

# Summary | Properties of Materials

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## 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

At extremely low temperatures, some metals tend to be superconductors.

## 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** contain too many alloying elements (maybe even 20).

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

Ductile easily change shape by applying force.

Brittle easily break when applying force.

# Ceramics

Inter-molecular bonds: covalent and/or ionic.

## Properties

- Non metallics
- 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.

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

Some ceramic materials are:

- magnetic
- piezoelectric - converts mechanic energy (sound) <> electrical energy (electric current)
- 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 in strength
- generally high in toughness
- poor conductors of electricity & heat (= good insulators)

We also have conducting polymers.

## Examples

### Plastics

- Polyvinylchloride (PVC)
- Polyethylene / Polythene (PE)

- Polypropylene (PP)
- Polystyrene (PS)
- Polypropylene - used in kitchen-were
- Polymethylmethacrylate (PMMA) Perspex
- Polytetrafluoroethylene (PTFE) Teflon

PMMA Perspex is

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

## Rubber

- Polyisoprene / Natural rubber
- Styrenebutadiene rubber (SBR)

# Composites

Advantages of two materials combined together.

## 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 arrangements 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).
- Metals and Ceramics.

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

## Amorphous (or Non Crystalline)

- Random arrangement 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

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

## 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)
- Orthorhombic
- 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.

We are only going to study about 4 of them.

- 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**.

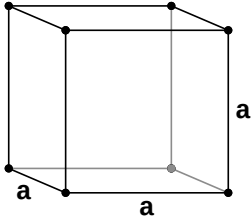
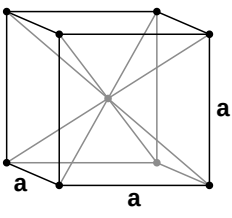
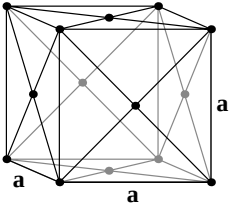
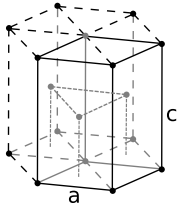
## Interstitial sites (aka holes, voids)

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

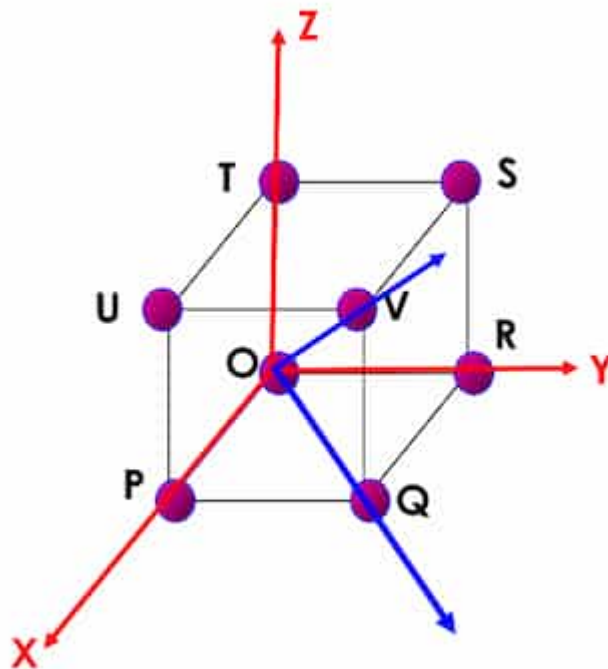
	sc	bcc	fcc	hcp
Unit cell				
Constants	$a$	$a$	$a$	$a, c$ (where $c > a$ )
With atom radius	$a = 2r$	$a = \frac{4}{\sqrt{3}}r$	$a = \frac{4}{\sqrt{2}}r$	$a = 2r; c = \sqrt{\frac{8}{3}}a$
Volume	$a^3$	$a^3$	$a^3$	$\frac{3}{2}\sqrt{3}a^2c$
Atoms per unit cell	1	2	4	6

	sc	bcc	fcc	hcp
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**
- $\langle 110 \rangle$  - 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

#####  $\langle 100 \rangle$

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

#####  $\langle 110 \rangle$

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

#####  $\langle 111 \rangle$

- 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  $(\frac{1}{3}, 1, \frac{2}{3})$ . 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.  $\infty$  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.  $\infty$  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.

## Defects in Crystals

There won't be a crystal with 100% of perfect arrangement. Defects 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.

## 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.

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