Basics

Introduction

Revise the second unit of Chemistry in G.C.E (A/L).

Materials

Materials can be divided into 4 sub-classifications.

- Metals
- Ceramics
- Polymers
- Composites

Materials can also be categorized based on their usage or their functionalities.

> (i) **Note**
>
> Previously wood was considered as a separate classification, along with the above-mentioned ones.

Property

The response given by a material to a specific stimulus.

- Mechanical properties – stress
- Electrical properties – electric field
- Magnetic properties – magnetic field
- Optical properties – electromagnetic or light radiation

Definitions

Anisotropic

Different properties in different directions.

Isotropic

Same properties in all different directions.

Structure of Atoms

Bohr theory

Presented by Neil Bohr.

1. Electrons of an atom can have only very distinct energy values. Therefore, the electrons are restricted to specific "energy levels" or "stationary states".
2. Electrons in these energy levels rotate about the nucleus in fixed orbits, without radiating or absorbing any energy.
3. When an electron receives energy, it moves from a lower to a higher energy level.
4. Emission of radiant energy (electromagnetic radiation) is due to the movement of the electrons from the higher level to the former lower level of energy.

Bohr Theory **can't** be used to describe the energy characteristics of atoms containing many electrons. Consequently, in the Modern Atomic Theory, four quantum numbers were introduced to describe the energy levels.

Quantum numbers

Principal quantum number

The number given in Bohr's original stationary states corresponds to the principal quantum number (n). Relates to the distance between the nucleus and the principal energy levels.

Secondary quantum number

Represents the various secondary sub-levels within the main energy level. Relates to the shape of the electron cloud. Denoted by l. Values goes from 0 to $n - 1$.

Magnetic quantum number

Represents the direction of maximum extension in space of the electron cloud in the sub shells p, d, and f. which has the dumb - bell shape. Denoted by m. Values goes from $-l$ to l (in total $2l + 1$ different values).

Spin quantum number

Represents the electron spin. $+\frac{1}{2}$ for clockwise and $-\frac{1}{2}$ for counterclockwise spin.

Principles

Pauli's exclusion principle

No two electrons in a single atom can have all four-quantum numbers the same.

Aufbau Principle

Sub-levels with the lowest energy are filled before those with higher energy.

Hund's Rule

The sublevels p, d, and f are occupied by single electrons before any pairing of electrons with opposed spins take place.

Atomic bonding

Primary (strong) bonds

Form when valence electrons are present (outer shell not completely filled).

Ionic

Forms between highly electropositive elements (metals) and highly electronegative elements (non-metals). Non-directional.

Covalent

Forms within electronegative elements that are close to each other in the periodic table. Directional.

Metallic

Forms in metals. Arrangement of positive ion cores in a sea of electrons. Non-directional.

Secondary (weak) bonds

Form when there are no valence electrons (outer shell filled completely).

Van Der Waal's

Forms between inert gases and between symmetric molecules. Forms because of the dipolarity caused inside molecules. Non-directional.

Hydrogen

Forms between polar covalently bonded molecules containing H. Polarity is due to the asymmetry of the molecule. Directional.

Properties of bonds

Property	Order
Hardness, Melting point, Crystalline percentage	Ceramics > Metals > Polymers
Directionality	Covalent > Ionic > Metallic
Brittleness	Ionic > Covalent > Metallic

Metals

Generally isotropic, and crystalline. Can be made amorphous by melting and then suddenly cooling a sample. Metals can be categorized into 2 types.

Pure Metals

Inter-molecular bonds: Metallic bonds. Commonly not used in the pure form.

Pure metals might be:

- not strong enough
- too weak to corrosion

Alloys

Which contain more than one metallic element.

Examples:

- Steel $[Fe + C]$

- Cast Iron $[Fe + C]$

- Brass $[Cu + Zn]$

- Bronze $[Cu + Sn]$

- Gold jewelry $[Au + Cu]$

- Duralumin $[Al + Cu]$ - used for aircraft body

- Stainless steel $[Fe + C + Cr + Ni]$,

- Cast iron $[Fe + C]$

Alloys have a parent metal (mostly used metal, percentage-wise) and one or more alloying elements (all elements other than parent metal).

> ⓘ **Note**
>
> Steel has maximum of $2\% \ C$ and it's ductile (won't break easily). Cast Iron has $2\% - 4\% C$ and it's brittle (will break easily).

Super Alloys

Alloys containing too many alloying elements (maybe even 20).

Properties

- Fe, Co, Ni , and their alloys are magnetic

- Good electrical conductivity

- Good thermal conductivity

- High strength

- High stiffness (= high young's modulus)

- Good ductility

Ceramics

Inter-molecular bonds: covalent and/or ionic.

Properties

- Non metallic

- Inorganic

- Produced by shaping and firing

- High melting temperatures (some can survive upto $8000°\text{C}$)

- Low density

- High strength, stiffness, hardness

- Corrosion-resistant

- Generally good insulators (electrical and thermal)

- Brittle as glass. Behaves glass-like mostly.

> ⓘ **Glass**
>
> **Not** an element of ceramics. Hugely differs in structure. Can be used to store liquids. Soluable in HF.

Some ceramic materials are:

- magnetic

- piezoelectric

- superconductors (only few, and only at very low temperatures)

Refractory ceramics

Ceramics that can withstand high temperatures. Can provide thermal insulation.

Types

2 types:

- Traditional - clay-based items like pottery, porcelain, and tiles

- Advanced - like silicon carbide, boron nitride, zirconia

Examples

- Alumina
- Sand
- Tiles
- Cement
- Concrete

Polymers

Polymers can be made 100% amorphous but not 100% crystalline. Inter-molecular bonds: Covalent and Van der Waals or Hydrogen.

Elastomers are a type of polymers.

Properties

- Has a repeating structure
- lightweight
- corrosion-resistant
- easy to process at low temperatures
- generally inexpensive
- generally low strength
- generally high toughness
- good heat, electrical insulators (but conductive polymers exist)

Examples

Plastics

- Polyvinylchloride (PVC)
- Polyethylene / Polythene (PE)
- Polypropylene (PP)
- Polystyrene (PS)
- Polypropylene used in kitchen-were
- Polymethylmethacrylite (PMMA) Perspex

  It's transparent and lightweight. Used in aircraft windows and contact lenses.
- Polytetrafluoroethylene (PTFE) Teflon
- Polysiloxane or Silicone (not to be confused with silicon which is a metalloid)

Rubber

- Polyisoprene / Natural rubber
- Styrenebutadiene rubber (SBR)

Composites

Materials that are a mixture of 2 different-typed materials. Materials are combined together to get the advantages of two materials.

Examples

- Concrete (conventional one)
- Fiber glass (GFRP)

  A combination of glass and plastic. Not brittle.

> ⓘ **Note**
>
> The procedure of creating fiber glass:
>
> - Glass is converted into fiber (which is a shape; not a material)
> - Add plastic

Crystal Structure

Materials are categorized into 2, based on the arrangement of atoms or molecules.

- Crystalline
- Amorphous

Crystalline

Atoms or molecules are arranged in a ordered structure. Long-order is present. Situated in a repeating array over large atomic distances (long-range order).

Examples:

- Metals
- Ceramics

Atomic arrangement is usually described by **space lattice**.

Amorphous (or Non Crystalline)

Atoms or molecules are randomly arranged. Long-range order is absent.

Example:

- Glass
- Polymers are semi-crystalline

Space Lattice

An infinite set of equally-spaced **points** in a space.

Set of lines are used to connect these points to provide a useful guide to the eye. They are not part of the lattice.

Unit Cell

Smallest repeating parallelepiped inside the lattice. By stacking in all directions, the lattice can be formed.

Density

$$\rho = \frac{\text{Mass/unit cell}}{\text{Volume/unit cell}} = \frac{Mn}{vL}$$

Here:

- M - molar mass
- n - atoms per unit cell
- v - volume of the unit cell
- L - avagadro's number

> ⓘ **Note**
>
> The total number of atoms stays the same when one structure transitions into another.

Crystalline systems

- All crystalline materials fall within one of the 7 possible shapes and 4 variants.

The shapes

Don't have to memorize.

- Cubic
- Hexagonal
- Tetragonal
- Rhombohedral (Trigonal)
- Orthorrhombic
- Monoclinic
- Triclinic

The variants

- Simple: atoms at the corners only.
- Base-centered: atoms at the corners and center of 2 opposing sides only.
- Body-centered: atoms at the corners and center only.
- Face-centered: atoms at the corners and center of all faces only.
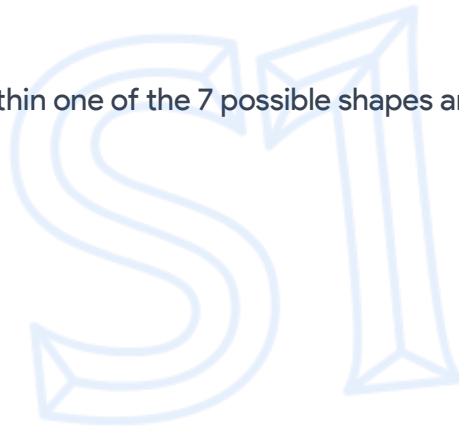
Bravais showed that only **14** of 28 (7 shapes x 4 variants) are possible in real life.

Only 4 of them are studied in s1.

- Simple cubic (**sc**)
- Body-centered cubic (**bcc**)
- Face-centered cubic (**fcc**)
- Hexagonal close packed or Close packed hexagonal (**hcp/cph**)

Coordination number

Coordination number of a lattice system is the number of particles that each particle contacts.

Atomic Packing Factor (APF)

$$\text{APF} = \frac{\text{True volume}}{\text{Bulk volume}} = \frac{\text{Volume of atoms/unit cell}}{\text{Volume/unit cell}}$$

Geometrically maximum APF in real life (assuming spherical and identical atoms) is 74%. If a structure has 74% APF, the structure is called a **close-packed structure**. The APF can be increased to a maximum of 79% by adding impurities.
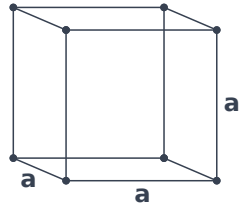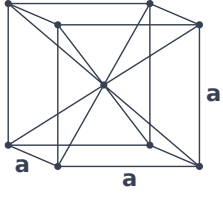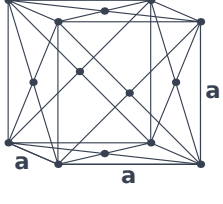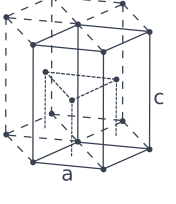
Interstitial sites (aka holes, voids)

Empty space that exists between the packing of atoms in a crystal structure.

Octahedral interstices

Locations of void spaces available in an FCC. Located at the center of each edge and body-center of the unit cell.

Summary of the 4

	sc	bcc	fcc	hcp
Unit cell				
Constants	a	a	a	a, c (where $c > a$)
With atom radius	$a = 2r$	$a = \frac{4}{\sqrt{3}}r$	$a = \frac{4}{\sqrt{2}}r$	$a = 2r; c = \sqrt{\frac{8}{3}}a$
Volume	a^3	a^3	a^3	$\frac{3}{2}\sqrt{3}a^2c$
Atoms per unit cell	1	2	4	6
Composition	$8 \cdot \frac{1}{8}$	$8 \cdot \frac{1}{8} + 1$	$8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2}$	$3 + 12 \cdot \frac{1}{6} + 2 \cdot \frac{1}{2}$
Near-neigbour distance	a	$\frac{\sqrt{3}a}{2}$	$\frac{a}{\sqrt{2}}$	a
Coordination number	6	8	12	12
APF	52.36%	68%	74%	74%
Examples	Po	Fe, Cr, W	Al, Cu, Ni	Mg, Zn

Sources of the images:

- Simple cubic: [Original file @ Wikipedia](#)
- Body-centered cubic: [Original file @ Wikipedia](#)
- Face-centered cubic: [Original file @ Wikipedia](#)
- Hexagonal close-packed: By [Original: Dornelf](#) Vector: [DePiep](#) - Own work based on: [Hexagonal close packed.png](#), [CC BY-SA 3.0](#), [Link](#)

Miller Indices
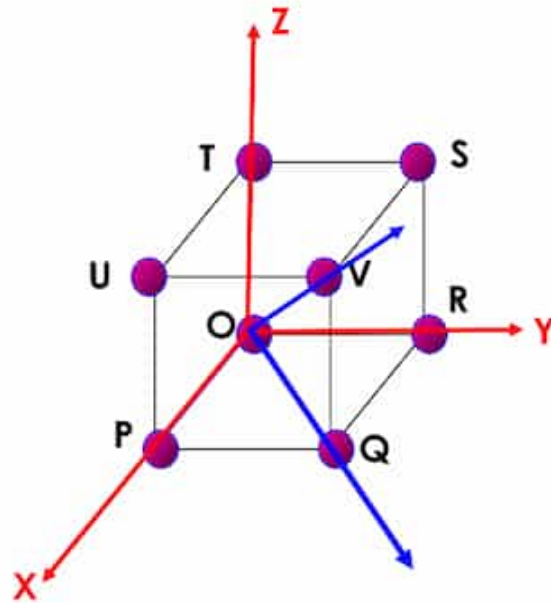
Any vertex can be chosen as the origin.

Notation

- Minus noted with a bar
- Addition and subtraction is carried out like vectors
- $(1, 1, 0)$ - Atom/Vertex
- $[110]$ - Direction, **no commas**
- $<110>$ - Family of directions
- (100) - Plane, **no commas**
- $\{100\}$ - Family of planes
- Always will be whole numbers. Fractions must be multiplied by LCM.

Direction

Equivalent directions are grouped into a **family**.

Direction families

<100>

- No of planes: 6
- $[100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]$

<110>

- No of planes: 12
- $[011], [01\bar{1}], [0\bar{1}1], [0\bar{1}\bar{1}], [101], [10\bar{1}], [\bar{1}01], [\bar{1}0\bar{1}], [110], [1\bar{1}0], [\bar{1}10], [\bar{1}\bar{1}0]$

<111>

- No of planes: 8
- $[111], [11\bar{1}], [1\bar{1}1], [\bar{1}11], [\bar{1}\bar{1}1], [\bar{1}11], [1\bar{1}\bar{1}], [\bar{1}\bar{1}\bar{1}]$

The above are the common directions. There are other directions as well.

Show the direction

To show the direction $[132]$, for example:

Take the point $(1, 3, 2)$. Divide by the highest number (3, in this case) to bring the point inside the unit cell. The resulting point will be $\left(\frac{1}{3}, 1, \frac{2}{3}\right)$. The direction is given by vector from $(0, 0, 0)$ to the resulting point.

Close packed direction

All neighbour atoms in a direction touch each other. For example: (110) of fcc.

Plane

Steps

- If sitting on any axes, move the origin.
- Find the intercepts. ∞ if parallel.
- Find the reciprocals.

Plane families

100

- Denotes as $\{100\}$
- No of planes: 6
- $(100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

110

- Denotes as $\{110\}$
- No of planes: 12
- $(011), (01\bar{1}), (0\bar{1}1), (0\bar{1}\bar{1}), (101), (10\bar{1}), (\bar{1}01), (\bar{1}0\bar{1}), (110), (1\bar{1}0), (\bar{1}10), (\bar{1}\bar{1}0)$

111

- Denotes as $\{111\}$
- No of planes: 8
- $(111), (11\bar{1}), (1\bar{1}1), (\bar{1}11), (\bar{1}\bar{1}1), (\bar{1}1\bar{1}), (1\bar{1}\bar{1}), (\bar{1}\bar{1}\bar{1})$

The above are the common planes. There are other planes as well.

Show the plane

- Divide by the smallest non-zero number.
- Find the reciprocals. ∞ means parallel to the axis.

Close packed plane

All neighbour atoms in a crystal plane touch each other. For example: (111) of fcc.

Planar Density / Aerial Density

Number of atoms in a unit area in a specific plane. Differs between different planes in a single crystal structure.

Allotropy

Ability of a single substance to exist in more than one physical form.

Examples

Iron

- $\alpha - \text{Fe}$ (Ferrite) - Below $912\,^\circ\text{C}$
- $\gamma - \text{Fe}$ (Austenite) - Between $912\,^\circ\text{C}$ and $1394\,^\circ\text{C}$
- $\delta - \text{Fe}$ - Above $1394\,^\circ\text{C}$
- $\epsilon - \text{Fe}$ (Hexaferrum)

First 3 exist in atmospheric pressure. Forth one exists in very high pressure.

Carbon

- Graphite
- Diamond
- [Carbon nanotubes](#)

Buckminsterfullerene

Aka. bucky ball. Has $60\ \mathrm{C}$ atoms inside a molecule. A molecule is truncated icosahedron shaped. Diameter of the molecule is approx. $1\ \mathrm{nm}$. Each carbon atom is bonded to another 3. Not chemically inert.

Defects in Crystals

There won't be a crystal with 100% of perfect arrangement. Defects are advantages in materials most of the time.

Types of defects:

- Point defects
- Line defects / Dislocations
- Planar defects
- Bulk defects - Related to volumetric defects. Common for any materials. Example: crack, holes.

> ⓘ **Note**
>
> Bulk defects are not covered in s1.

Point defects

Related to a single atom.

- Vacancy - Missing parent atom

- Self-interstitial atom - A self atom entered into an interstitial site

- Interstitial impurity atom - A foreign atom entered into an interstitial site

- Substitutional impurity atom - A foreign atom replaced a parent atom or a vacancy

Line defects

Related to a line of atoms. Three types:

- Edge dislocation - only covered in s1

- Screw dislocation

- Mixed dislocation (combination of above 2)

Edge dislocation

Caused by removal of a half plane.

Half plane

Remaining part of a plane of atoms after a set of planes are gone missing.

Slip plane

Plane that is perpendicular to the half plane and on a boundary.

Dislocation line

Intersecting line of half plane and slip plane.

Planar defects

Related to a plane of atoms.

Solidification

The process of conversion liquid to solid. Occurs in 3 steps:

- Nucleation

- Growth of crystals

- Formation of grain structure

Tiny solid particles forms. Called as Nuclei (nothing related to atom's nucleus). Each nucleus grows bigger and forms a crystal. And then forms grains.

Grain

A group of atoms packed in a particular orientation that is different from that of the neighbor ones.

Each grain is usually in micrometer in size. Grain structure can only be observed through a microscope after careful preparation of samples (microstructure).

Grain boundaries

The boundary between 2 adjacent grains. These are the planar defects found in crystalline materials.

Functional Materials

Classification of materials based on whether most important function they perform is either mechanical, structural, biological, electronic, magnetic, or optical.

These materials have one or more properties that can be significantly changed in a controlled fashion with an external stimuli.
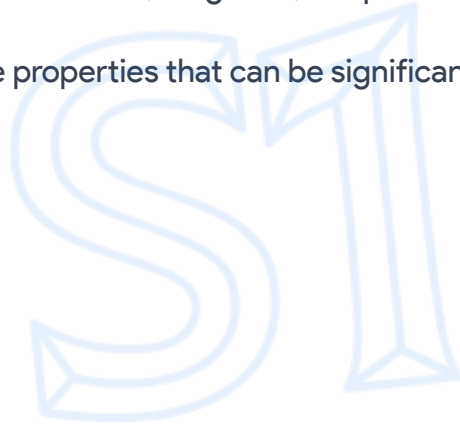
List of properties

- Electrical properties
  - [Piezoelectricity](#)
  - Ferroelectricity
  - Superconductivity
  - Capacitance

- Optical properties
  - Photoluminescence
  - Photochromism
  - Fluorescence
  - Photoelectricity

- Magnetic Properties
  - Diamagnetism
  - Ferromagnatism
  - Ferrimagnetism
  - Paramagnetism
  - Anti-ferri magnetism

- Chemical Properties / Reactivity properties
  - reactivity with other substances
  - catalytic properties

- Others
  - Photocatalytic - a material that uses light energy to catalyze a chemical reaction.
  - Electroluminescent - a material that emits light under an electric current or strong electric field

Examples

Gas sensing

Graphene based field effect transistor is used as the sensor. When gas molecules get absorbed into the graphene surface, graphene's charge carrier concentration and resistance changes. Large surface means higher sensitivity. Can be done for NO, CO, NH_3.

Ethanol sensing

Metal oxide nanoparticles are used as the sensor. Nanoparticles are used because of high surface area, which means more sensitive.

O_2 gas is adsorbed on the metal oxide. It turns into O^{2-} as shown below. Number of free electrons will decrease as this series of reactions is happens. Hence conductivity will decrease.

$$O_2 + e^- \longrightarrow O_2{}^-$$

$$O_2{}^- + e^- \longrightarrow 2\,O^-$$

$$O^- + e^- \longrightarrow O^{2-}$$
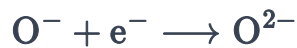
When ethanol gas is present, it will also be adsorbed.

$$CH_3CH_2OH + 6\,O^{2-} \longrightarrow 2\,CO_2 + 3\,H_2O + 6\,e^-$$

The above reaction will release the electrons back into the conduction band, and conductivity will be increased.

2 types of metal oxides are used.

- n-type
    - TiO_2
    - ZnO

- p-type
    - NiO
    - Cu_2O

Li-ion battery

Positive electrode is made of $LiCoO_2$. During discharge, Li^+ are released from cathode to the electrolyte. Connected using Al.

Negative electrode is made of graphite. Li^+ are stored in graphite layers during charging. Connected using Cu.

The electrolyte is either a liquid or gel, containing Li salts. The anode and cathode are separated using a porous membrane which only allows Li^+ to pass through.

While charging:

- Anode - Graphite
- Cathode - $LiCoO_2$

While discharging:

- Anode - $LiCoO_2$
- Cathode - Graphite

The reactions are:

$$LiC_6 \longrightarrow C_6 + Li^+ + e^-$$

$$CoO_2{}^- + Li^+ + e^- \longrightarrow LiCoO_2$$

Self-cleaning surfaces

The surface is coated with nano-scale layer of TiO_2 which is photocatalytic. It causes a series of chemical reactions, which loosen the dust particles from the surface. The glass surface turns superhydrophilic because of TiO_2.

Superhydrophilic material is a material that attract water strongly which causes water to spread out into a thin layer on its surface.

When raining, a thin layer of water will be formed on the surface of TiO_2-coated glass. This layer of water washes the dust particles away.

LEDs

LEDs are electroluminescent. Electrons and holes recombine at the p-n junction, and emit light.

The color of a LED depends on the energy band gap of the semiconductor material.

Blu-ray disk

Writing media of the blu-ray disc is a phase-changable material. The material can transition between crystalline and amorphous when hit by laser.
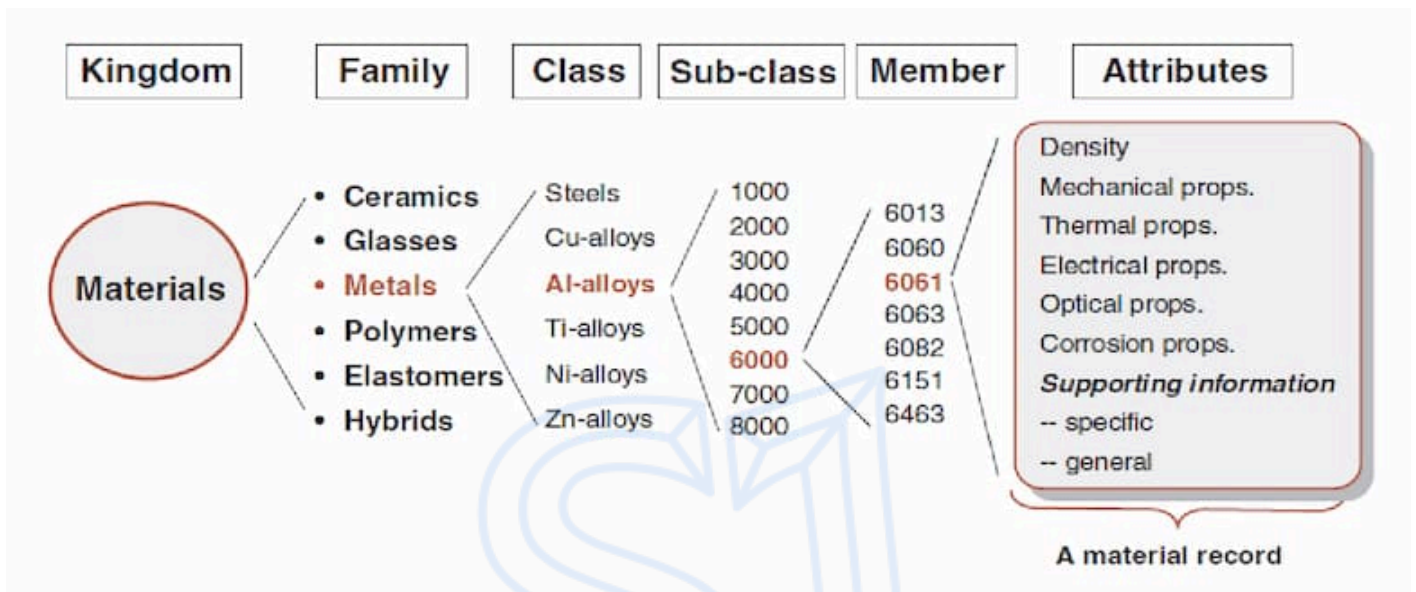
Example for phase-changable material: $Ge_8Sb_2Te_{11}$.

Selection of Materials

> **ⓘ Note**
>
> This is a separate unit itself and taught as the last thing in the module.

Materials are categorized into a tree.

In computerized selection software, materials are stored in the above structure.

Selection process

Seeking the best match between design requirements and property profiles of materials. Has 4 main steps.

Translation

Identification of requirements. The requirements include:

- Function - what does it have to do?
- Constraints - what non-negotiable conditions must be bet?
- Objective - what is to be maximized or minimized?
- Free variables - what parameters of the problem are free to be changed?

Screening

Eliminating materials that do not meet the constraints.

Ranking

Materials are ranked according to certain criteria involving multiple dimensions. Done based on objectives.

Material index

Property of property group that maximizes performance for a given design.

Supporting information

A few materials are filtered through the above steps. After this, additional information (such as listed below) are considered to choose one.

- Price
- Availability

> ⓘ **Note**
>
> Nowadays software is used to select materials. World-wide accepted software is Cambridge Engineering Selector (CES). Expensive and powerful.