# Introduction to Properties of Materials

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

**Glass is not an element of ceremics**. 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-resistent
- 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
- Polymethylmethacrylite (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 arrangments of atoms or molecules.

- Crystalline
- Amorphous

## Crystalline

- Ordered arrangment 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 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

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

# 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)
- 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.

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)

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

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**.

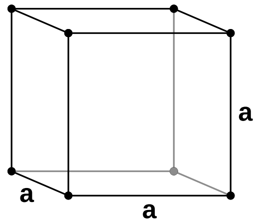
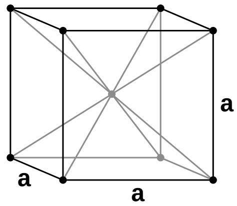
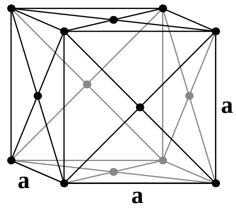
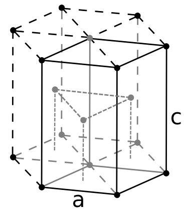
# Interstitial sites (aka holes, voids)

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.

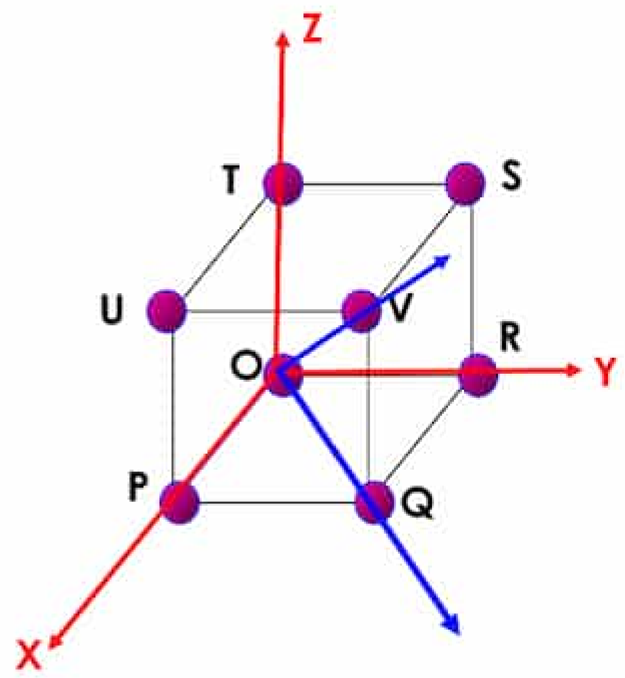
# Summary of the 4

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