

Fundamentals of Materials (EG-080)

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Introduction

Lecturer Dr Shirin Alexander, available in room 204 ESRI building. Office hours are Friday 1-3pm, although she needs to be emailed before you turn up.

0.1 Recommended Reading

- Chemistry : molecules, matter, and change / Peter Atkins, Loretta Jones.
- General Chemistry E2 *Free* Aie by BELLAMA
- Engineering materials 1 : an introduction to properties, applications and design / Michael F. Ashby and David R. H. Jones.
- Materials science and engineering : an introduction / William D. Callister, Jr.

0.2 Testing

There will be three Blackboard tests, worth a total of 25%, each test being worth 8%, 9%, and 8% respectively. There will also be a final exam in January worth 75%

1 Atoms and Elements

Matter - Has volume and mass

Substance - A pure form of matter, containing only a single type. For example, pure water

Element - A substance composed of a single kind of atom

Isotope - An atom with the same atomic number but a different molecular weight

Homogenous Mixture - A solution that will naturally separate if left

Heterogeneous Mixtures - A mixture of substances that require a physical technique to separate

1.1 Atomic Configuration

Proton Mass (Positive) = 1.67×10^{-24}

Neutron Mass (Neutral) = 1.67×10^{-24}

Electrons (Negative) = 9.11×10^{-28}



Where:

Z - Is the atomic number, the number of protons

A - Is the atomic weight, the total number of protons and neutrons

X - Is the atomic symbol

Quantum numbers for an atom's electrons can be used to calculate properties of the electrons, such as their energy

n - Principal quantum number (or Shell number) represents the energy of the electron. The greater n, the higher the shell's energy level and the weaker it's bound to the nucleus

l - Orbital angular quantum number. This specifies the shape of the orbital

m_l - Magnetic quantum number. This specifies the individual orbital of a particular shape and is also associated with the orbital direction

The number of electrons that can occupy a single shell is $2n^2$

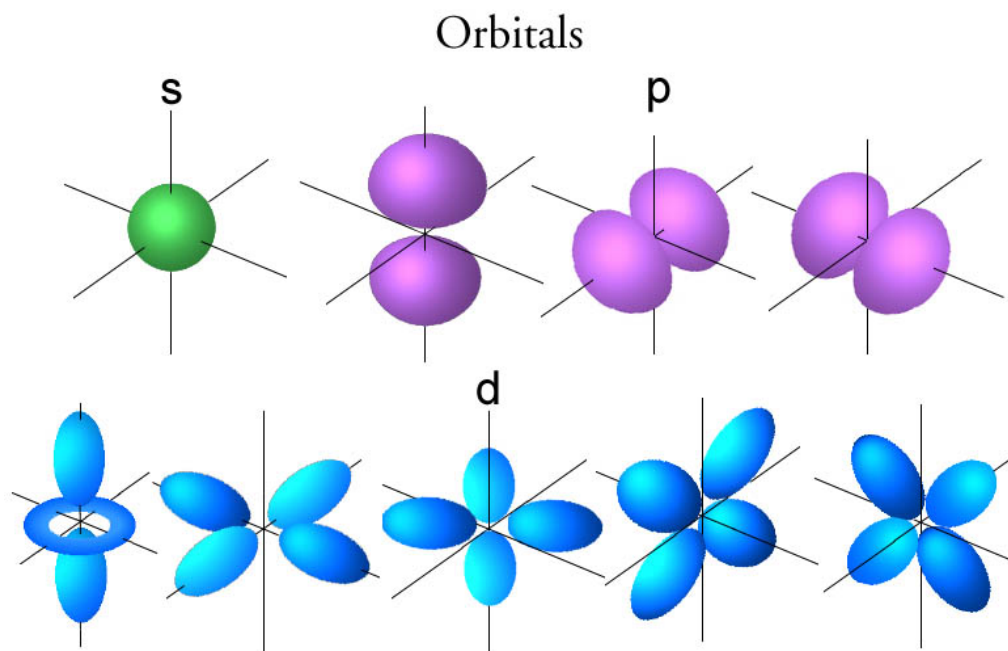


Figure 1: The different possibilities for s, p, and d orbitals

1.2 Implications of Quantum Physics

- Electrons can only occupy discrete orbitals
- Orbitals have different energies, shapes and directions
- There are only a maximum of 2 electrons per orbital (spinning opposite ways)
- Electrons will fill empty shells first before doubling up
- Orbitals are clouds of probability, not true orbits
- Orbitals can be represented using a number for the energy level and a letter for the shape. For example 1s, 2p, 3d

Electrons in electron shells can be represented using written notation. For example, $\text{Mg} = 1s^2 2s^2 2p^6 3s^2$. This can be written shorthand by using the previous noble gas to represent complete shells. For example, $\text{Mg} = [\text{Ne}] 3s^2$

Energy levels of orbitals:

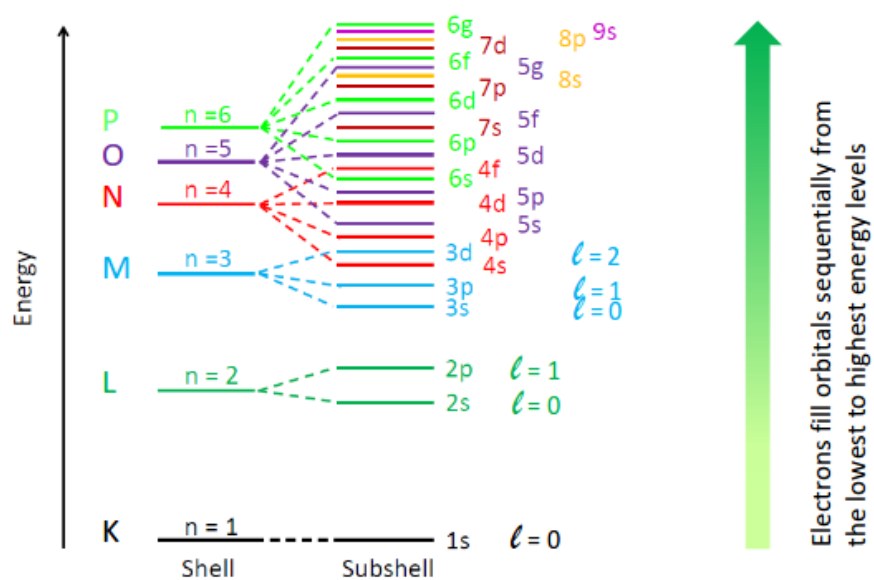


Figure 2:

How to fill orbitals?

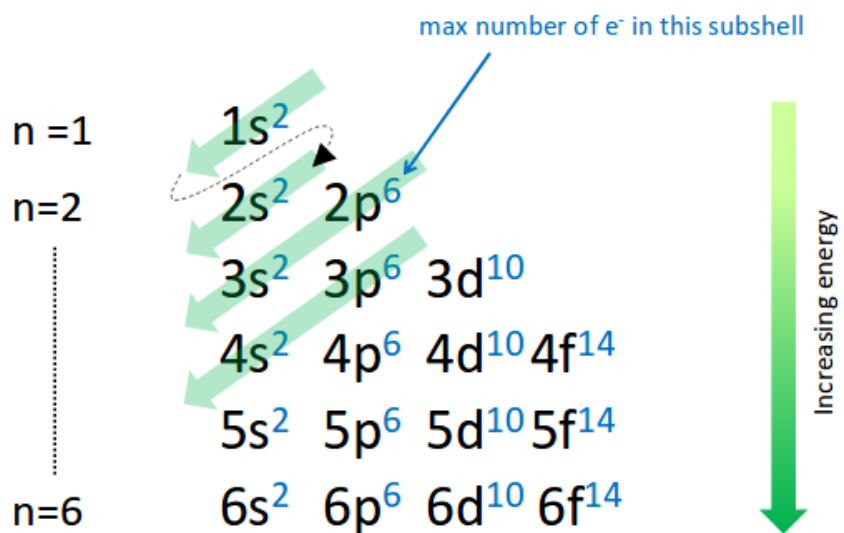


Figure 3:

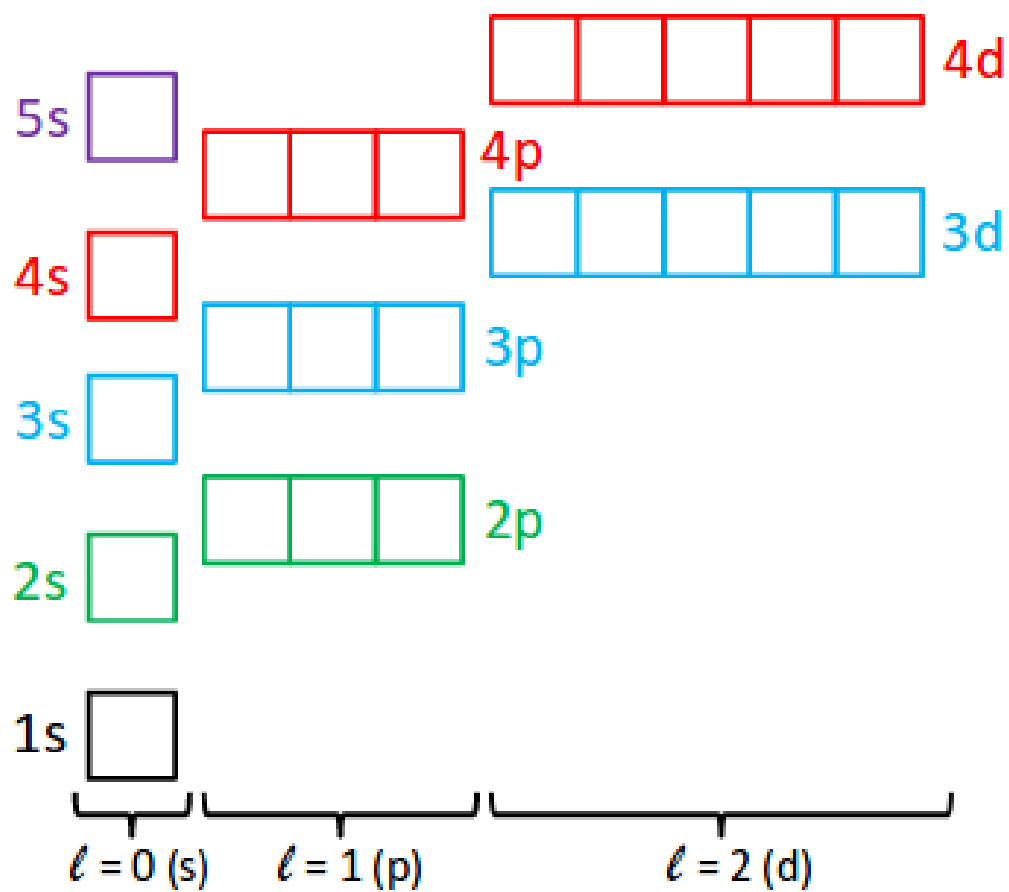


Figure 4: This diagram can be used to show how electrons fill shells. Within each row electrons will always go to an empty box before filling a box completely. These boxes represent the different options within each shell layer (reference Figure 1)

23 V 50.94 $3d^34s^2$	24 Cr 52.00 $3d^54s^1$	25 Mn 54.94 $3d^54s^2$	26 Fe 55.85 $3d^64s^2$	27 Co 58.93 $3d^74s^2$	28 Ni 58.71 $3d^84s^2$	29 Cu 63.54 $3d^{10}4s^1$
41 Nb 92.91 $4d^45s^1$	42 Mo 95.94 $4d^55s^1$	43 Tc 98.91 $4d^55s^2$	44 Ru 101.07 $4d^75s^1$	45 Rh 102.91 $4d^85s^1$	46 Pd 106.4 $4d^{10}$	47 Ag 107.87 $4d^{10}5s^1$
73 Ta 180.95 $4f^{14}5d^36s^2$	74 W 183.85 $4f^{14}5d^46s^2$	75 Re 186.2 $4f^{14}5d^56s^2$	76 Os 190.2 $4f^{14}5d^66s^2$	77 Ir 192.2 $4f^{14}5d^76s^2$	78 Pt 195.09 $4f^{14}5d^96s^1$	79 Au 196.97 $4f^{14}5d^{10}6s^1$

Figure 5: These are the exceptions to these rules. They may ask about the highlighted ones

2 Atomic Bonding

The Valence Electrons (VE) of an atom are the electrons in the outer shell of an atom, so are the ones involved in forming bonds to adjacent atoms. Lewis symbols can be used to show the valence electrons in an atom. For example,



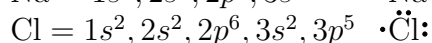
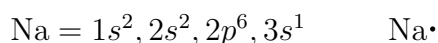
Atoms aim to gain stability by gaining or losing electrons with an aim to gain the same electronic configuration of the closest (in terms of atomic number) noble gas. The interaction of atoms through chemical bonding leads to an overall decrease in the energy. The energy is stored as potential energy.

Ionic and covalent are terms used to describe two extremes of chemical bonds. In most substances the bonds lie between purely covalent or covalent. When describing bonds between non-metals covalent bonding is a good model, while when the bond is between metals and non-metals ionic bonding is a good model.

2.1 Ionic Bonding

Ionic bonding occurs when one atom loses at least one electron from its valence band to another atom to gain stability. Atoms that undergo ionic bonding become positively/ negatively charged.

Salt, NaCl



For Na and Cl the third shell holds the valence electrons. Na loses one electron while Cl gains it, producing $\text{Na}^+ \cdot\ddot{\text{Cl}}^-$

Ionic solids tend to stack together in regular crystalline structures as the charged electrons in the molecule attract to the other charged atoms in other molecules. This strong electrostatic attraction between oppositely charged ions in ionic solids accounts of their typical properties such as high melting and boiling points, as well as brittleness.

When an ionic solid is hit the positive ions that normally line up with negative ions now line up with positive ions, forcing the lattice apart. This is why ionic solids are brittle.

In the lattice strong coulomb forces ionically bond each Na^+ ion to six neighbouring Cl^- , meaning it takes a lot of energy to break all of these bonds. This accounts for the high melting and boiling points.

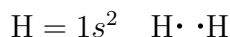
The ionisation energy of an atom increases as its position in the periodic table moves down and to the right. This is based on the distance of the nucleus to the valence shell.

2.2 Covalent Bonding

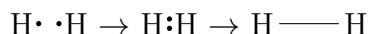
Covalent bonding occurs when pairs of valence electrons are shared between two atoms. This means that neither atom gains or loses any charge. Non-metal elements tend to interact via covalent bonding (instead of ionic) because their ionisation energy is too high.

Covalent bonds are very strong; it takes a large amount of energy to separate atoms bonded in this way. For example, diamond is 100% covalent bonds, while graphite is only partially covalent.

Hydrogen

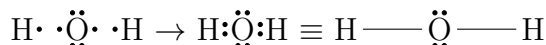
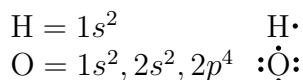


Hydrogen wants to be as stable as the closest noble gas, Helium. The sum of attractive electrostatic forces (nucleus \leftrightarrow electrons) and repulsive electrostatic forces (electron \leftrightarrow electron, nucleus \leftrightarrow nucleus) is overall attractive therefore bonding occurs.



Here the two hydrogen atoms share their bond, resulting in a single covalent bond being formed.

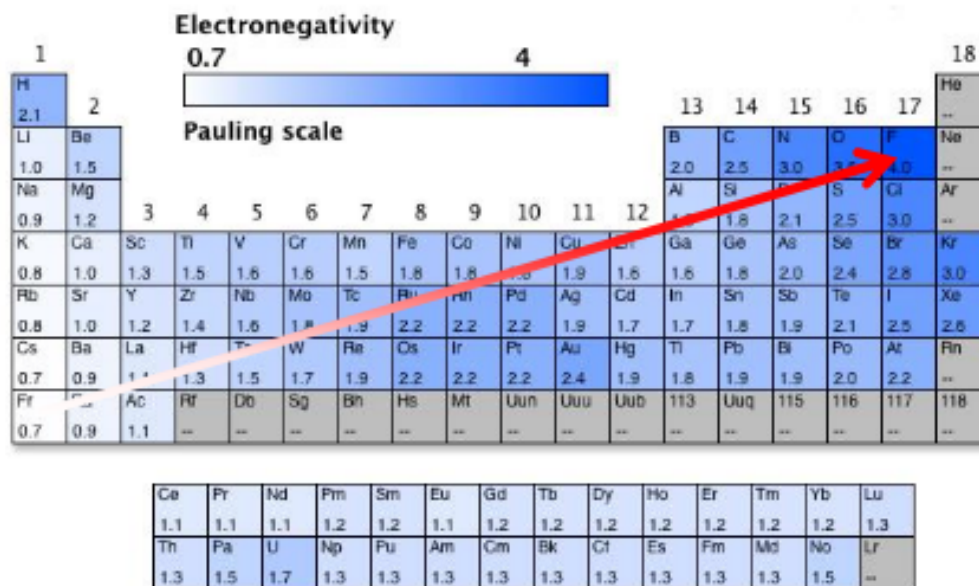
Water



The presence of the doublet of negative electrons the two hydrogens are squeezed together as the two doublets repel from each other. This force results in water having a bond angle of 104.5° . The oxygen atom pulls on the shared electrons in each hydrogen, meaning one side of the molecule is positively charged and the other side is negatively charged. This means it is a polar molecule.

In liquid water these partial charges cause weak electrostatic attraction between molecules, called hydrogen bonds, that keep the molecules together.

2.3 Electronegativity



Electronegativity defines the power of an atom in a bond to draw electrons from the other atom. We can use the difference in electronegativity between two elements to predict the most appropriate bonding model for a chemical bond between them. In general, if the electronegativity difference, x , between the two elements is:

$$x \geq 1.7 \rightarrow \text{Ionic Bond}$$

$$x < 0.5 \rightarrow \text{Covalent Bond}$$

$$0.5 \leq x < 1.7 \rightarrow \text{Polar Covalent Bond}$$

3 Metallic Bonding

Delocalisation - When an electron is freed from its orbital

Malleable - Can be pressed to form sheets

Ductile - Can be stretched to form wires

Metallic bonding can be explained according to the Drude model, which is a simplistic model. It was developed to explain the transport of electrons in metals, although does not explain all of their electronic properties.

The drude model assumes a 'sea of free, vibrating, electrons' which are rebounding off of heavier, relatively immobile ions. Valence electrons are free to drift through the entire metal as they are not bound to any single atom, while the nonvalence electrons and the atomic nuclei form the ion cores. When metallic atoms come close the valence electrons become delocalised as orbitals overlap and lose energy. This lowers the overall energy and holds the atoms together, forming the sea of free electrons, or "Drude Glue".

3.1 Metallic properties within the Drude model

Partially explains melting points

The overall energy is lowered significantly when the atoms are close together so a lot of energy needs to be added to separate them. The electrons are homogeneously shared, meaning there is a strong bonding between metal atoms. This gives metals their solid structure.

The more outer electrons an atom has the more "Drude Glue" there is between atoms, meaning there is a higher melting points, although this is only true to a certain extent. Some examples:

- Sodium ($1s^2, 2s^2, 2p^6, 3s^1$): 98°C
- Magnesium ($[\text{Ne}] 3s^2$): 650°C
- Aluminium ($[\text{Ne}] 3s^2, 3p^1$): 660°C

There are exceptions to this, such as mercury ($[\text{Xe}] 4f^{14}, 5d^{10}, 6s^2$) which has very weak atomic interaction, so very little Drude Glue.

Explains conductivity

The outer electrons are free to move so can carry electric charge (current). Also, the more valence electrons there are the higher the conductivity. Valence electrons also carry heat through vibrations, so metals are good thermal conductors.

Explains shininess

When a photon of light hits a metal surface, knocks an electron up to one of the many empty orbitals of a higher energy. This electron is unstable so drops back down, re-emitting the energy as a photon identical to the first. This is called reflection.

Explains malleability

Metallic bonding is non-directional, so atoms can move along slip planes by a small amount. As long as the atoms stay close together the metallic bonds stay in place, meaning metals can be deformed.

4 Introduction To Metals

Smelting - A process where metals are extracted from an ore by using a combination of heat and a reducing agent.

Monoatomic - A stable molecule composed of a single atom (such as noble gases)

4.1 Crystalline vs Amorphous

- Atoms in a crystalline material are in a repeating/ orderly array over large atomic distances.
- All metals (and many ceramics) form crystalline structures
- Amorphous materials are characterised by no/ very little ordering of their atoms. Their layout is random

Crystalline materials have a small energy difference between the conduction band and the valence band, while amorphous materials have a large energy difference. This is why amorphous materials are insulators, while crystalline materials are conductors or semiconductors.

4.2 How atoms in a metal stack

There are three main ways in which atoms stack -

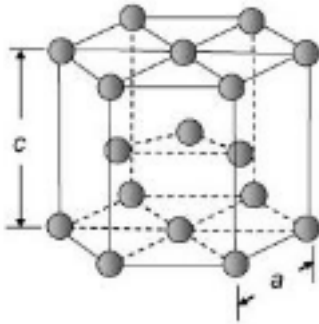
- Hexagonal close packing (HCP)
- Cubic close/ face-centered cubic packing (CCP/ FCP)
- Body-centered cubic packing (BCC)

This stacking controls the ductility, electronic and magnetic properties of metals.

Coordination Number - The number of near neighbours, at equal distance, to a central atom in a crystal

Packing Density - The fraction of space filled by the atoms (assuming the atoms are perfect spheres)

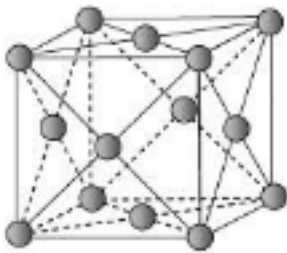
Unit Cell - The smallest hypothetical unit that when stacked together repeatedly with no gaps will produce an entire crystal



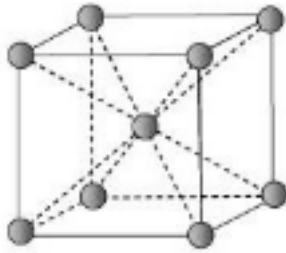
Hexagonal Close Packing (HCP)

- Each atom is surrounded by 6 others in each layer
- Coordination number of 12
- 74 % packing density
- 3 slip systems
- Examples - Magnesium, Zinc

Cubic Close Packing (CCP)



- Each atom is surrounded by 6 others in each layer
- Coordination number of 12
- 74 % packing density
- 12 slip systems (4 slip planes, 3 directions)
- Examples - Aluminium, Copper, Gold



Body Centred Cubic (BCC)

- More open structure
- Coordination number of 8
- 68 % packing density
- 48 slip systems (but planes are not closely packed, so more force is required)
- Examples - Iron, Sodium, Potassium

4.3 Slip in metals

Metals deform in planes, with one plane of atoms sliding over another plane. Atoms want to stay as close to each other as possible, meaning slip is easiest on closely packed planes in closely packed directions.

A slip system describes the set of symmetrically identical slip planes and the associated family of slip directions for which dislocation motion can easily occur and lead to plastic deformation.

HCP

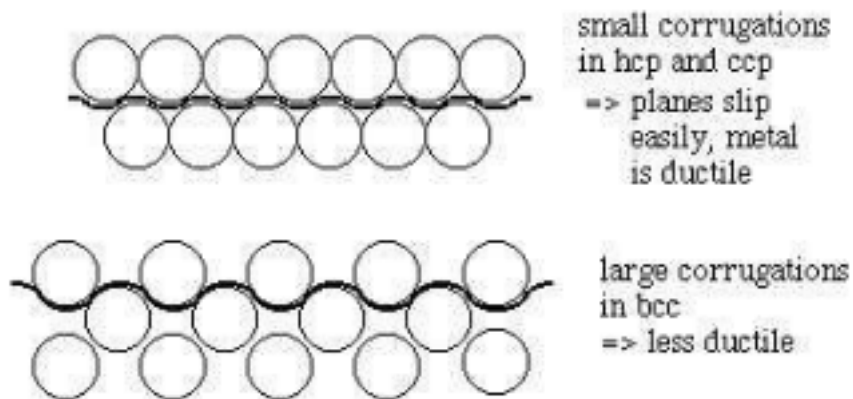
HCP has only one close packed plane, with three directions, so three slip systems. This means it is limited to slipping only if force is applied in certain directions. In most cases, it is quite brittle.

CCP/ FCC

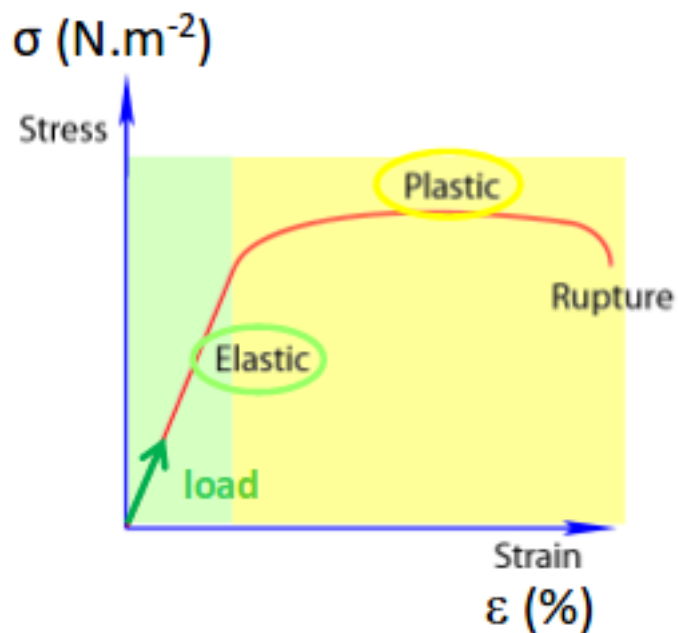
CCP has four close packed planes, each with three close packed directions, so 12 slip planes. It can slip in many arrangements, meaning it is ductile.

BCC

BCC has the most slip systems (up to 48) but the planes are not tightly packed, meaning a higher force or higher temperature is needed.



4.4 Plastic vs Elastic Deformation



Elastic deformation is one in which stress and strain are directly proportional. The deformation is also reversible. The equation for elastic deformation is

$$\sigma = E\epsilon$$

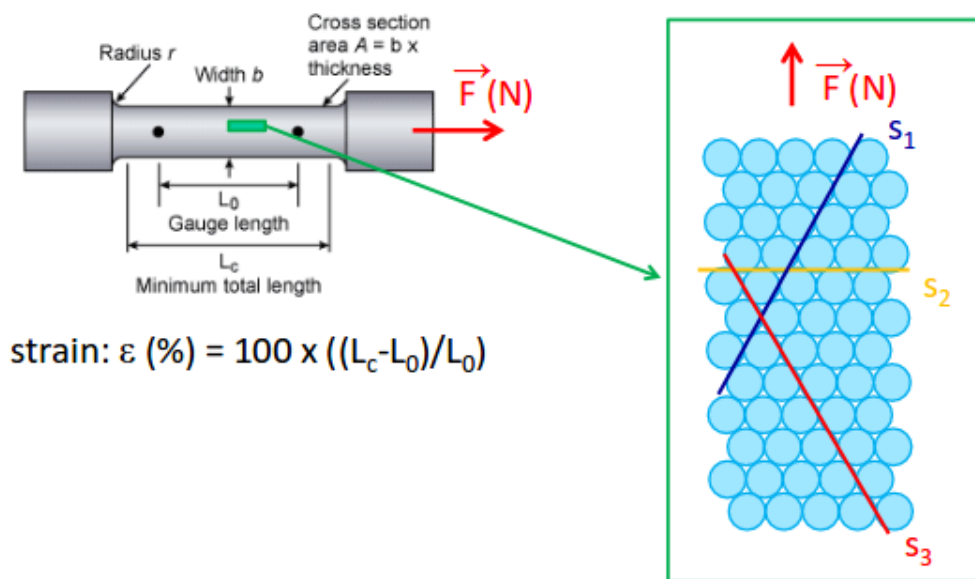
Where:

σ = Stress

E = Young's modulus

ϵ = Strain

Plastic deformation is one in which stress and strain are no longer proportional. This deformation is not reversible.

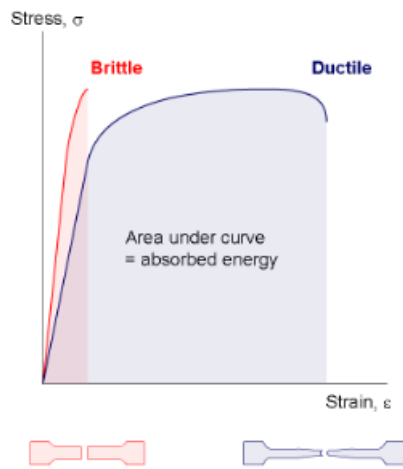


4.5 Ductile vs Brittle

Ductility - A measure of the extent of plastic deformation a material can sustain before fracture; a ductile metal can be stretched into a wire without breaking

Malleability - The ability of a solid to deform under pressure

Brittle - A material is brittle if it fractures at less than $\sim 5\%$ strain



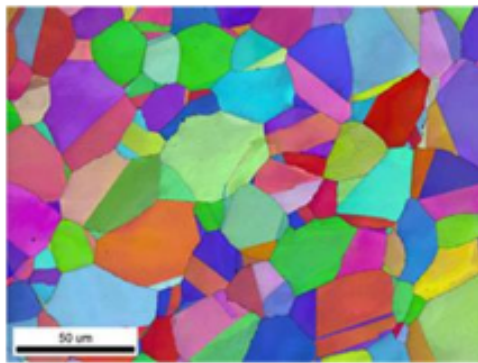
Brittle metals have very clean breaks when they fracture, while malleable metals will deform and tear before they break. Metals can change from ductile to brittle, for example below 912°C Iron and steel transform from CCP to BCC, from ductile to brittle.

5 Properties of metals

5.1 Metallic Grains

As a metal starts to solidify crystals start growing in many different directions. These crystals merge, giving the metal a grain structure. Every grain has its own crystalline orientation.

Figure 6: Orientation map of an Inconel 600 superalloy sample (Ni- based corrosion resistant alloy)



EBSD is magic! (Electron Back-Scattered Diffraction analyses) Each colour corresponds to a specific grain orientation. How pretty!

Slip is difficult across a grain boundary. Smaller grains means more boundaries, reducing slip so forming a harder/ stronger metal. Small grains can be obtained by fast cooling, use of a chemical agent (such as a very strong acid), or through physical treatment, like ultrasounds.

Reducing slip in a metal makes the metal harder, normally stronger, but sometimes more brittle. There are two ways to make it harder for atoms to slip, these are:

- Alloying
- Decreasing the grain size

Alloying

Alloy - An alloy is a metallic substance which is composed of two or more elements with a metallic structure.

A mix of differently sized atoms makes it harder for atoms to slip over each other, the the more alloying the harder it is for atoms to slip. For example:

Mild steel -0.15% Carbon

Malleable and ductile

Used for rolled structural sections (tubes, round bars etc.)

Cast iron - 4% Carbon

Much harder and brittle

Used in foundaries to make complex objects

Interstitial alloying is where the alloying atoms fit between the metal atoms, such as carbon in steel. Substitutional alloying is where the alloying atoms replace the other metal atoms, such as in Brass with Copper and Zinc.

Decreasing the grain size

Grain size can be decreased through chemical treatment, such as an acid wash, or through the use of ultrasound as the metal solidifies. Smaller grains normally lead to stronger metals, although in high temperature applications, such as in a jet turbine, small grains are actually unwanted. This is because a T-induced slip or failure can occur along grain boundaries. For these applications, it is better to reduce the density of grain boundaries, ideally aiming for a single crystal microstructure, meaning the metal is a single crystals, therefore has no grain boundaries.

5.2 Advanced Materials

Metallic Glass

This is a metal but with a disordered, non-crystalline structure, the same as glass. This provides high strength, high elastic limit, high corrosion resistance, resistance to scratches, dents, or wear. It does however make the metal brittle, although less brittle than mineral glass (normal glass, SiO_2).

Shape-Memory Alloys

This is an alloy that 'remembers' its original shape, so that when it is deformed it returns to its original shape upon heating. These alloys have applications in industries such as automobile, aerospace, and robotics.

5.3 Choosing a Metal

There are five main things to consider when deciding if a metal is appropriate for use. These are:

- Is it suitable for the task (strength, chemical stability)?
- Is it abundant as an ore?
- Is it easy to extract and purify?
- Is it cheap (This is a combination of the above two)?

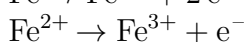
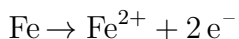
6 The Chemical Behaviour of Metals

How stable and how easy to extract a metal is is mainly determined by oxidation and reduction. These are the most common types of chemical reaction and they normally occur together, with one chemical oxidising while another reduces. This is a redox reaction, and the system hosting both the reactions is called a redox system

6.1 Oxidation

Oxidation is a chemical reaction associated with a loss of electrons (remember OIL RIG). Within our environment this normally involves oxygen, although not always. Any chemical which causes oxidation is known as an oxidising agent. Metal corrosion is an oxidation reaction.

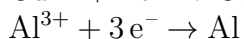
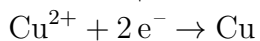
Examples:



6.2 Reduction

Reduction is a chemical reaction associated with the gain of electrons (again, remember OIL RIG). Any chemical which causes the reduction of another is known as a reducing agent. The extraction of metals from ores is done through the reduction of metals.

Examples:



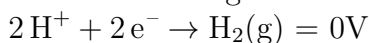
7 Electrochemical Potential

Electrochemical potential is an alternative way of measuring the oxidising/reducing power of elements. It is a measure (J/ mol) of the chemical potential of a compound which takes electrostatic forces into account.

It can be used to understand; the use of electricity to extract metals, corrosion, batteries, and fuel cells. It also provides another way to predict the occurrence of redox chemical reactions.

7.1 Standard Potential

The standard potential is an electrochemical potential which measure the ability of compounds to oxidize/ reduce other compounds in comparison to the H^+ / H_2 redox couple under standard conditions. Standard potential (E^0) is in volts and the sign and magnitude is an indication of a substance to act as a reducing or oxidizing agent.



Standard Potentials at 25 °C		E^0 (V)
Reduction Half-Reaction		
Stronger oxidizing agent	$F_2(g) + 2e^- \rightarrow 2F^-(aq)$	2.87
	$H_2O_2(aq) + 2H^+(aq) + 2e^- \rightarrow 2H_2O(l)$	1.78
	$MnO_4^-(aq) + 8H^+(aq) + 5e^- \rightarrow Mn^{2+}(aq) + 4H_2O(l)$	1.51
	$Cl_2(g) + 2e^- \rightarrow 2Cl^-(aq)$	1.36
	$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^- \rightarrow 2Cr^{3+}(aq) + 7H_2O(l)$	1.33
	$O_2(g) + 4H^+(aq) + 4e^- \rightarrow 2H_2O(l)$	1.23
	$Br_2(l) + 2e^- \rightarrow 2Br^-(aq)$	1.09
	$Ag^+(aq) + e^- \rightarrow Ag(s)$	0.80
	$Fe^{3+}(aq) + e^- \rightarrow Fe^{2+}(aq)$	0.77
	$O_2(g) + 2H^+(aq) + 2e^- \rightarrow H_2O_2(aq)$	0.70
	$I_2(s) + 2e^- \rightarrow 2I^-(aq)$	0.54
	$O_2(g) + 2H_2O(l) + 4e^- \rightarrow 4OH^-(aq)$	0.40
	$Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$	0.34
	$Sn^{4+}(aq) + 2e^- \rightarrow Sn^{2+}(aq)$	0.15
	$2H^+(aq) + 2e^- \rightarrow H_2(g)$	0
	$Pb^{2+}(aq) + 2e^- \rightarrow Pb(s)$	-0.13
	$Ni^{2+}(aq) + 2e^- \rightarrow Ni(s)$	-0.26
	$Cd^{2+}(aq) + 2e^- \rightarrow Cd(s)$	-0.40
	$Fe^{2+}(aq) + 2e^- \rightarrow Fe(s)$	-0.45
	$Zn^{2+}(aq) + 2e^- \rightarrow Zn(s)$	-0.76
	$2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$	-0.83
	$Al^{3+}(aq) + 3e^- \rightarrow Al(s)$	-1.66
	$Mg^{2+}(aq) + 2e^- \rightarrow Mg(s)$	-2.37
	$Na^+(aq) + e^- \rightarrow Na(s)$	-2.71
Weaker oxidizing agent	$Li^+(aq) + e^- \rightarrow Li(s)$	-3.04
	Stronger reducing agent	

By convention, the standard potential is associated to a reduction reaction: $M^{n+} + ne^- \rightarrow M$ where M represents a metal. $E^0 = E_{red(uction)}^0$. This equation can be shown as $E_{red}^0(M^{n+}/M) = \text{Standard potential (V)}$. For example:

$$E_{red}^0(Cu^{2+}/Cu) = +0.34 \text{ V}$$

$$E_{red}^0(Zn^{2+}/Zn) = -0.76 \text{ V}$$

If $E_{red}^0 > 0$ Then M^{n+} tends to be reduced by $H_2(g)$:
 $M^{n+}(aq) + H_2(g) \rightarrow M(s) + 2H^+(aq)$

If $E_{red}^0 < 0$ Then M^{n+} tends to reduce $H^+(aq)$:
 $M(s) + 2H^+(aq) \rightarrow M^{n+}(aq) + H_2(g)$

For example:
 $Cu^{2+} + H_2 \rightarrow H^+ + Cu$
 $Zn^{2+} + H^+ \rightarrow Zn + H_2$

For a redox reaction the total voltage produced is $E_{red} - E_{ox}$

7.2 Group Metals

Group 1

Very reactive, strong reducing agent, and soft with low melting points

Group 2

Less reactive than group 1, weaker reducing agents, they are harder and have higher melting points.

Group 3

Weaker reducing agents than group 2 and not very reactive. They are harder and have higher melting points (due to more "drude glue")

7.3 Transition Metals

Transition metals are metals with partially filled d-orbitals. This controls many properties of transition metals and make the elements all behave similarly. They generally engage in strong bonding as atoms are small and heavy. They are also not very reactive due to their valence electrons having a high

ionization energy. They have more than one oxidation state and often show catalytic activity.

8 Extraction of Iron, production and corrosion of steel

9 Aluminium

Aluminium is a light-weight metal that is mechanically stronger than group one and two metals, has a higher melting point and is less reactive (as there is more 'Drude Glue'). It is the most common metallic element in the Earth's crust, and the third most abundant of all the elements, after oxygen and silicon.

9.1 Aluminium Extraction vs Iron Extraction

Aluminium is a good reducing agent, better than iron, meaning it is difficult to reduce it chemically in an economic way



For aluminium it is more economically viable to use electrolysis, in which electricity is used to force the reduction reaction.

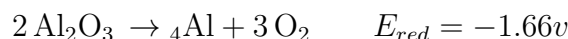
9.2 Electrolysis

Electrolysis uses a direct current to force a non-favourable reaction to occur. Cations migrate to the cathode where they are reduced while anions migrate to the anode where they are oxidised.

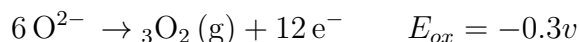
Electrolysis requires the reacting material to allow movement of charged ions, however solid Al_2O_3 (alumina) doesn't allow this as the atoms are in a fixed position. A solution of the material would normally be used, but alumina doesn't easily dissolve in anything. Melting the material would also work, although the melting point of alumina is 2050 °C, so this is impractical.

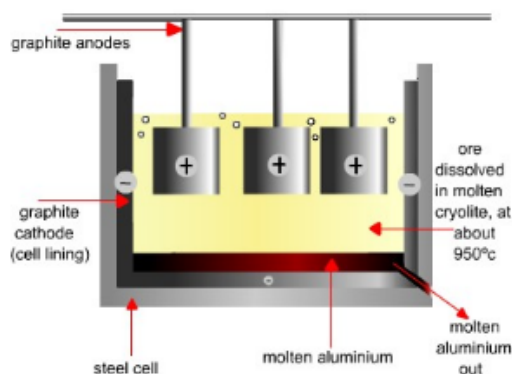
The solution is to decompose the alumina into molten cryolite (Na_3AlF_6), which occurs at about 950 °C. The fluoride here lowers the melting point of the cryolite-alumina mix, allowing the alumina to dissolve in the molten cryolite, meaning it can conduct electricity.

At the graphite cathode:



At the graphite anode:





The lifetime of these graphite anodes is only 20-28 days, meaning that they need to be replaced every 28 days as the carbon gradually burns away and reacts with oxygen. Modern cells operate between 4.0-4.5 volts, and between 150,000 and 300,000 amps! A single cell can normally produce 1-2 tonnes of aluminium per day.

9.3 Economical considerations

Aluminium extraction is very expensive as it requires a lot of electrical power (3 moles of e^- to produce 1 mol of Al), meaning the plants are normally located nearby cheap electricity, such as hydroelectric. It is also costly due to the replacing of the graphite rods, the fabrication of cryolite, and the transport of bauxite (aluminium ore).

Recycling Al requires around 5% of the energy needed to extract it from bauxite, making recycling incredibly valuable. Unfortunately 58% of cans go to landfill in Europe, around 45000 tonnes of Aluminium cans go to landfill in the UK per year.

9.4 Properties of Aluminium

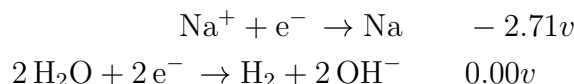
Aluminium has stronger bonds than group one or two metals as the atom is smaller and there is more Drude glue. This means it is harder, has a higher melting point, is more dense, and is a good conductor of heat and electricity.

10 Extraction and Corrosion of Other Metals

The more reactive a metal the higher its tendency to bond with other elements, so the harder it is to extract

10.1 Group One and Two

Group one and two metals are very reactive, having only one or two valence electrons, meaning they tend to occur as salts such as sodium chloride and magnesium chloride. These metals are extracted using electrolysis as they are some of the strongest reducing agents so they can't be chemically reduced. When electrolysis of these salts we must start with molten salt, not just a salt solution, such as sea water in the case of sodium chloride. This is because the easiest reaction (the one which requires less energy) will always occur first, so using sea water we would just reduce the water to hydrogen, not reduce the sodium.



These metals also corrode incredibly easily because of how reactive they are.

10.2 Transition Metals

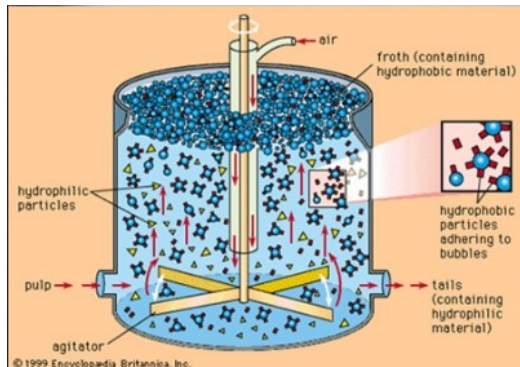
Iron is the most important because of how much it is used. Nearly all of these can be extracted by chemical reduction of an ore.

Copper

Copper occurs mainly as sulphides (Cu_2S and CuFeS_2) and has a ccp structure, making it very malleable. It is also an excellent electrical and thermal conductor.

In extraction, crushed ore is separated from excess rock using froth flotation. In this process, the copper ore is mixed with water and stirred by a agitator. Air is then bubbled through, along with a small amount of alcohol which binds to the copper sulphide, allowing it to bind to the air bubbles and float to the surface where it can then be scraped off. The process is shown below.

This copper is then extracted from its ore using either high temperatures (air roasting) or using an aqueous solution with electrolysis. Copper has catalytic properties and slowly corrodes to form a green outer



later which then protects it from further corrosion. It can be used to make various alloys:

- Brass (10-50% Zinc)
- Bronze (22% Tin, 9-16% Aluminium)
- Cupro-nickel coins (with Nickel)
- Gold blends (5-30% Copper in Gold to lower the carat, making it cheaper and harder)

Titanium

Titanium is a relatively abundant element, but on its own it is not very strong, although is quite light. When alloyed with tin, aluminium or vanadium it has high strength and is quite ductile, meaning it's widely used for strong, tough and light alloys. However, because of the extraction process it is quite expensive.

The main titanium ores are rutile (TiO_2) and ilmenite (FeTiO_3), although rutile is scarcer and more expensive than ilmenite it is more commonly used as it doesn't contain iron compounds so is easier to process. When processing rutile it is first converted to titanium(IV) chloride, which is then reduced to titanium using either magnesium or sodium.

Like copper, titanium has catalytic properties. It also should corrode but, like aluminium, forms a thin stable, self-healing, corrosion-resistant layer of TiO_2 that protects the metal.

TiO_2 is very white so is widely used as a pigment and whitener in paint.

It is as strong as steel but less dense, and can withstand very high temperatures. This gives it a lot of uses in the fabrication of aircraft, space craft and missiles.

11 Non-Metallic Elements and Compounds

11.1 Primary and Secondary bonds

Atoms have two types of bonds, primary and secondary bonds. Primary bonds are strong, short range and include Covalent, Ionic and Metallic bonds, while secondary bonds are weak, long range and include Polar/ Hydrogen bonds and Van der Waals bonds. Primary bonds are rarely pure bonds, and most compounds are partially one type of bonding and partially another type.

Pure Covalent

Between atoms of the same group or element

Very strong, directional bonds

Insoluble in water

Some form giant structures with very high melting points

Others form isolated molecules with very low melting points

Pure Ionic

Between group one, two and seven

Strong, non-directional bonds

Soluble in water

High(ish) melting points

Ionic with some Covalent

Between groups two, three (metals) and five and six (non-metals)

Higher strength bonds than Ionic

More directional bonds than pure Ionic

Less soluble than pure Ionic

Higher melting points than pure Ionic solids

Covalent with some Ionic

Between different atoms (non-metals)

Quite strong directional bonds

Partially soluble in water

Polar molecules

12 Secondary Bonding

The behaviour of gases is often non-ideal, meaning that the relationships between pressure, volume and temperature are not accurately described by the ideal gas law, $PV = nRT$.

Cohesion is used when describing intermolecular forces while adhesion is used to describe when a foreign object interacts with the molecules in a substance. These forces explain capillary action.

Surface Tension - The elastic tendency of liquids which makes them acquire the least surface area possible

Capillary Action - The ability of a liquid to flow in narrow spaces without the assistance of external forces, such as gravity

Vapor Pressure - The pressure exerted by a vapor in thermodynamic equilibrium with its condensed phases at a certain T in a closed system

Miscibility - The property of substances to mix in all proportions to form a homogenous solution (for example water and oil are immiscible as they wont mix)

Solubility - The ability for a substance, called the solute, to dissolve in a solvent

12.1 Bonding Strength

Primary Bonding

Force	Basis of Attraction	Energy (Kj/mol)	Example
Ionic	Cation-anion	400-4000	NaCl
Covalent	Nuclei-shared e ⁻ pair	150-1100	H-H
Metallic	Cations-delocalised electrons	75-1000	Fe

Secondary Bonding

Force	Basis of Attraction	Energy (Kj/mol)
Ion - dipole	Ion charge - dipole charge	40-600
H bond	Polar bond to H^- dipole charge	10-40
Dipole - dipole	Dipole charges	5-25
Ion-induced dipole	Ion charge - polarised e^- cloud	3-15
Dipole-induced dipole	Dipole charge - polarizable e^- cloud	2-10
Dispersion	polarizable e^- clouds	0.05-40

13 Properties of Non-Metallic Elements

13.1 Groups 1, 2, 3 (except Boron) and transition metals

All of these have metallic bonding and across the periods, as the number of electrons increases the melting point, conductivity and strength all increase as there's more Drude glue.

13.2 Metalloids of groups 3, 4 and 5

These all have giant covalent structures, have very high melting points and are very strong. Most are semi-conductors and have a low level of conductivity

13.3 Carbon

Carbon can have one of three crystalline forms, all of which are giant structures

13.3.1 Diamond

Incredibly hard, often used as a cutting tool and an abrasive. It has a completely covalent giant structure, giving it poor electrical conductivity because of the strong covalent bonds. However it is a good thermal conductor due to the rigid giant covalent structure.

13.3.2 Graphite

A layered structure with very strong covalent bonds within the layers and weaker Van der Waals bonding between the layers. This allows some electrical conductivity and allows the layers to slip, meaning it can act as a lubricant and pencil lead.

13.3.3 Buckminster Fullerene

Carbon atoms are arranged in a football shape, and the structure has similar bonding to that in graphite. It can be made into tubes and has potentially useful electrical, chemical, and lubricant properties.

13.4 Non-metals of groups 5, 6 and 7

These are small molecules with strong intramolecular covalent bonding, meaning they are not conductors as all electrons are strongly fixed in these bonds. Most elements form pairs of atoms, such as N_2 , O_2 , F_2 , although some do form larger molecules (P_4 , S_8). Their intermolecular bonding is weak however due to weak Van der Waals force, meaning they have low melting points.

13.5 Group 8

These are the noble gases, and they are isolated, inert atoms. They become liquid at very low temperatures due to the weak Van der Waals bonding.

14 Carbon, Oil and Lubricants

14.1 Sources of organic chemicals

Crude Oil

Crude oil is a major source of organic compounds. It is a mixture of hydrocarbons, mainly alkanes along with some alkenes and aromatic compounds. These are used for fuel and in grease, asphalt, polymers and pharmaceuticals.

Natural gas

Is mainly methane with some other alkanes, such as ethane, propane, butane and pentane. It is used as fuel and in fabric, paint and plastics.

Coal

Coal is primarily carbon but also contains aromatic compounds and heavier alkanes. It is used in fuel and tar (which is used to prevent wooden ships from rotting)

Plants

These are natural sources for sugars, alcohols, natural oils and polymers (cellulose and rubber). They are used in fuel, polymers and pharmaceuticals.

Waste Plastics

Plastic is a sustainable source of recyclable materials which contains hydrocarbons and aromatics.

14.2 Oil

Oil is aquatic in origin and is believed to be formed from marine plants. The oldest reserves are found in sedimentary rocks over a billion years old. Above the oil there is a layer of natural gas, and these can both be contained within the pores of the rock, like a sponge. Above the porous rock is a layer of non-porous rock that traps the oil and gas.

14.2.1 Extraction

Primary Recovery (5-15%) - This method harvests the natural flow of the oil

Secondary Recovery (20-40%) - The oil cavern is flooded with pressurised water from one side which forces oil out of the other side

Tertiary recovery (50-60%) -Can use gas injection where very high pressure gas is injected in to force oil out; steam or hot water can also be used. This method can also use a chemical method using polymer and surfactant.

14.2.2 Refining

Paraffins - (straight or branched alkanes) : gases (methane, lightest), liquids (few to many C atoms) or some very thick waxes and tars (very large molecules with many C atoms, heaviest).

Aromatics - Benzene rings with chains attached, normally liquid

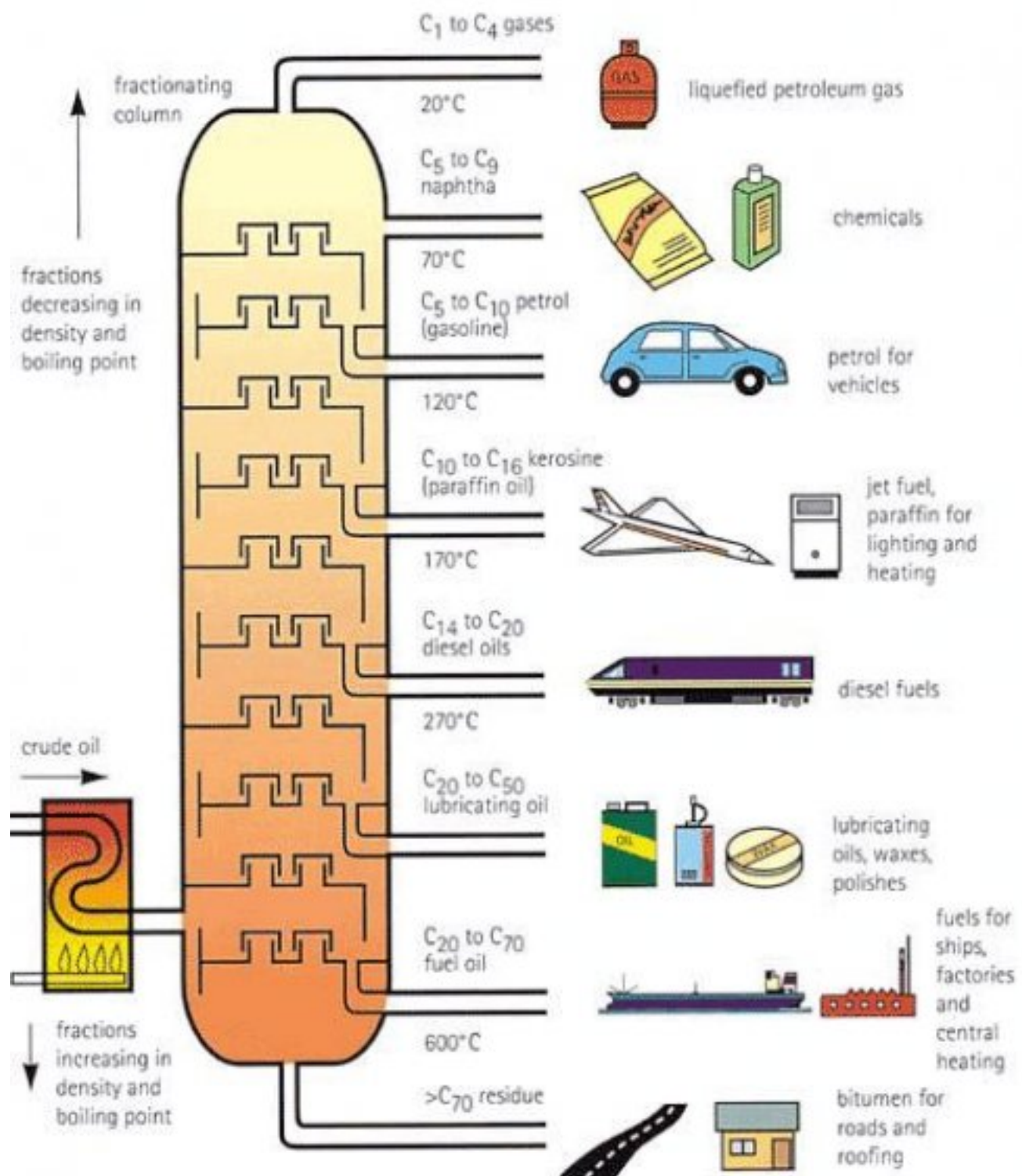
Cycloalkanes - Ringed alkanes, normally liquid

Single Alkenes - One double bond, can be either liquid or gas

Di-enes and Alkynes - More than one double or triple bond, can be either liquid or gas

14.2.3 Fractional Distillation

1. Crude oil is heated to around 400°C in an inert atmosphere (no oxygen, otherwise it would explode)
2. Most components evaporate and the gasses move to the top of the column
3. The column gets cooler towards the top
4. Different fractions condense back to liquids at different heights dependant on their boiling point
5. These fractions are then collected separately



Most fractions from the distillation column are not used directly, they must be further processed to make useful fractions. This further processing can include:

- Further fractional distillation and selective dissolution
- Unification which combines small molecules to make larger ones
- Cracking which is the breaking of large alkanes into smaller alkanes, alkenes and alkynes. It involves heating larger alkanes to high temperatures (around 800°C) which breaks some C–C bonds. The products of this process are highly dependant on the temperature used.

15 Polymers

A polymer is a large molecule, or macromolecule, composed of many repeated subunits, known as monomers. These are made up of long chain molecules with covalently bonded atoms. Polymers are created using a technique known as polymerisation, where many monomers are combined. They are often based on a carbon backbone, with two main types, synthetic polymers, such as plastic, and natural biopolymers, such as DNA and proteins.

Polymers can be subdivided into thermoplastics or thermosets, depending on how they react to heat.

15.1 Raw materials

Synthetic polymers can contain raw materials from many different sources, such as:

- | | |
|-------------------|---|
| Natural Sources | - Natural Rubber
- Cellulose
- Fermentation of plants |
| Oil and Gas | - Currently the main source |
| Coal | - Used extensively in the mid 1950's but has now been replaced with oil and gas |
| Recycled Plastics | - Being used more, although there are still some challenges |

15.2 Thermoplastics

Thermoplastics have discrete chains with no primary bonds between the chains, so they are held together only by secondary bonds and physical entanglement. These soften and melt on heating, as the secondary bonds break, and harden on cooling in a reversible process. This allows thermoplastics to be shaped and recycled. They are generally softer and more flexible, and some common thermoplastics include polyethylene, polypropylene, nylon, polystyrene and PVC.

15.3 Thermosets

These are an infinite network of chains which have primary bonding at cross-linking points. When heated these crosslinks and some main chain bonds

break, but do not reform when cooled. This means thermosets don't melt but instead degrade. This cross-linking provides good strength and stiffness to higher temperatures than thermoplastics and have good chemical and heat resistance, making them useful for insulation and car parts. They are made by mixing liquid or soft solid components which crosslink and harden when they react, because this process cannot be reversed they cannot be recycled. Thermosets include epoxies and polyesters.

15.4 Rubbers (Elastomers)

These are a type of thermoset. The chains are crosslinked but there are much fewer crosslinks than in regular thermosets, and these crosslinks are provided through vulcanization. These chains are much more flexible and the few number of crosslinks provides a memory effect so it returns to its original shape after being deformed. This crosslinking is normally achieved through the addition of sulphur to chains of thermosets.

15.5 Crystallinity

Thermoplastics can be either amorphous or semi-crystalline materials, while thermosets are always amorphous.

15.5.1 Amorphous Thermoplastics

Most clear plastics, such as acrylic and polycarbonates are amorphous thermoplastics, and these have no long-range structural order. When they cool from a liquid molecular motion is essentially 'frozen out' due to either:

- They cool too fast for crystallisation as the molecules need time to rearrange in an ordered fashion in a crystal
- The structure is too complex for crystallisation as an ordered arrangement becomes difficult

Both of these conditions can also occur in the same material.

This means that these materials have a random, glassy structure with no major secondary bonds between chains. Their entanglement provides their strength, they have good impact resistance and high stiffness.

Glass Transition Temperature (T_g) - When a polymer is cooled below this temperature it becomes hard and brittle, like glass, as the motion of chain molecules freezes out significantly.

This transition is not as sudden as a melting point, unless the material is a crystalline polymer, and is affected by the type of polymer. The higher the T_g the stiffer the chains and the more energy is needed to move the chains. If an amorphous polymer has a $T_g > T_{amb}$ it will be a hard solid while if $T_g < T_{amb}$ it will be soft and rubbery. This difference means some polymers are used above their T_g while others are used below their T_g .

A flexible polymer will have a very low T_g , while one that is stiffer will have a higher T_g . The flexibility of the chains is determined by their chemical structure. For example flexibility decreases with $C=C$ or $C-O-C$ bonds as they are rigid and don't allow twisting or rotation in the molecule. Large side groups also decrease flexibility while a non-carbon backbone, such as silicons or sulphur based polymers, increase the flexibility.

Some examples of amorphous thermoplastics are:

Name	Uses
Polystyrene	- Cheap mouldings and packaging foams
PMMA (Polymethyl methacrylate)	- Known as acrylic, used in windows and light covers
PVC	- Packaging, window frames and pipes
Polycarbonate	- Tough glazing, electrical goods (tough and strong due to rigid $C-O-C$ bonds and aromatic chain groups, with a high T_g of 145-150°C)

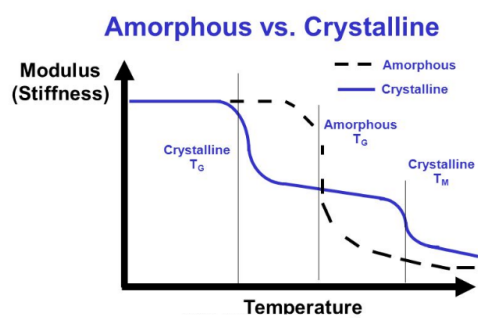
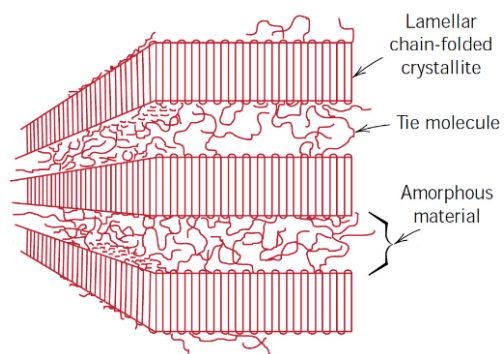
15.5.2 Semi-Crystalline Thermoplastics

The materials have some regions where the chains are arranged in a regular crystalline manner with the chain folding and stacking on itself. Secondary bonds between the chains in these regions provide the strength. These materials have a definite melting point, T_m . Between the crystalline regions the chains are arranged in a random manner, forming an amorphous region. Chains extend between the two regions, providing mechanical strength.

Factors affecting the melting point:

- Flex

Some examples of semi-crystalline thermoplastics are:



Name	Uses
Polyethylene	- Packaging, bottles and toys
Polypropylene	- Casings, crates and pipes
Nylons	- Gears, zips, wheels and casings