Biomaterials Journal
http://www.biomatj.com
Online ISSN: 2812-5045

Type of the Paper (Review Article)

Atomic structure and interatomic bonding

Menna S. Gaber [1,*]

[1] *Teaching assistant of dental materials science/ Dental Biomaterials department/ Faculty of Dentistry/ Cairo University*

* Corresponding author e-mail: Menna.sayed@dentistry.cu.edu.eg

Abstract: Some of the important properties of solid materials depend on the atomic arrangement, and also the interactions that exist between constituent atoms or molecules. So, atomic structure, the periodic table, and the various types of primary and secondary interatomic bonds that hold together the atoms comprising a solid are fundamental and important concepts in materials science and engineering

Keywords: *bonding; atomic structure; periodic table.*

Citation: Menna S. Gaber. *Atomic structure and interatomic bonding. Biomat. J., 1 (3),17 – 25 (2022)*

https://doi.org/10.5281/znodo.5829408

Received: 10 February 2022

Accepted: 27 February 2022

Published: 20 March 2022

An important reason to understand interatomic bonding in solids is that the type of bond allows a material's properties to be explained. For example, carbon which exist as both graphite and diamond. Graphite is relatively soft and has a "greasy" feel to it while, diamond is the hardest known material. This large difference in properties is related to the type of interatomic bonding found in graphite that does not exist in diamond. (1)

II.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; electrons are negatively charged, protons are positively charged while neutrons are electrically neutral. (1)

⚜ 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, the highest of the naturally occurring elements. (1)

◎ The atomic mass (A) of a specific atom is 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)

III. Interatomic bonding:

III.1.Atomic models:

⚜ Bohr model and quantum model are models that explain the structure of an atom. The key difference between Bohr and quantum model is that Bohr model states that electrons behave as particles whereas quantum model explains that the electron has both particle and wave behavior. (1)

Bohr Model:

- The electrons move around the nucleus in spherical orbitals which have a fixed size and energy. Each orbit has a different radius and is named from nucleus to the outside as n=1, 2, 3, etc. or n= K, L, M, etc. where n is the fixed energy level number.

- When an electron is moving in a certain orbital, the energy of that electron is constant. Electrons can move from one energy level to another by absorbing or releasing energy. This movement causes radiation. Bohr model perfectly fit the hydrogen atom which has a single electron but have some limitations.

◎ Limitations: It does not explain the spectra of atoms having more than one electron. (ii) Bohr's atomic model failed to explain the effect of the magnetic field (Zeeman Effect) or electric field (Stark effect) on the spectra of atoms or ions. (1)

Wave-mechanical model:

⚜ 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 considered to be the probability of an electron's being at various locations around the nucleus. In other words, position is described by a probability distribution or electron cloud. Figure 1 compares Bohr and wave-mechanical models for the hydrogen atom. (1)

Quantum Numbers:

Using wave mechanics, every electron in an atom is characterized by four parameters called quantum numbers.

Principal quantum number n: letters K, L, M, N, O, …… This quantum number is related to the distance of an electron from the nucleus, or its position.

The second quantum number l "the subshell": which is denoted by a lowercase letter….. s, p, d, or f; it is related to the shape of the electron subshell.

The number of energy states for each subshell is determined by the third quantum number (n-1). 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). Spin moment is the fourth quantum number ms : Associated with each electron is a spin moment, which must be oriented either up or down. Related to this, for which two values are possible (+1/2 and-1/2), one for each of the spin orientations.

N.B.: The smaller the principal quantum number, the lower the energy level; for example, the energy of a 1s state is less than that of a 2s state, which in turn is lower than the 3s.

◎ Second, within each shell, the energy of a subshell level increases with the value of the l quantum number. For example, the energy of a 3d state is greater than a 3p, which is larger than 3s.

◎ However, there may be overlap in energy of a state in one shell with states in an adjacent shell, which is especially true of d and f states; for example, the energy of a 3d state is greater than that for a 4s.

• To determine the manner in which these states are filled with electrons, we use the Pauli exclusion principle, which states that each electron state can hold no more than two electrons, which must have opposite spins(one is clockwise and the other is counter-clockwise). Thus, s, p, d, and f subshells may each accommodate, respectively, a total of 2, 6, 10, and 14 electrons.

For example, the electron configurations for hydrogen, helium, and sodium are, respectively, 1s1, 1s2, and 1s22s22p63s1.

III.2.Valence electrons:

⚜ The valence electrons are those that occupy the outermost shell. These electrons are extremely important; as they participate in the bonding between atoms to form molecules. Furthermore, many of the physical and chemical properties of solids are based on these valence electrons.

◎ In addition, some atoms have what are termed "stable electron configurations"; where the outermost or valence electron shell are completely filled. These elements (Ne, Ar, Kr, and He) are the inert gases, which are unreactive chemically.

◎ Some atoms of the elements that have unfilled valence shells assume stable electron configurations by gaining or losing electrons to form charged ions, or by sharing electrons with other atoms. This is the basis for some chemical reactions, and also for atomic bonding in solids. (1)

III.3.The Periodic table:

⚜ All the elements have been classified according to electron configuration in the periodic table. The elements are situated, with increasing atomic number, in seven horizontal rows called periods. All elements present in a given column or group have similar valence electron structures, as well as chemical and physical properties. (1)

◎ Electropositive elements are capable of giving up their few valence electrons to become positively charged ions.

◎ Electronegative elements situated on the right-hand side of the table are that accept electrons to form negatively charged ions, or share electrons with other atoms,(Figure2) (1).

◎ The electronegativity value: indicates the attraction of an atom for shared electrons.

◎ As a general rule, electronegativity increases in moving from left to right and from bottom to top with fluorine as the highest.

III.4.Bonding Energies and Forces:

⚜ Between any two atoms, there are forces of attraction drawing them together and forces of repulsion pushing them apart. The magnitude of each depends on the separation or interatomic distance.

◎ Both forces increase as the distance between the atoms decreases. Attractive forces (FA) arise from primary bonding between the two atoms. Repulsive forces (FR) arise from interactions between the negatively charged electron clouds or between the positively charged nuclei for the two atoms and are important only at small interatomic distances (1)(2)

⚜ The position at which both forces are equal in magnitude but opposite in direction is considered the equilibrium position of the atoms where the net force (FN) equals to zero.

◎ The interatomic distance at equilibrium (r0) represents the distance between the centers of the two adjacent atoms, where any attempt to move the two atoms farther apart is counteracted by the attractive force, while pushing them closer together is resisted by the increasing repulsive force. (1)(2)

◎Integration of the interatomic force over the interatomic distance yields the interatomic energy (EN). It represents the energy required to separate the two atoms.

◎ In contrast to the resultant force, the interatomic energy does not change much initially as two atoms come closer together. As the resultant force approaches zero, the energy value decreases and finally reaches a minimum when the resultant force becomes zero (at equilibrium interatomic distance). Thereafter, the energy increases rapidly because the resultant repulsive force increases rapidly with little change in interatomic distance **(1)(2)**

⚜ Correlation between Bonding Energy and Materials Properties

1- Coefficient of thermal expansion: is a material property that indicates the extent to which a material expands upon heating and increase in the average distance between the atoms. The energy-distance curve is in the form of an energy trough, the minimal energy required to maintain equilibrium is indicated by the bottom of the trough.

As the temperature increases, the amplitude of the atomic vibration increases. Consequently, the mean interatomic distance and internal energy increase. For all materials, the higher the atomic bonding energy, the deeper and narrower this energy trough (Figure 5A). As a result, the increase in interatomic separation with a given rise in temperature is lower, yielding a lower coefficient of thermal expansion than that of a material with lower bonding energy and shallower energy trough (1)(2)

2-Melting and boiling temperatures: The linear coefficient of thermal expansion of materials tends to be inversely proportional to the melting temperature. If the temperature continues to increase, the increase of interatomic distance will result in change of state. For a solid with greater minimum energy (a deeper trough depth), greater amounts of energy are required to achieve melting and boiling, which corresponds to higher melting and boiling temperatures. (1)(2)

3- Modulus of elasticity: is measured by the slope of the force-distance curve

near equilibrium. A steep slope means that a greater force is required to stretch

the bond thus the material has a high modulus of elasticity .

N.B. Ionic bonds tend to have the highest bond energy due to the large difference

in electronegativities between the ions followed by the covalent bonds, and then finally the metallic bond.(1)(2)

III.5.Types of bonds:

III.5.A.Primary interatomic bonding:

It includes three types of bonding, arises from the tendency of the atoms to assume stable electron structures, by completely filling the outermost electron shell.(1)

III.5.A.1.Ionic bonding:

- 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, has a large electronegativity difference (1.8 or more).

- Atoms of a metallic element easily give up their valence electrons to the nonmetallic atoms and acquire stable an electrical charge as become ions.

- Sodium chloride (NaCl) is the classic ionic material. A sodium atom acquire and a net single positive charge by a transfer of its one valence electron to a chlorine atom. (1)

- After such a transfer, the chlorine ion has a net negative.

- Ionic bonding is non-directional. The magnitude of the bond is equal in all directions around an ion. This is because ionic bonds are a result of the electrostatic fields that surround ions, and these fields will interact with any other ions in the vicinity.

- Dental Examples such as in gypsum structures,phosphate-based cements, and ceramic materials.(1)(3)

III.5.A.2.Covalent bonding:

Two atoms that are covalently bonded will share at least one electron to the bond.

Example: Methane(CH_4):The carbon atom has four valence electrons, whereas each of the four hydrogen atoms has a single valence electron. Each hydrogen atom and the carbon atom now has four additional shared electrons, one from each hydrogen.

- The covalent bond is directional as it lies between specific atoms and may exist only in the direction between one atom and another that participates in the electron sharing.

- This type of bonding is found in elemental solids such as diamond(carbon) where in each carbon atom covalently bonds with four other carbon atoms.

- Dental example: Covalent bonding occurs in many organic compounds, such as in dental polymers.(1)(3)

- A nonpolar covalent bond: is an equal or almost equal sharing of electrons and has almost no electronegativity difference (0.0 to 0.4).

◎ A polar covalent bond: occurs between nonmetal atoms, is an unequal sharing of electrons and has a moderate electronegativity difference (0.5 to 1.7).

Example: O-Cl (3.5 - 3.0) = 0.5 ………Polar covalent.

III.5.A.3.Metallic Bonding:

⚜ Metallic bonding is found in metals and their alloys which have one, two or three valence electrons able to drift throughout the entire metal forming a "sea of electrons" or an "electron cloud." The remaining non valence electrons and atomic nuclei form what are called ion cores.

◎ 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. (1)(3)

III.5.B.Secondary bonds:

⚜ Secondary, van der Waals, or physical bonds are weak in comparison to the primary or chemical ones. Secondary bonding exists between virtually all atoms or molecules, but its presence may be masked if any of the three primary bonding types is present.

◎ Secondary bonding forces arise from atomic or molecular dipoles. An electric dipole exists whenever there is some separation of positive and negative portions of an atom or molecule. The bonding results from the attraction between the positive end of one dipole and the negative region of an adjacent one. (1)

III.5.B.1. Fluctuating Induced Dipole Bonds:

⚜ A dipole may be created or induced in an atom or molecule that is normally electrically symmetric (the overall spatial distribution of the electrons is symmetric with respect to the positively charged nucleus), also may be present between inert gases.

◎ All atoms experience constant vibrational motion that can cause instantaneous and short-lived distortions of this electrical symmetry creating 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 and temporarily attracted or bonded to the first.

◎ Melting and boiling temperatures are extremely low in materials with induced dipole bonding as they are the weakest of all intermolecular bonds. (1)

III.5.B.2. 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. hydrogen chloride molecule; 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.(1)

III.4.B.3. 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 type of polar molecule bonding. It occurs between molecules in which hydrogen is covalently bonded to fluorine (as in HF), oxygen (as in H2O), and nitrogen (as in NH3). For each H—F, H—O, or H—N bond, the single hydrogen electron is shared with the other atom.

⚜ Thus, the hydrogen end of the bond is essentially a positively charged bare proton that is unscreened by any electrons. This highly positively charged end of the molecule is capable of a strong attractive force with the negative end of an adjacent molecule, as demonstrated in for HF. (1)

◎ Melting and boiling temperatures for hydrogen fluoride and water are abnormally high considering their low molecular weights, as a consequence of hydrogen bonding. (1)

III.5.C. Mixed bonds:

⚜ The four bonding types (ionic, covalent, metallic and van der Waals) are represented on a three-dimensional bonding tetrahedron (a tetrahedron with one of these "extreme" types located at each vertex).

◎ Many real materials, the atomic bonds are mixtures of two or more of these extremes (i.e., mixed bonds). (1)

◎ Three mixed bond types: (included on edges of this tetrahedron)

III.5.C. 1.Mixed covalent–ionic bonds:

⚜ There is some ionic character to most covalent bonds and some covalent character to ionic ones.

◎ 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. (1)

◎ The wider the separation (both horizontally and vertically in the periodic table) from the lower left to the upper right corner (i.e., the greater the difference in electronegativity), the more ionic is the bond.

◎ Conversely, the closer the atoms are together (i.e., the smaller the difference in electronegativity), the greater is the degree of covalency. (1)

III.5.C. 2.Mixed metallic and covalent bonds:

⚜ Are called the metalloids or semi-metals, and their properties are intermediate between the metals and nonmetals. (1)

III.5.C. 3.Mixed metallic–ionic bonds:

⚜ They are observed for compounds composed of two metals when there is a significant difference between their electronegativities. This means that some electron transfer is associated with the bond. (1)

Example: There is little ionic character to Titanium–aluminum bond for the intermetallic compound TiAl3 because electronegativities of both Al and Ti are the same (1.5). However, a much greater degree of ionic character is present for AuCu3;the electronegativity difference for copper and gold is 0.5. (1)

IV.Influence of Bond Type on Structure and Properties:

IV.1.Structure and density:

⚜ Neither the metallic nor the ionic bond is directional and this allows metal atoms to pack closely together in a regular crystalline array.

◎ The majority of metals form closely packed arrangements with coordination numbers of either 12 (close packed hexagonal or face centred cubic systems) or 8 (body centred cubic systems) and this explains the high density of metals.(4)

◎ The coordination number for ionic crystals is frequently 4, 6 or 8 and so, on average, ionic crystals possess lower packing densities than metals. The reasons for this are:

A.an ionic compound contains at least two types of ion which may be of different size, compared with a pure metal where all atoms are identical

B.The ions possess opposing charges. (4)

- Covalent bonds are directional and this will affect the structures of covalent crystals. The coordination number for diamond is four with each carbon atom bonded to four other atoms of carbon.

- Metals and ceramics are fully crystalline but polymers and glasses are either partially crystalline or completely amorphous.

- In amorphous structures, the atoms or molecules are not packed in a regular and symmetrical pattern and the amount of void space is greater than within a crystal.

- Polymer molecules are very large and, in many instances, of complex shape so that void spaces of considerable size can occur within the structure, which is reflected as lower density compared to metals and ceramics. (4)

IV.2.Stability and melting point:

- The stability of a substance is related to the bond strength. One indicator of bond strength and stability is the melting point of a substance. (4)

- In covalently bound crystals, the strength of the bonds lessens as the atomic number of the element increases and the distance of the outer shell, or valence,

- In metals, although the strength of the metallic bond tends to be less than that of ionic and covalent bonds, the close packing of atoms leads towards relatively high melting points

- Polymers have low melting points in the range 100-400°C. Although the bonding within molecules is covalent, only weak van der Waal's bonds exist between molecules and it is these secondary bonds that influence melting temperatures. (4)

IV.3. Stiffness:

- The modulus of elasticity E (Young's modulus) is a measure of the stiffness of a material. Crystalline structures, metals and ceramics, have high values of E, generally within the range 40-450 GPa while polymer materials have low stiffnesses, usually in the range 0.7-3.5 GPa. (4)

IV.4. Electrical properties:

- Metals are electrically conductive. In an electric field, the electrons in the electron cloud will move preferentially in one direction producing an electric current.

- Ionic and covalent solids are insulators because their valency electrons are localized around one or a pair of atoms.

- However, the ions in ionic crystals become mobile in solutions. These mobile ions move preferentially when influenced by an electric field. This ionic conduction is termed electrolytic conduction and the solution is termed an electrolyte.(4)

References:

1. Callister WD. Materials science and engineering : an introduction. 7 th. John Wiley & Sons,New York; 2007.

2. Anusavice, Kenneth J., Ralph W. Phillips, Chiayi Shen and HRR. Phillips' science of dental materials. St. Louis, Mo: Elsevier/Saunders. 2003.

3. Noort R Van. Introduction to dental materials. 2002.

4. John V. Introduction to Engineering Materials. 1992.