Summary | Properties of Materials

Introduction

Be sure to 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.

Property

A property is 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

Metals

Metals can be categorized into 2 types.

- Pure metals
- Alloys

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]
- 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).

> ⓘ **Super Alloys**
>
> Alloys containing too many alloying elements (maybe even 20).

> ⓘ **Note**
>
> Steel (Fe + C) has maximum of 2% C. Won't break easily (ductile).
> Cast Iron (Fe + C) has 2%-4% C. Will break easily (brittle).

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

> **Note**
>
> Ductile - easily changes shape by applying force.
> Brittle - easily breaks when applying force.

Ceramics

Inter-molecular bonds: covalent and/or ionic.

Properties

- Non metallic
- Inorganic
- Produced by: shaping => firing.
- High melting temperatures (some can survive upto 8K deg C)
- Low density
- High strength, stiffness, hardness
- Corrosion-resistant
- Generally good insulators (electrical and thermal)
- Brittle as glass. Behaves glass-like mostly.

> **Note**
>
> **Glass is not an element of ceramics**. Hugely differs in structure.

Some ceramic materials are:

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

Examples

- Sand
- Tiles
- Cement
- Concrete

2 types:

- Traditional - clay-based items (like pottery, porcelain, tiles)
- Advanced - (like silicon carbide, boron nitride, zirconia)

Polymers

Inter-molecular bonds: Covalent and Van der Waals or Hydrogen.

Properties

- Has a repeating structure.
- lightweight
- corrosion-resistant
- easy to process at low temperatures
- generally inexpensive
- generally low strength
- generally high toughness
- poor conductors of electricity & heat (= good insulators) (but conductive polymers exists as well)

Examples

Plastics

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

> **Note**
>
> PMMA Perspex is

> - transparent (like glass)
> - lightweight
> - used in aircrafts’ windows & contact lenses.

Rubber

- Polyisoprene / Natural rubber
- Styrenebutadiene rubber (SBR)

Composites

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

Examples

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

Fiber glass is a combination of glass and plastic. Not brittle. The procedure to creating fiber glass:
glass => fiber (a shape not material) => add plastic == fiber glass

Crystal Structure

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

- Crystalline
- Amorphous

Crystalline

- Ordered arrangement of atoms or molecules.
- Situated in a repeating array over large atomic distances (long-range order).
- Example: Metals and Ceramics.

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

Amorphous (or Non Crystalline)

- Random arrangment of atoms or molecules.
- 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 generated.

Density

$$\rho = \frac{\text{Mass/unit cell}}{\text{Volume/unit cell}} = \frac{1}{v}(\frac{M}{L} \times n)$$

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 atoms) is 74%. If a structure has 74% APF, the structure is called a **close-packed structure**.

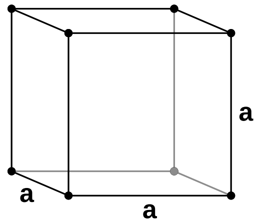
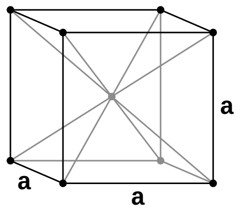
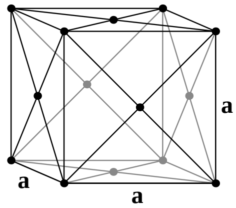
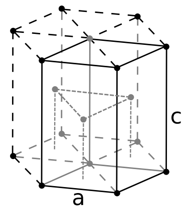
Interstitial sites (aka holes, voids)

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.

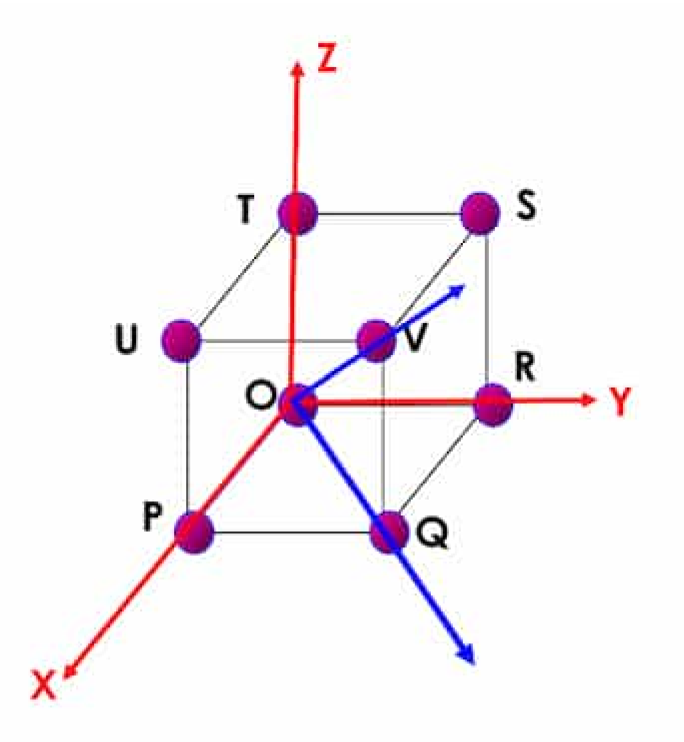
Summary of the 4

	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	$8 \cdot \frac{1}{8}$	$8 \cdot \frac{1}{8} + 1$	$8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2}$	$3 + 12 \cdot \frac{1}{6} + 2 \cdot \frac{1}{2}$
Coordination number	6	8	12	12
APF	52.36%	68%	74%	74%
Examples	Po	Fe, Cr, W	Al, Cu, Ni	Mg, Zn

The unit cell images are taken from Wikipedia.

- Simple cubic: [Original file @ Wikipedia]
- Body-centered cubic: [Original file]
- Face-centered cubic: [Original file]
- 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 as 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
- $[111], [11\bar{1}], [1\bar{1}1], [\bar{1}11], [\bar{1}\bar{1}1], [\bar{1}1\bar{1}], [1\bar{1}\bar{1}], [\bar{1}\bar{1}\bar{1}]$

Show the direction

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

Take the point $(1, 3, 2)$. It **must be** inside the unit cell. 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:

- Fe
- C
  - Graphite
  - Diamond
  - Buckminsterfullerene
  - Carbon nanotubes
  - Graphene

Defects in Crystals

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

1. Point defects
2. Line defects / Dislocations
3. Planar defects
4. Bulk defects - Related to volumetric defects. Common for any materials. Example: crack, holes. Not covered in s1.

Point defects

Related to a single atom.

- Vacancy - Missing parent atom
- Self-interstitial atom - A parent 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

TODO

Slip plane

Plane that is perpendicular to the half plane.

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

Boundary between 2 adjacent grains is **grain boundary**.

Planar defects found in crystalline materials.

Nanomaterials

A material with

- any external dimension in the nanoscale (size range from approximately $1\text{–}100\ \mathrm{nm}$).
- having internal structure or surface structure in the nanoscale.

At nanoscale, materials exhibit very unusual and very interesting properties. Examples: Graphene has very high young’s modulus and very high carrier mobility.

Nano object

An object with any external dimension is in the nanoscale.

Examples: carbon nanotube, bucky ball.

Nano structured material

A material where its internal or surface structure is in the nano scale.

Examples: TiO_2 nanotube films.

Nano in nature

- Lotus leaves being superhydrophobic
- Gecko adhesive system

Nanoscience

Study of structures and materials on the nanoscale.

Nanotechnology

Development of materials and devices by exploiting the characteristics of particles on the nanoscale.

Applications

- Nanoscale transistors
  - Higher-performance
  - Improved energy efficiency
- Magnetic data storage
  - High data density and data capacity
  - Ultra compact
- Nanomedicine and drug delivery
- Energy storage

Preparation of nanomaterials

Top-down approach

Nanoscale dimensions are created using larger components, by externally controlled devices.

Examples: Lithography, Etching techniques.

Photolithography

Can be used to create nanoscale patterns in thin films or bulk substrates.

The steps:

1. Coat Si wafer with a photosensitive material.
   A material which changes its properties when exposed to electromagnetic radiation
2. Allow the radiation to pass through the mask on to photosensitive material.
3. Developer solution removes either reacted or unreacted material.
4. The silicon wafer is etched to transfer the pattern onto silicon wafer.
5. Photosensitive material is removed.

Bottom-up approach

Molecular components arrange themselves into more complex nano materials/objects.

Examples: Molecular self-assembly, Chemical vapour deposition

Graphene

Carbons arranged to a hexagonal network. 2D crystal based.

Unit Cell

- A rhombus with 120° .
- Lattice parameter is $2d\cos 30^\circ$ where d is the $\mathrm{C-C}$ bond length.
- 2 atoms per unit cell.

> **Note**
>
> Single layer of graphene was discovered using scotch tape method and the discovery won a Nobel prize in 2010.

Synthesis

- Top-down approaches
  - Exfoliation (eg: Scotch tape method)
- Bottom-up approaches
  - Chemical vapor deposition

> **Note**
>
> Graphene has a band gap of 0.