electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any electron is well defined in terms of its orbital.

Electrons are permitted to have only specific values of energy. An electron may change energy, but in doing so it must make a quantum jump either to an allowed higher energy (with absorption of energy) or to a lower energy (with emission of energy). Often, it is convenient to think of these allowed electron energies as being associated with *energy levels* or *states* (1).

The Bohr model represents an early attempt to describe electrons in atoms, in terms of both position (electron orbitals) and energy (quantized energy levels). This model was eventually found to have some significant limitations because of its inability to explain several phenomena involving electrons (3).

Wave-mechanical model:

It is a 3D model where the electron is considered to exhibit both wave-like and particle-like characteristics. With this model, an electron is no longer treated as a particle moving in a discrete orbital; rather, position is the probability of an electron's being at various locations around the nucleus. The position is described by a probability distribution or *electron cloud* (3). Figure (1) is a schematic representation for electron distribution in (a) Bohr and (b) wave-mechanical models.

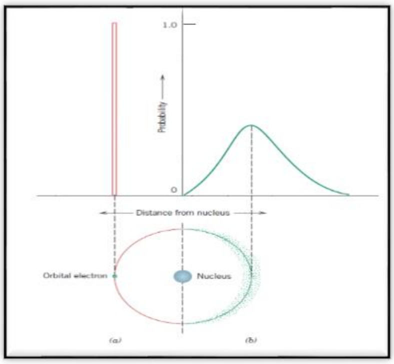


Figure 1 (*a*) Bohr and (*b*) wave-mechanical atom models in terms of electron distribution.

Quantum numbers:

1.3.1. Using wave mechanics, every electron in an atom is characterized by four parameters called **quantum numbers. Principal quantum number (n):** Specifies the shell number,

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. This quantum number is only associated with Bohr model (1). Figure (2) is a schematic representation of shells and sub shells in Bohr and wave mechanical models.

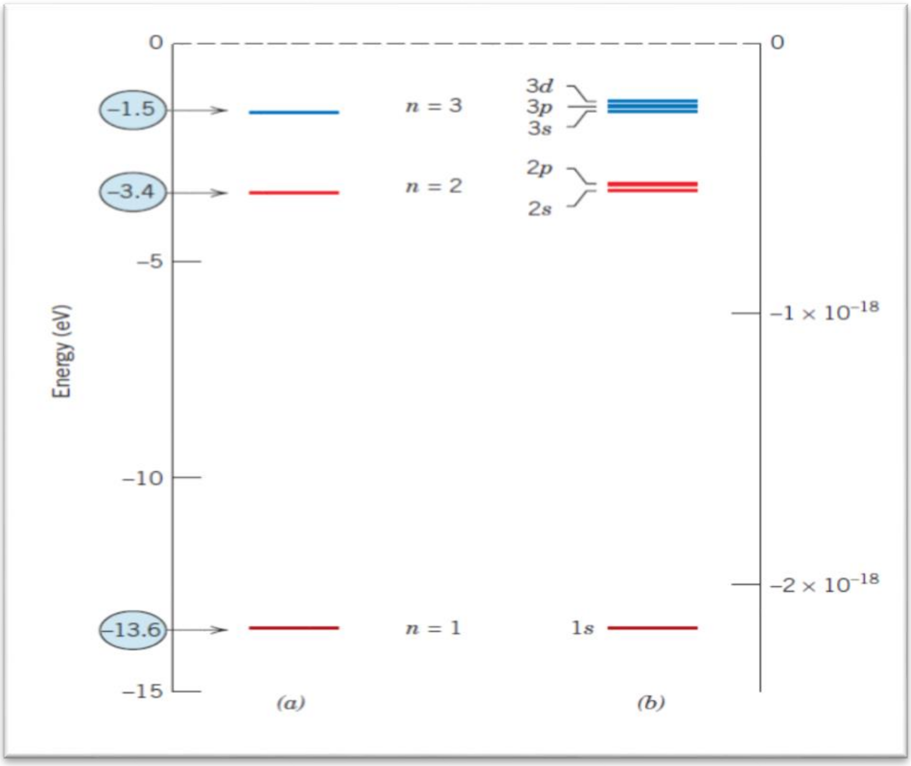


Figure (2) Schematic representation of shells and sub shells in (a) Bohr and (b) wave mechanical models.

1.3.2. Second quantum number (l):

signifies the subshell, which is denoted by a lowercase letter— *s*, *p*, *d*, or *f*; it is related to the shape of the electron subshell. Each shell has definite allowable number of subshells (1).

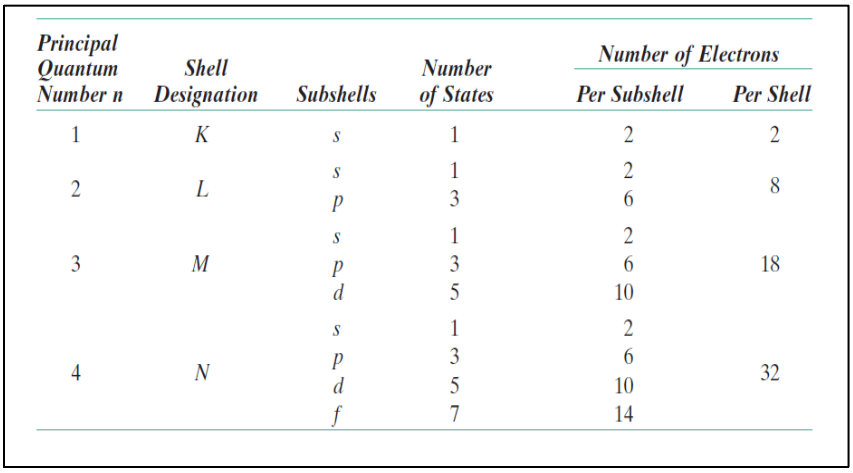
1.3.3. Third quantum number (m_l):

It is related to the number of energy states for each subshell. For an *s* subshell, there is a single energy state, whereas for *p*, *d*, and *f* subshells, three, five, and seven states exist, respectively (1).

1.3.4. Fourth quantum number (m_s):

Related to this spin moment which must be oriented either up or down. for which two values are possible (+ ½ and – ½), one for each of the spin orientations. The smaller the principal quantum number, the lower the energy level; for example, the energy of a 1*s* state < 2*s* state < 3*s*. Also, within each shell, the energy of a subshell level increases with the value of the *l* quantum number. For example, the energy of a 3*d* > 3*p* > 3*s* (1).

Table (1) Illustrates the different quantum numbers and 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	

Pauli exclusion principle:

It is a quantum-mechanical concept that is designated to determine the way the energy states are filled with electrons. Each electron state can hold no more than two electrons, which must have opposite spins. Thus, *s*, *p*, *d*, and *f* subshells may each accommodate, respectively, a total of 2, 6, 10, and 14 electrons. Electrons fill up the lowest possible energy states in the electron shells and subshells, two electrons (having opposite spins) per state. When all the electrons occupy the lowest possible energies in accordance with the foregoing restrictions, an atom is said to be in its ground state.

- **Valence electrons** are those that occupy the outermost shell. These electrons are extremely important; as will be seen, they participate in the bonding between atoms to form atomic and molecular aggregates. Furthermore, many of the physical and chemical properties of solids are based on these valence electrons. Some atoms have what are termed *stable electron configurations;* that is, the states within the outermost or valence electron shell are completely filled. Those are the inert gases (Ne, Ar, Kr and He). Atoms of the elements that have unfilled valence shells tend to assume stable electron configurations by gaining or losing electrons to form charged ions, or by sharing electrons with other atoms. Electropositive elements are those which can give up their few valence electrons to become positively charged ions. While electronegative elements readily accept electrons to form negatively charged ions (1).

Bonding forces and Energies:

Force as a function of interatomic separation between two atoms:

The interatomic forces that bind the atoms together directly affects the physical properties of the materials. At large distances, interactions are negligible, because the atoms are too far apart to have an influence on each other; however, at small separation distances, each atom exerts forces on the other. These forces are of two types, attractive (F_A) and repulsive (F_R). The magnitude of each depends on the separation or interatomic distance (r). The origin of an attractive force depends on the bonding that exists between the two atoms, while repulsive forces arise from interactions between the negatively charged electron clouds for the two atoms and are important only at small values of r as the outer electron shells of the two atoms begin to overlap. Figure (3) is a schematic plot of F_A and F_R versus r (1).

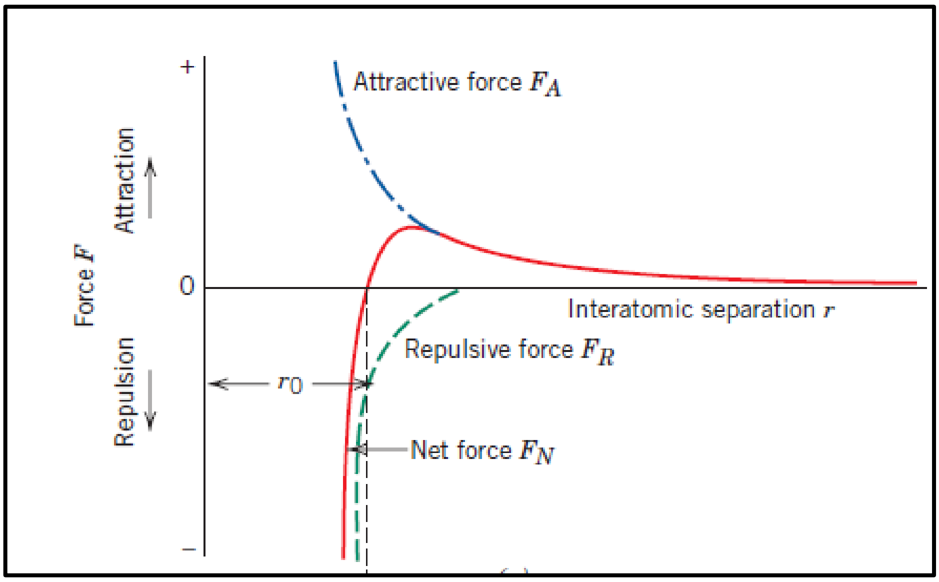


Figure (3) The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms.

The net force F_N between the two atoms is just the sum of both attractive and repulsive components: ($F_N = F_A + F_R$)

When F_A and F_R balance, or become equal, there is no net force; ($F_N+F_A=0$).

In that case, a state of equilibrium exists. The centers of the two atoms will remain separated by the equilibrium spacing r_0. In this equilibrium position, any attempt to move the two atoms farther apart will be counteracted by the attractive force, while pushing them closer together will be resisted by the increasing repulsive force (1).

Potential energy as a function of interatomic separation for two atoms:

Sometimes it is more convenient to work with the potential energies between two atoms instead of forces. Mathematically, energy (E) and force (F) are related as or, for atomic systems: $E= \int F dr$

$E_N= \int FNdr$, = $\int FAdr + \int FRdr$, $\mathbf{E_N = E_A+E_R}$

Figure (4) plots attractive, repulsive, and net potential energies as a function of interatomic separation for two atoms. The net curve is the sum of the attractive and repulsive curves. The minimum in the net energy curve corresponds to the equilibrium spacing, r_0 (1).

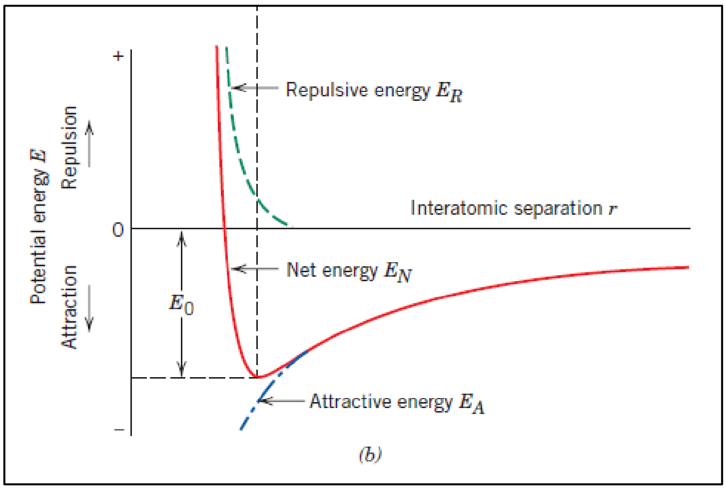


Figure (4) The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

The Bonding energy (E_0): Is the energy required to separate two atoms in equilibrium to an infinite distance (1).

The magnitude of this bonding energy and the shape of the energy versus interatomic separation curve vary from material to material, and they both depend on the type of atomic bonding (1).

Significance of bonding forces and energies:

Several material properties depend on E_0, the curve shape, and bonding type. For example, materials having large bonding energies typically also have high melting temperatures; at room temperature, solid substances are formed for large bonding energies, whereas for small energies the gaseous state is favored; liquids prevail when the energies are of intermediate magnitude (1).

In addition, the modulus of elasticity of a material depends on the shape of its force–versus–interatomic separation curve. The slope for a relatively stiff material at the r _ r_0 position on the curve will be quite steep; slopes are shallower for more flexible materials. Furthermore, how much a material expands upon heating or contracts upon cooling (that is, its linear coefficient of thermal expansion) is related to the shape of its E_0-versus-r_0 curve. A deep and narrow "trough," which typically occurs for materials having large bonding energies, normally correlates with a low coefficient of thermal expansion and relatively small dimensional alterations for changes in temperature (1).

Atomic Bonding

Primary or chemical bonds are three types found in solids. Those are ionic, covalent, and metallic. For each type, the bonding necessarily involves the valence electrons; furthermore, the nature of the bond depends on the electron structures of the constituent atoms. In general, each of these three types of bonding arises from the tendency of the atoms to assume stable electron structures, like those of the inert gases, by completely filling the outermost electron shell. **Secondary** or physical forces are also found in many solid materials; they are weaker than the primary ones, but even so influence the physical properties of some materials (1).

Primary bonds:

Ionic bonds:

It is always found in compounds that are composed of both metallic and nonmetallic elements, elements that are situated at the horizontal extremities of the periodic table. Atoms of a metallic element easily give up their valence electrons to the nonmetallic atoms. In the process all the atoms acquire stable or inert gas configurations and, in addition, an electrical charge; that is, they become ions. Sodium chloride (NaCl) is the classic ionic material. A sodium atom can assume the electron structure of neon (and a net single positive charge) by a transfer of its one valence 3*s* electron to a chlorine atom. After such a transfer, the chlorine ion has a net negative charge and an electron configuration identical to that of argon. In sodium chloride, all the sodium and chlorine exist as ions (1).

The attractive bonding forces are **coulombic;** that is, positive and negative ions, by virtue of their net electrical charge, attract one another. This type of bonding is illustrated schematically in Figure (5).

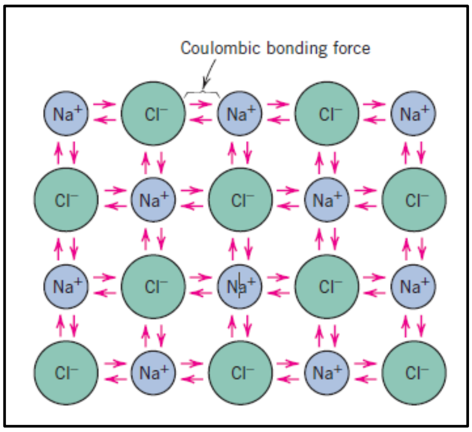


Figure (5) Schematic representation of ionic bonding in sodium chloride (NaCl).

Ionic bonding is termed *nondirectional;* that is, the magnitude of the bond is equal in all directions around an ion. It follows that for ionic materials to be stable, all positive ions must have as nearest neighbors negatively charged ions in a three-dimensional scheme, and vice versa. (1).

Ionic solids:

Ionic substances such as chlorides, nitrides and oxides of metals are the basic building blocks of ceramic materials. Bonding energies are relatively large and are reflected in high melting temperatures. Ionic materials are characteristically hard and brittle, also they are electrically and thermally insulative. These materials are very stable because of their high ionic bond strengths (4).

The ionic solids are hard and brittle because the ions in ionic solids are held in a lattice due to the electrostatic forces of attraction in cations and anions as well as the repulsion with the like charges. If a large enough force is applied along a certain plane this causes ions to shift along that layer which displaces that layer with respect to the next so, there will be the repulsion between like charges with ionic compounds. Because the ionic solids are localized, these solids tend to be stiff and brittle like covalent solids (5).

Covalent bonds:

In covalent bonding, stable electron configurations are assumed by sharing of electrons between adjacent atoms. Two atoms that are covalently bonded will each contribute at least one electron to the bond, and the shared electrons may be considered to belong to both atoms (1).

Covalent bonding is schematically illustrated in Figure (6) for a molecule of methane (CH4). The carbon atom has four valence electrons, whereas each of the four hydrogen atoms has a single valence electron. Each hydrogen atom can acquire a helium electron configuration (two 1*s* valence electrons) when the carbon atom shares with it one electron. The carbon now has four additional shared electrons, one from each hydrogen, for a total of eight valence electrons, and the electron structure of neon.

The covalent bond is directional; that is, it is between specific atoms and may exist only in the direction between one atom and another that participates in the electron sharing. Many nonmetallic elemental molecules (H_2, Cl_2, F_2,) as well as molecules containing dissimilar atoms, such as CH_4, H_2O, HNO_3, and HF are covalently bonded. Furthermore, this type of bonding is found in elemental solids such as diamond (carbon) and silicon (1).

Bond Polarity:

The electron pairs shared between two atoms are not necessarily shared equally.

- ***Non-polar covalent bond*** is one in which the electrons are shared *equally* between two atoms**.**
- ***Polar covalent bond*** is one in which one atom has a greater attraction for the electrons than the other atom. If this relative attraction is great enough, then the bond is an ionic bond (2).

The polarity of a bond—the extent to which it is polar—is determined largely by the relative electronegativities of the bonded atoms. Thus, there is a direct correlation between electronegativity and bond polarity. A bond is *nonpolar* if the bonded atoms have equal electronegativities. If the electronegativities of the bonded atoms are not equal, however, the bond is *polarized* toward the more electronegative atom (2).

Mixed bonds:

It is possible to have interatomic bonds that are partially ionic and partially covalent, and, in fact, very few compounds exhibit pure ionic or covalent bonding. For a compound, the degree of either bond type depends on the relative positions of the constituent atoms in the periodic table or the difference in their electronegativities. The wider the separation (both horizontally— relative to Group IVA—and vertically) from the lower left to the upper right-hand corner (i.e., the greater the difference in electronegativity), the more ionic the bond. Conversely, the closer the atoms are together (i.e., the smaller the difference in electronegativity), the greater the degree of covalency (1).

Significance of bond polarity:

The degree of ionic character in covalent compounds directly affects their chemical and physical properties. The viscosity, melting and boiling points of covalent compounds exhibiting polarity are higher than those of non-polar compounds. For example, diatomic fluorine (F2), boiling point –188°C, is purely covalent as both small atoms are 'pulling' equally on each other's electrons (EN difference = 0). Whereas in hydrogen fluoride (HF), the EN difference is 1.9, resulting in HF having around 44% ionic character and a boiling point of 19.5°C (6).

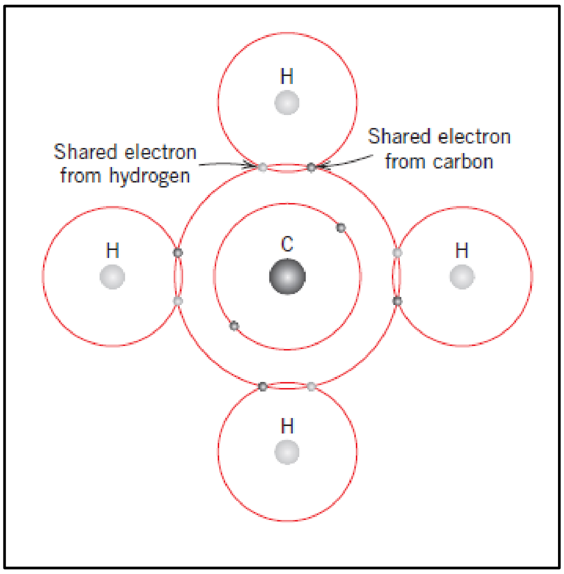


Figure (6) Schematic representation of covalent bonding in a molecule of methane (CH4).

Covalent solids:

An example of a covalently bonded solid is diamond, which is a form of carbon. Carbon has an arrangement of electrons in its outer shell such that it needs four more electrons to obtain a configuration similar to neon; in the case of diamond, it achieves this by sharing electrons with neighboring carbon atoms.

Metallic bonds:

The final primary bonding type is found in metals and their alloys. Metallic materials have one, two, or at most, three valence electrons. These valence electrons are not bound to any atom in the solid and are free to drift throughout the entire metal. They may be thought of as belonging to the metal as a whole or forming an "electron cloud." The remaining non valence electrons and atomic nuclei form what are called *ion cores*, which possess a net positive charge equal in magnitude to the total valence electron charge per atom. Figure (7) is a schematic illustration of metallic bonding. The free electrons shield the positively charged ion cores from mutually repulsive electrostatic forces, which they would otherwise exert upon one another; consequently, the metallic bond is nondirectional in character. In addition, these free electrons act as a "glue" to hold the ion cores together (4).

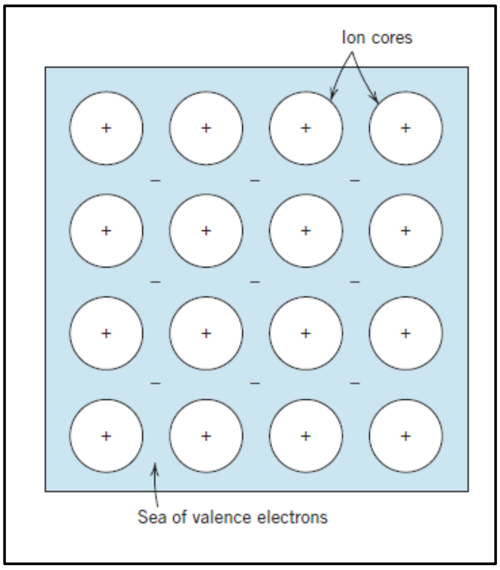


Figure (7) Schematic illustration of metallic bonding.

Factors affecting the strength of metallic bond:

- The number of electrons delocalized from the metal, the greater the number of delocalized electrons, the stronger the bond.
- Charge held by the metal cation, the greater the magnitude of the charge, the stronger the force of attraction between the electron sea and the cations.
- Size of the cation; the smaller the ionic radius, the greater the effective nuclear charge acting on the electron sea (7).

Metallic solids:

Some general behaviors of the various material types may be explained by bonding type. For example, metals are good conductors of both electricity and heat, because of their free electrons. On the other hand, ionically and covalently bonded materials are typically electrical and thermal insulators because of the absence of large numbers of free electrons (1).

Furthermore, that at room temperature, most metals and their alloys fail in a ductile manner; that is, fracture occurs after the materials have experienced significant degrees of permanent deformation. This behavior is related to the characteristics of the metallic bond. While at room temperature, ionically bonded materials are intrinsically brittle because of the electrically charged nature of their component ions (1).

Effect of metallic bond on the properties:

The presence of the mobile valence electrons, as well as the non-directionality of the binding force between metal ions, account for the malleability and ductility of most metals. When a metal is shaped or drawn, it does not fracture, because the ions in its crystal structure are quite easily displaced with respect to one another. Moreover, the nonlocalized valence electrons act as a buffer between the ions of like charge and thereby prevent them from coming together and generating strong repulsive forces that can cause the crystal to fracture (7).

Secondary intermolecular bonds (Van Der Waals bonding)

Secondary, Van der Waals, or physical **bonds** are weak in comparison to the primary or chemical ones. Secondary bonding exists between nearly all atoms or molecules. Secondary bonding is evidenced for the inert gases, which have stable electron structures, and, in addition, between molecules in molecular structures that are covalently bonded (1).

The consequence of sharing of electrons by two or more atomic nuclei is that the electrons will spend a relatively longer time in one particular position. The effect of this is that one end of the molecule may acquire a slight positive charge and the other end a slight negative charge, resulting in an electrical imbalance known as ***an electric dipole***. These dipoles allow molecules to interact with one another, and to form weak secondary bonds (4).

Fluctuating induced dipole bonds:

A dipole may be created or induced in an atom or molecule that is normally electrically symmetric; that is, the overall spatial distribution of the electrons is symmetric with respect to the positively charged nucleus.

All atoms are experiencing constant vibrational motion that can cause instantaneous and short-lived distortions of this electrical symmetry for some of the atoms or molecules, and the creation of small electric dipoles. One of these dipoles can in turn produce a displacement of the electron distribution of an adjacent molecule or atom, which induces the second one also to become a dipole that is then weakly attracted or bonded to the first; this is one type of van der Waals bonding. These attractive forces may exist between large numbers of atoms or molecules, which forces are temporary and fluctuate with time (8).

Melting and boiling temperatures are extremely low in materials for which induced dipole bonding predominates; of all possible intermolecular bonds, these are the weakest (1).

The molecules in which fluctuating induced dipole forces can be seen include, halogens (F_2, Cl_2, I_2, and Br_2), homoatomic gases (O_2, N_2, H_2), noble gases (He, Ne, Kr), and hydrocarbons (CH_4, C_2H_3) (6).

Polar molecule-Induced dipole bonds:

Permanent dipole moments exist in some molecules by virtue of an asymmetrical arrangement of positively and negatively charged regions; such molecules are termed **polar molecules.** A permanent dipole moment arises from net positive and negative charges that are respectively associated with the hydrogen and chlorine ends of the HCl molecule. Polar molecules can also induce dipoles in adjacent nonpolar molecules, and a bond will form as a result of attractive forces between the two molecules. Furthermore, the magnitude of this bond will be greater than for fluctuating induced dipoles (1).

Permanent dipole bonds:

Van der Waals forces will also exist between adjacent polar molecules. The associated bonding energies are significantly greater than for bonds involving induced dipoles. The strongest secondary bonding type, the hydrogen bond, is a special case of polar molecule bonding (1).

Hydrogen bonding, a special type of secondary permanent dipole bonding, is found to exist between some molecules that have hydrogen as one of the constituents. The hydrogen atom can be imagined as a proton on the end of a covalent bond, but, unlike other atoms, the positive charge of the proton is not shielded by surrounding electrons. Therefore, it will have a positive charge and will be attracted to the electrons of atoms in other molecules. A necessary condition for the formation of a hydrogen bond is that an electronegative atom should be in the proximity of the hydrogen atom, which is itself bonded to an electronegative atom (4).

Molecular solids:

It is possible to create a wide variety of different molecules, some of which can be solid at room temperature. If the molecules are sufficiently large, they are bonded together due to numerous dipole– dipole interactions. The low bond strength means that such solids will have a very low melting temperature and the upper limit for molecular solids is approximately 100°C (4).

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