

PHYSICS FUNDAMENTALS-Atoms and bonding

Introduction

You will probably be familiar from your schooldays with the ways in which atoms bind, together, but we thought a quick review of the basics would be a sensible precursor to a number of these fundamental concepts. If this section breaks new ground, then you should read up the subject in more detail: suitable sources are Chapter 4 in Bolton, Engineering Materials Technology and Chapter 2 in Shackelford, Materials Science for Engineers. Or browse at <http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html> under Atoms and elements and Chemical bonding in the Chemistry section.

Electrons in orbit

Although the reality is much more complicated, for our purpose we can use a simple planetary model of atomic structure, where electrons (the planets) orbit around a nucleus (the sun). The nucleus contains almost all the mass of the atom, and is made up of protons (positively charged) and neutrons (no charge), both of which weigh around 1.66×10^{-24} g. There are a lot of atoms in each gram of material!

Electrons are much lighter (0.911×10^{-27} g), but have a negative charge of 0.16×10^{-18} C (C = coulomb). Protons have an equal but positive charge; the number of electrons in orbit is the same as the number of protons in the nucleus, so atoms have no overall charge.

Electrons are grouped at fixed orbits about the nucleus, each distance from the nucleus being characterised by a different energy level. For reasons which quantum mechanics can explain, but aren't required here:

Electrons can occupy only certain specific distances/energy levels, intermediate levels being 'forbidden'.

Only a limited number of electrons can cohabit each energy level or 'orbital shell'. The inner shell, which is the most tightly bound to the nucleus, can contain two electrons, the next layer out up to eight electrons, and so on.

The bonding of adjacent atoms is an electronic process. Strong 'primary' bonds are formed when electrons in outer shells are actually transferred or shared between atoms; weaker 'secondary' bonds are the result of electron-proton attraction without transfer or sharing.

Ionic bonds

Ionic bonds are formed when electrons are transferred from one atom to another. Transfer takes place when the resulting electron configuration is more stable, producing full orbital shells for each of the atoms. When sodium and chlorine combine, the sodium loses its lone electron in the outermost shell, and chlorine plugs the only gap in its outer shell, giving two charged but stable ions, described as Na^+ and Cl^- . These particular ions lose and gain only one electron, but other types of atom may lose or gain as many as three. For example, in a plating solution, copper exists as the cupric ion, with two charges, denoted as Cu^{++} .

The bond between the atoms comes from electrostatic attraction between these unlike transferred charges, which increases as the atoms move closer together. What keeps them from colliding is the repulsion between like charges in the shells of electrons. The equilibrium bond length is the point of balance between these opposing forces, and is the lowest-energy state of the system. [Note that moving the atoms away from this point of balance always needs energy to be applied, for example by stressing the material.]

If we think of the whole atom as taking up a spherical space, with the radius of the sphere being approximately that of the outermost completed orbital shell, the bond length can be visualised as the sum of the atomic radii of the two ions.

Whilst the ionic bond is actually inherently non-directional, the structures that result are generally regular. This is because the atoms pack together to create the most stable (lowest energy) state. The ratio of the individual atomic radii in an ionic bond determines which of the many possible configurations will be adopted: you will see some examples of this in Metal basics.

Covalent bonds

Covalent bonds between adjacent atoms are created by the sharing of the electrons in the outer shells, the so-called 'valence' electrons. This is sharing rather than transfer of electrons, but covalent bonds often have some directional nature, one partner becoming more positive and the other more negative.

As with ionic bonding, the driving force is the requirement to reach the lowest-energy state. Covalent bonds may exist between atoms of the same kind (found in gases such as oxygen, whose molecules are pairs of atoms) and between atoms of different types. The bonds to carbon atoms are the basis of life, as well as organic chemistry!

In Polymer basics you will come across the conventional depiction of a covalent bond using lines between the atoms. Each line represents the sharing of one pair of valence electrons. In some molecules, two (or much less frequently three) pairs of

electrons will form a double (triple) covalent bond and this is shown by a double (or triple) line joining the atoms.

Although their bonding forces are lower than with ionic bonds, structures made with covalent bonds have well-defined bond lengths. However, unlike ionic bonds, the directional nature of valence electron sharing also determines a 'bond angle'. For example, carbon tends to form bonds which are equally spaced around a tetrahedron. The angle between bonds on a carbon atom depends on whether the bond is single or double, and on the type of the other atom to which the bond is made, but varies very little from its ideal value of 109.5° .

Metallic bonds

Metallic bonds involve electron sharing, but are not directional, because the valence electrons are 'delocalised', with an equal probability of being associated with any of a large number of adjacent atoms. In a typical metal, valence electrons may be found anywhere in the entire material, giving the effect of an 'electron cloud', which is the reason for their high electrical conductivity.

The lowest-energy requirement, and the concept of atomic radius, again comes into play in determining how the atoms are arranged in the solid. However, the effective radius of metal atoms can be lower than expected, because the outer electrons are being shared.

Van der Waals bonds

The bonds so far described have been strong 'primary' bonds, but weaker bonds are important, especially between molecules in fluids and gases. The bonding force is electrostatic attraction, but no electrons are transferred. Instead, the attraction results from uneven distribution of charge within the molecule. This asymmetry produces a small static 'dipole', combining balanced positive and negative charges.

In some cases, a distortion of the charge distribution between two adjacent atoms can create a weak 'induced' dipole in otherwise neutral molecules. However, higher bond energies are found between 'permanent' dipoles, where the charge asymmetry is built into the molecular structure. The most important example of such 'polar molecules' is probably water. In water, the hydrogen atoms are at an angle to each other, and not in line with the oxygen atom. As the electron sharing tends to make the hydrogen atoms more positive, and the oxygen atoms more negative, there is an in-built imbalance of charge, as shown in Figure 1.

Figure 1: The 'hydrogen bridge' after Shackelford 1999

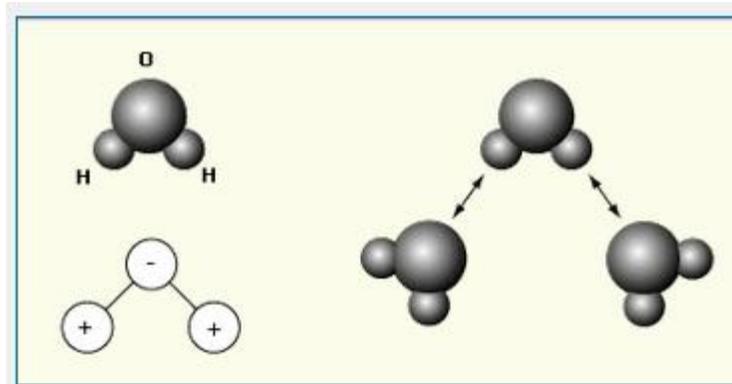


Figure 1: The 'hydrogen bridge'

The bond formed between permanent dipoles in adjacent molecules is referred to as the 'hydrogen bridge'. When water freezes, this bridge aligns the molecules into a regular and relatively open structure, which is why ice is less dense than water: on melting, adjacent molecules pack together closely in a more random arrangement.

Author: Martin Tarr

Source: http://www.ami.ac.uk/courses/topics/0204_aab/index.html