

# Fundamentals of Materials (EG-080)

## 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.

## 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.

## 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

03/10/2017

**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

## Atomic Configuration

Proton Mass (Positive) =  $1.67 \times 10^{-24}$

Neutron Mass (Neutral) =  $1.67 \times 10^{-24}$

Electrons (Negative) =  $9.11 \times 10^{-28}$



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<sub>l</sub>** - 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  $2n^2$

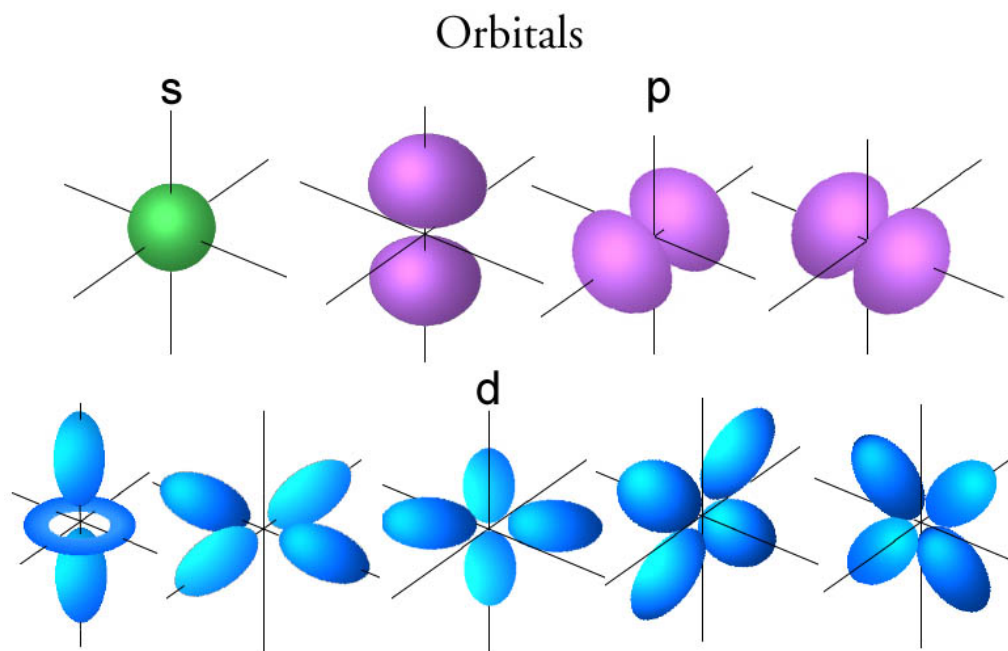


Figure 1: The different possibilities for s, p, and d orbitals

## 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:

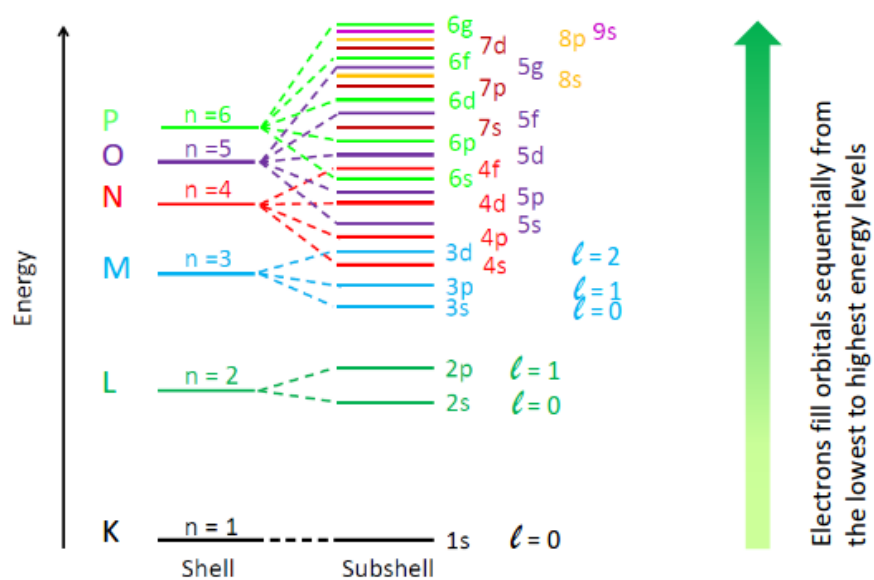


Figure 2:

How to fill orbitals?

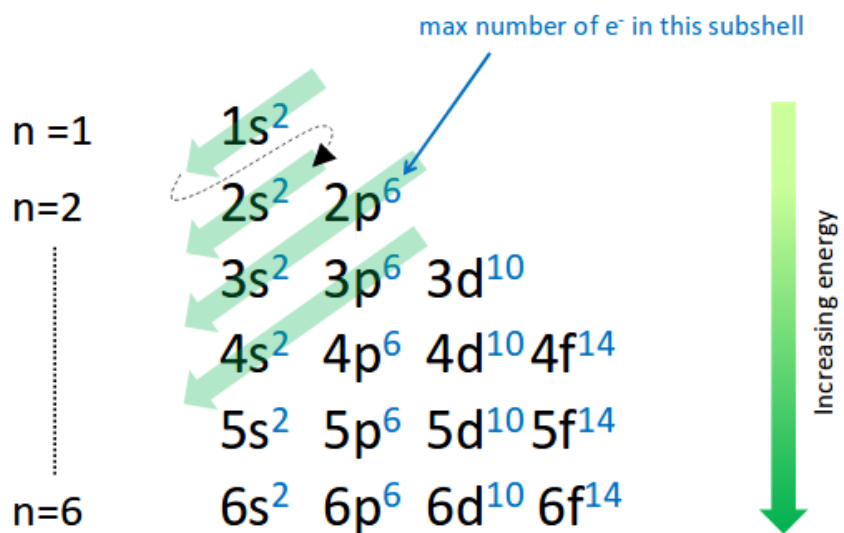


Figure 3:

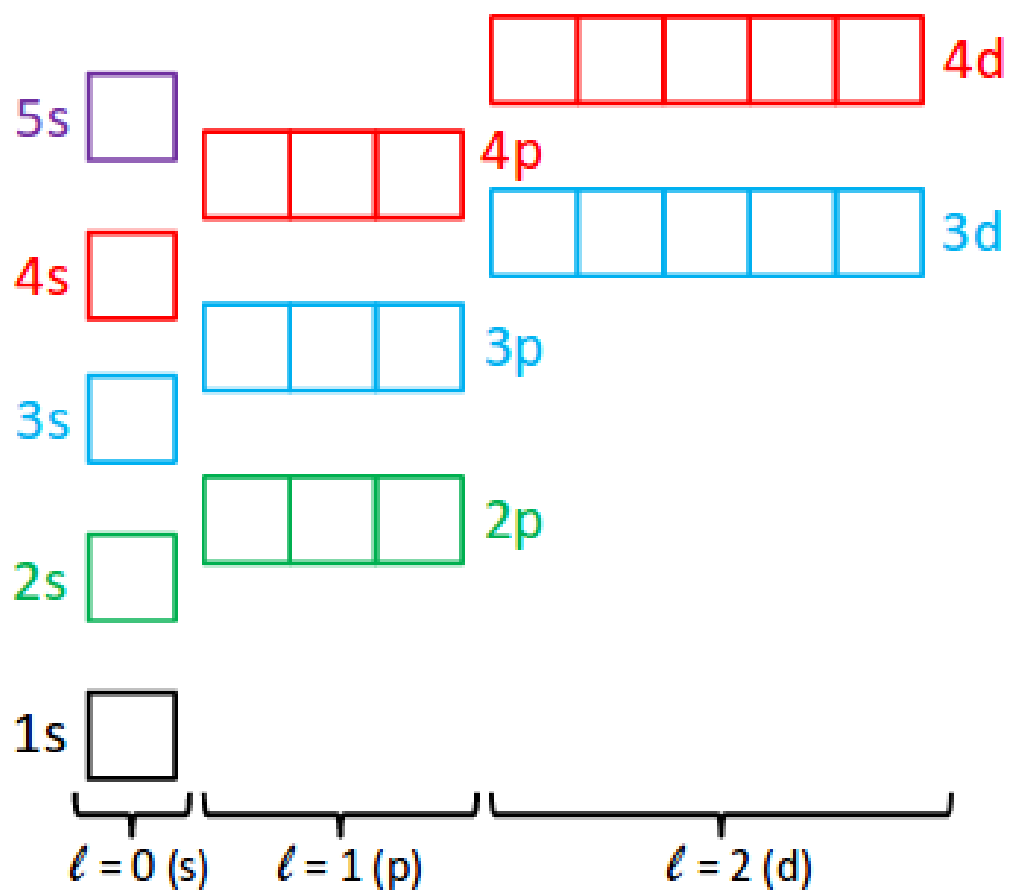


Figure 4: This diagram can be used to show how electrons fill shells. Within each row electrons will always go to an empty box before filling a box completely. These boxes represent the different options within each shell layer (reference Figure 1)

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

10/10/17

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,  $\cdot\dot{\text{C}}\cdot$

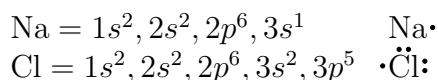
Atoms aim to gain stability by gaining or losing electrons with an aim to gain the same electronic configuration of the closest (in terms of atomic number) noble gas. The interaction of atoms through chemical bonding leads to an overall decrease in the energy. The energy is stored as potential energy.

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.

### 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  $\text{Na}^+$  ion to six neighbouring  $\text{Cl}^-$ , meaning it takes a lot of energy to break all of these bonds. This accounts for the high melting and boiling points.



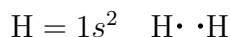
The ionisation energy of an atom increases as its position in the periodic table moves down and to the right. This is based on the distance of the nucleus to the valence shell.

## Covalent Bonding

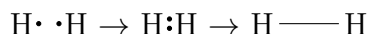
Covalent bonding occurs when pairs of valence electrons are shared between two atoms. This means that neither atom gains or loses any charge. Non-metal elements tend to interact via covalent bonding (instead of ionic) because their ionisation energy is too high.

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

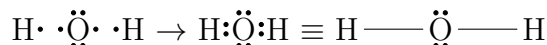
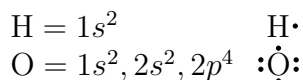


Hydrogen wants to be as stable as the closest noble gas, Helium. The sum of attractive electrostatic forces (nucleus  $\leftrightarrow$  electrons) and repulsive electrostatic forces (electron  $\leftrightarrow$  electron, nucleus  $\leftrightarrow$  nucleus) is overall attractive therefore bonding occurs.



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

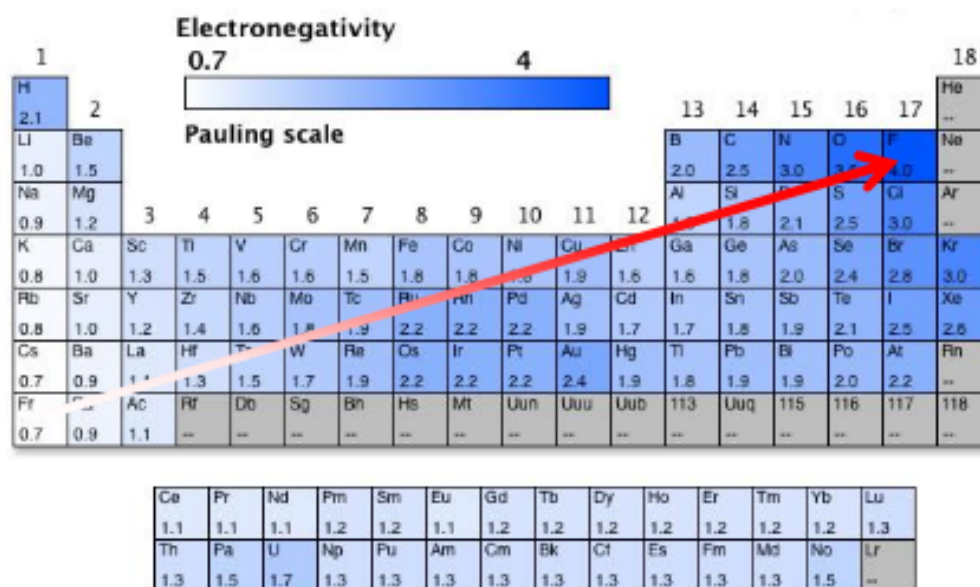
## Water



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  $104.5^\circ$ . 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.

## 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

17/10/17

**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".

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

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

19/10/17

**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)

### 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.

### How atoms in a metal stack

There are three main ways in which atoms stack -

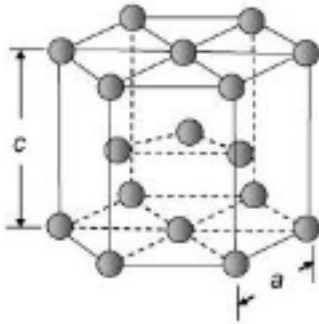
- Hexagonal close packing (hcp)
- Cubic close/ face-centered cubic packing (ccp/fcc)
- Body-centered cubic packing (bcc)

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)

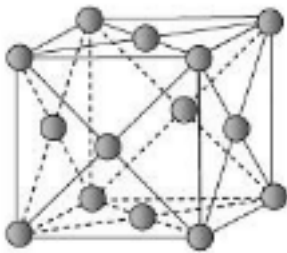
**Unit Cell** - The smallest hypothetical unit that when stacked together repeatedly with no gaps will produce an entire crystal



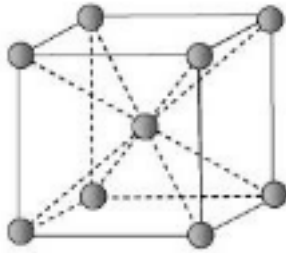
### Hexagonal Close Packing

- 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 (fcc)



- Each atom is surrounded by 6 others in each layer
- Coordination number of 12
- 74 % packing density
- 12 slip streams (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

### 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

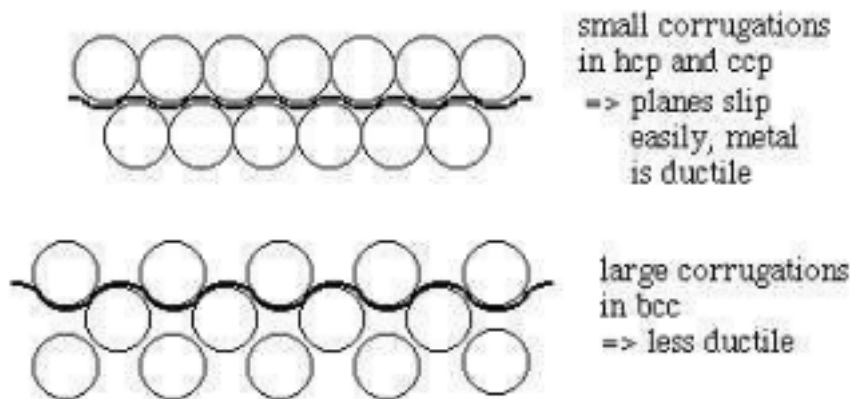
HCP has only one close packed plane, with three directions, so three slip systems. This means it is limited to slipping only if force is applied in certain directions. In most cases, it is quite brittle.

### CCP/ FCC

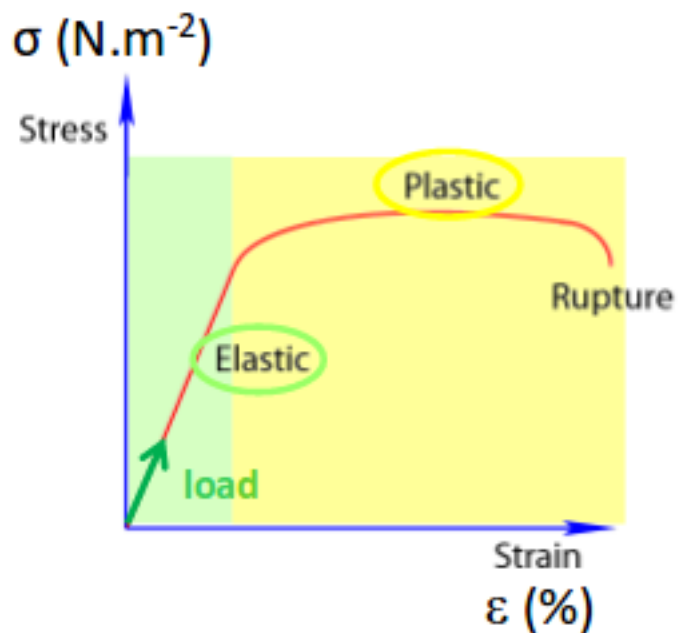
CCP has four close packed planes, each with three close packed directions, so 12 slip planes. It can slip in many arrangements, meaning it is ductile.

## 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.



## 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



$$\sigma = E\epsilon$$

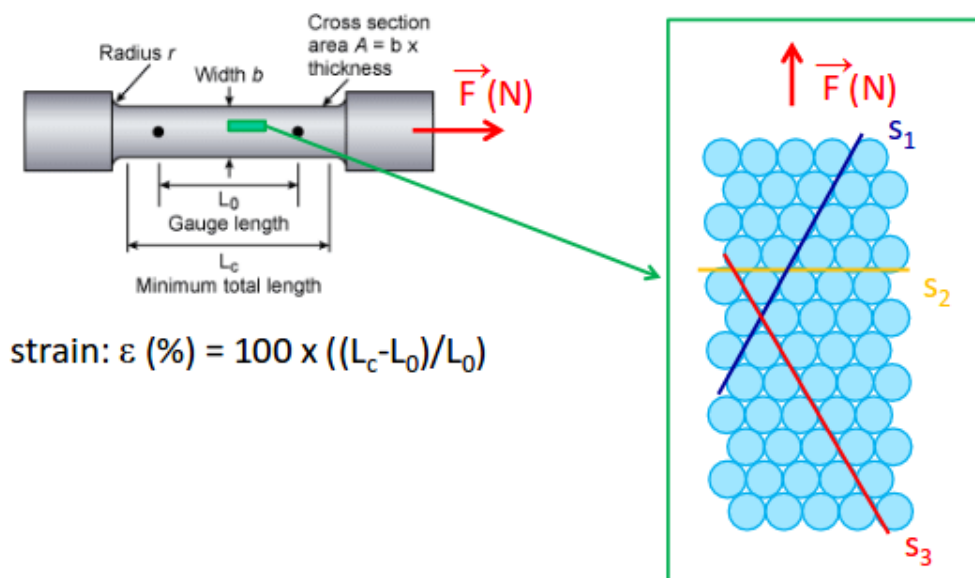
Where:

$\sigma$  = Stress

$E$  = Young's modulus

$\epsilon$  = Strain

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

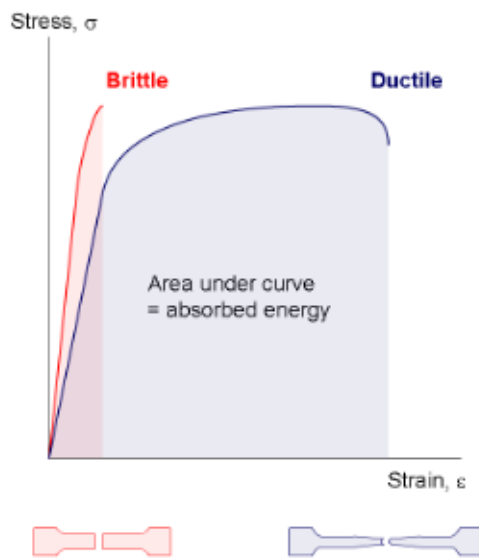


## Ductile vs Brittle

**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  $912^{\circ}\text{C}$  Iron and steel transform from CCP to BCC, from ductile to brittle.