

Inter atomic Bonding

There are four important mechanisms by which atoms are bonded in engineered materials. These are:

1. Metallic bond.
2. Covalent bond.
3. Ionic bond.
4. Van der Waals bond.

In the first three of these mechanisms, bonding is achieved when the atoms fill their outer s and p levels. These bonds are relatively strong and are known as primary bonds (relatively strong bonds between adjacent atoms resulting from the transfer or sharing of outer orbital electrons). The van der Waals bonds are secondary bonds and originate from a different mechanism and are relatively weaker.

1.The Metallic Bond: It is the atomic bonding mechanism in pure metals and metal alloys. The metallic bond forms when atoms give up their valence electrons, which then form an electron sea. The positively charged atom cores are bonded by mutual attraction to the negatively charged electrons.

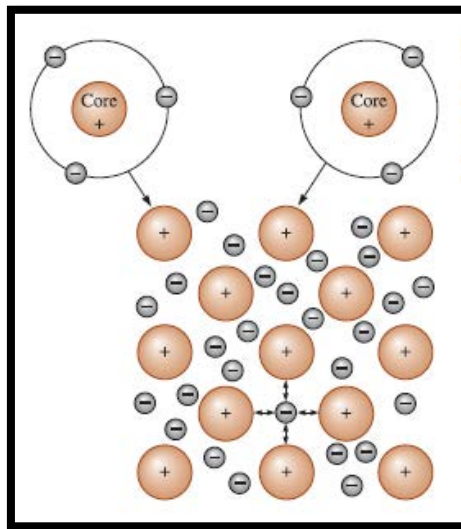


Figure 1. Diagrammatic Representation of the "Metallic Bond".

Because their valence electrons are not fixed in any one position, most pure metals are good electrical conductors of electricity at relatively low temperatures ($T < 300 \text{ K}$). Under the influence of an applied voltage, the valence electrons move, causing a current to flow if the circuit is complete. Because of the general distribution of electrons and their freedom to move within the metal, metallic bonding provides typical properties of materials characterized such as good electrical conductivity, good conduction of heat and good ductility.

2.The Covalent Bond: In the covalent bond, electrons are shared (as opposed to transferred) between atoms in their outermost shells to achieve a stable set of eight. For example, a silicon atom, which has a valence of four, gets eight electrons in its outer energy shell by sharing its electrons with four surrounding silicon atoms (Figure 2). Each instance (case) of sharing represents one covalent bond; thus, each silicon atom is bonded to four neighboring atoms by four covalent bonds. In order for the covalent bonds to be formed, the silicon atoms must be arranged so the bonds have a fixed directional relationship with one another. Solids with covalent bonding generally possess high hardness and low electrical conductivity.

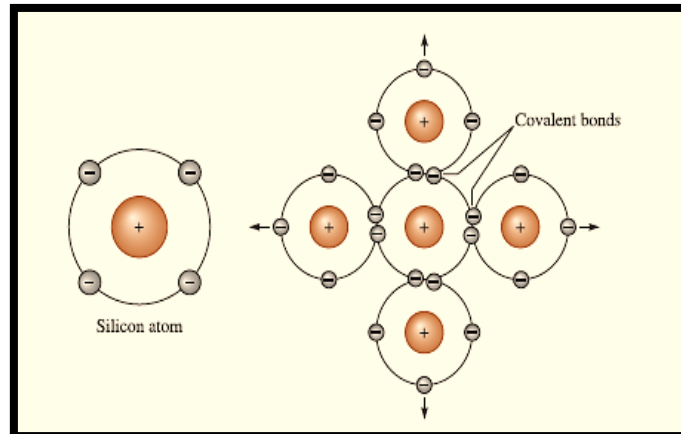


Figure 2. Covalent bonding requires that electrons be shared between atoms in such a way that each atom has its outer **sp** orbital filled. In silicon, with a valence of four, four covalent bonds must be formed for every atom.

3.The Ionic Bond: In the ionic bond, when more than one type of atoms are present in a material, one atom may donate its valence electrons to a different atom, filling the outer energy shell of the second atom. Both atoms now have filled (or emptied) outer energy levels, but both have acquired an electrical charge and behave as ions. The atom that contributes the electrons is left with a net positive charge and is called a **cation**, while the atom that accepts the electrons acquires a net negative charge and is called an **anion**. The oppositely charged ions are then attracted to one another and produce the **ionic bond**. This bond is naturally provides a very strong bond between atoms and as a properties of solid materials with the ionic bonding include low electrical conductivity and poor ductility.

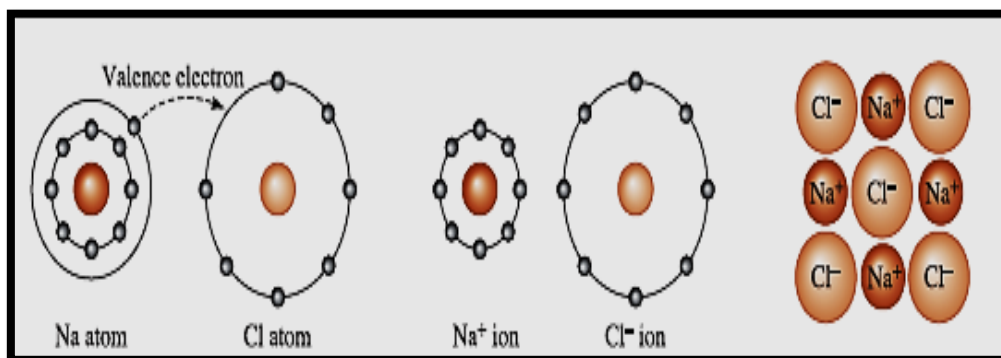


Figure 3. An ionic bond is created between two unlike atoms with different electronegativities. When sodium donates its valence electron to chlorine, each atom becomes an ion, and the ionic bond is formed.

Solids that exhibit considerable ionic bonding are also often mechanically strong because of the strength of the bonds. Electrical conductivity of ionically bonded solids is very limited. A large fraction of the electrical current is transferred via the movement of ions. Owing to their size, ions typically do not move as easily as electrons. However, in many technological applications we make use of the electrical conduction that can occur via movement of ions as a result of increased temperature, chemical potential gradient, or an electrochemical driving force. Examples of these include lithium ion batteries that make use of lithium cobalt oxide, conductive indium tin oxide (**ITO**) coatings on glass for touch sensitive displays, and solid oxide fuel cells (**SOFC**) based on compositions based on zirconia (**ZrO₂**).



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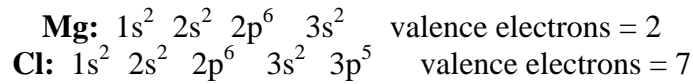


EXAMPLE.1 Describing the Ionic Bond Between Magnesium and Chlorine.

Describe the ionic bonding between magnesium and chlorine ???

SOLUTION

The electronic structures and valences are



Each magnesium atom gives up its two valence electrons, becoming a Mg^{+2} ion. Each chlorine atom accepts one electron, becoming a Cl^- ion. To achieve the ionic bonding, there must be twice as many chloride ions as magnesium ions present, and a compound, MgCl_2 , is formed.

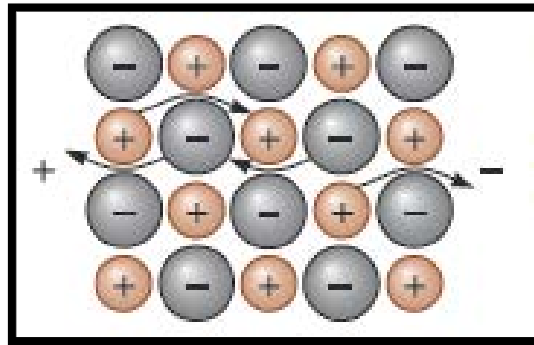


Figure 4. When voltage is applied to an ionic material, entire ions must move to cause a current to flow. Ion movement is slow and the electrical conductivity is poor at low temperatures (for Example 1).

4. Van der Waals Bonding: They are very small forces of attraction acting between atoms in cases where the formation of ionic or covalent bonds is not possible. Basically similar forces also act between atoms which are already bounded in neighboring molecules, giving rise to weak Van der Waal's forces between long-chain molecules in polymers.

Mixed Bonding: In most materials, bonding between atoms is a mixture of two or more types. **Iron**, for example, is bonded by a combination of metallic and covalent bonding that prevents atoms from packing as efficiently as we might expect.

Compounds formed from two or more metals (intermetallic compounds) may be bonded by a mixture of metallic and ionic bonds, particularly when there is a large difference in electronegativity between the elements. Because **lithium** has an electronegativity of **1.0** and **aluminum** has an electronegativity of **1.5**, we would expect **Al-Li** to have a combination of metallic and ionic bonding. On the other hand, because both **aluminum** and **vanadium** have electronegativities of **1.5**, we would expect **Al₃V** to be bonded primarily by metallic bonds.

Many **ceramic** and **semiconducting compounds**, which are combinations of metallic and nonmetallic elements, have a mixture of covalent and ionic bonding. As the electronegativity difference between the atoms increases, the bonding becomes more ionic. The fraction of bonding that is covalent can be estimated from the following equation:

$$\text{Fraction covalent} = \exp(-0.25 \Delta E^2)$$

Where

ΔE is the difference in electronegativities.