MATERIALS SCIENCE AND ENGINEERING

An Introduction





Part of Electric Engineering Materials



Prof. Simranjeet Singh Department of Electric Engineering

What are the kind of questions that a student of materials science would like answers for?

- Why is glass brittle, while copper is ductile? What is meant by a *ductile* material?
- □ If we take two rods, one of Al and one of steel, why is it easier to bend the Al rod as compared to the steel rod?
- □ How can I change properties like hardness, without changing the composition (say of 0.8% C steel)?
- □ Why is wire of copper conducting, while piece of brick or wood non-conducting?
- □ Why is glass transparent, while any typical metal is opaque?
- □ Why does the electrical conductivity of Cu decrease on heating, while that of Si increases?
- □ Why does Iron corrode easily, while Aluminium does not (or does not seem to?!)?
- How come I can hold a molten material in the liquid state below the melting point (e.g. water can be held at sub-zero (°C) temperatures), for at least some time (*in many cases this is not difficult*)?
 How come bubbles tend to form in a aerated drink glass around the straw and glass walls?
 - > What is the melting point? Is it different from the freezing point?
- Usually, good thermal conductors are also good electrical conductors. Why is this so?
 Why is diamond a good thermal conductor, but not a good electrical conductor?
- □ If I pull a spring and then release the load, it 'comes back' to its original shape. However, a if I bend an aluminium rod, does not come back to its original shape. How can one understand these observations?

What will you learn in this chapter?

- Where does Materials Science lie in the broad scheme of things?
- What are the common types of materials?
- What are the Scientific and Engineering parts of Materials Science & Engineering?
- What is the important goal of Materials Science?
- What determines the properties of Materials?





A polycrystalline vessel for drinking fluids is sometimes referred to as GLASS! And, a faceted glass object is sometimes referred to as a crystal!



Faceted glass objects are sometimes called crystals!

Continued...

- Based on state (phase) a given material can be Gas, Liquid or Solid Intermediate/coexistent states are also possible (i.e clear demarcations can get blurred). (Kinetic variables can also affect how a material behaves: e.g. at high strain rates some materials may behave as solids and as a liquid at low strain rates)
- Based on structure (arrangement of atoms/molecules/ions) materials can be Crystalline, Quasicrystalline or Amorphous.
 Intermediate states (say between crystalline and amorphous; i.e. partly crystalline) are also possible. *Polymers are often only partly crystalline*.
- Liquid Crystals ('in some sense') are between Liquids and Crystals.
- Similarly Solid Electrolytes (also known as* fast ion conductors and superionic conductors) are also between crystals and liquids. These materials have a sublattice which is 'molten' and the ions in this sublattice are highly mobile (these materials are similar to liquid electrolytes in this sense).
- Based on Band Structure we can classify materials into Metals, Semi-metals, Semiconductors and Insulators.
- Based on the size of the entity in question we can Nanocrystals, Nanoquasicrystals etc.
- There are other classifications we will encounter during the course (readers may want to check this out: <u>Slide 7</u>).



One way of classification does not interfere with another

- □ From a *state* perspective we could have a liquid, which is a metal from the *band structure/conductivity perspective*
 - \rightarrow Hg is liquid metal at room temperature.
- Or we could have a metal (band structure viewpoint), which is amorphous (structural viewpoint (atomic ordering))
 - \rightarrow ZrTiCuNiBe bulk metallic glass.
- □ Or we could have a ferromagnetic material (*from spontaneous spin alignment point of view- a physical property*), which is amorphous (e.g.) (*structural viewpoint*)
 → amorphous Co-Au alloys are ferromagnetic.

A Common Description

- Let us consider the common types of *Engineering Materials*.
- □ These are Metals, Ceramics, Polymers and various types of composites of these.
- A composite is a combination of two or more materials which gives a certain benefit to at least one property → A comprehensive classification is given in the next slide. The term Hybrid is a superset of composites.
- □ The type of atomic entities (ion, molecule etc.) differ from one class to another, which in turn gives each class a *broad 'flavour'* of properties.
 - Like metals are usually ductile and ceramics are usually hard & brittle
 - Polymers have a poor tolerance to heat, while ceramics can withstand high temperatures
 - Metals are opaque (in bulk), while silicate glasses are transparent/translucent
 - Metals are usually good conductors of heat and electricity, while ceramics are poor in this aspect.
 - If you heat semi-conductors their electrical conductivity will increase, while for metals it will decrease
 - Ceramics are more resistant to harsh environments as compared to Metals
- Biomaterials are a special class of materials which are compatible with the body of an organism ('biocompatible'). Certain metals, ceramics, polymers etc. can be used as biomaterials.



Diamond is poor electrical conductor but a good thermal conductor!! (phonons are responsible for this)

Bonding and structure are key factors in determining the properties of materials



Classification of composites.

- Based on the matrix: metal matrix, ceramic matrix, polymer matrix.
 - Based on the morphology of the reinforcement: particle reinforced (0D), fiber reinforced (1D), laminated (2D).



- In functionally graded materials (FGM) the property varies from one side of the material (structure) to the other.
- E.g the outer surface may be made hard and abrasion resistant, while the interior could be made tough.
- The gradation in function could be obtained by composition changes, microstructure differences (via heat treatment), etc.

Gradation of function

*Note: this use of the word 'lattice' should not be confused with the use of the word in connection with crystallography. Also known by other names: foams, cellular materials)



Common materials: *examples*

- Metals and alloys
 - Cu, Ni, Fe, NiAl (intermetallic compound), Brass (Cu-Zn alloys).
- Ceramics & glasses (usually oxides, nitrides, carbides, borides)
 - > Oxides (Alumina (Al₂O₃), Zirconia (Zr₂O₃)), Nitrides (Si₃N₄), Borides (MgB₂), Carbides (SiC)).
- Polymers (thermoplasts, thermosets) (Elastomers)
 - Polythene, Polyvinyl chloride, Polypropylene.

Based on Electrical Conduction

- □ Conductors ≻ Cu, Al, NiAl
- □ Semiconductors ≻ Ge, Si, GaAs
- □ Insulators > Alumina, Polythene* (also called 'dielectrics').

Based on Ductility (at room temperature $\sim 25 \,^{\circ}C$)

- \Box Ductile > Metals, Alloys.
- □ Brittle ≻ Ceramics, Inorganic Glasses, Ge, Si.

* Some special polymers could be conducting.

- □ The broad scientific and technological segments of Materials Science are shown in the diagram below.
- □ To gain a comprehensive understanding of materials science, all these aspects have to be studied.



The Materials Tetrahedron

- A materials scientist has to consider four 'intertwined' concepts, which are schematically shown as the 'Materials Tetrahedron'.
- When a certain performance is expected from a component (and hence the material constituting the

same), the 'expectation' is put forth as a set of properties.

- The material is synthesized and further made into a component by a set of processing methods (casting, forming, welding, powder metallurgy etc.).
- The structure (at various <u>lengthscales</u>*) is determined by this processing.
- The structure in turn determines the properties, which will dictate the performance of the component.
- Hence each of these aspects is dependent on the others.

The broad goal of Materials Science & Engineering is to understand and 'engineer' this tetrahedron

* this aspect will be considered in detail later



□ What determines the properties of materials?

Cannot just be the composition!

Few 10s of ppm of Oxygen in Cu can degrade its conductivity (that is why we have Oxygen free high conductivity copper (OFHC)).

- Cannot just be the amount of phases present!
 - → A small amount of cementite along grain boundaries can cause the material to have poor impact toughness.
- Cannot just be the distribution of phases!
 - → Dislocations can severely weaken a crystal.
- Cannot just be the defect structure in the phases present!
 - \rightarrow The presence of surface compressive stress toughens glass.
- The following factors put together determines the properties of a material:
 - Composition
 - Phases present and their distribution
 - Defect Structure (in the phases and between the phases)
 - > Residual stress (can have multiple origins and one may have to travel across lengthscales).
- □ These factors do NOT act independent of one another (*there is an interdependency*).



Hence, one has to traverse across lengthscales and look at various aspects to understand the properties of materials.



□ Properties of a material are determined by two important characteristics*:

Atomic structure

(The way atoms, ions, molecules arranged in the material).

Electromagnetic structure – the bonding character

(The way the electrons**/charge are distributed and spin associated with electrons).

(Bonding in some sense is the simplified description of valence electron density distributions).

Essentially, the electromagnetic structure and processing determine the atomic structure.



Note: the nuclear structure (at its interactions) is usually ignored in such considerations. "The nucleus gives atom its mass, the electrons its personality"!

* Both these aspects are essentially governed by (properties of) electrons and how they talk to each other! ** Including sharing of electrons.

- In the next three slides we will traverse across lengthscales to demarcate the usual *domain of Materials Science*.
- Many of the terms and concepts in the slide will be dealt with in later chapters.
- As we shall see the scale of Microstructures is very important and in some sense Materials Scientists are also 'Microstructure Engineers'! (Material scientists are microstructure engineers who 'worry' about mechanisms).
- There could be issues involved at the scale of the component (i.e. design of the component or its meshing with the remainder of the system), which are traditionally not included in the domain of Materials Science. E.g. sharp corners in a component would lead to stress concentration during loading, which could lead to crack
 - initiation and propagation, leading to failure of the component.
 - The inherent resistance of the material to cracks (and stress concentrations) would typically be of concern to materials scientists and not the design of the component.





Processing determines shape and microstructure of a component

Please spend time over this figure and its implications (notes in the next slide)

Structure could imply two types of structure:

- Crystal structure
- Electromagnetic structure

• Fundamentally these aspects are two sides of the same coin

Microstructure can be defined as:

(Phases^{*} + Defect Structure + Residual Stress) and their distributions (more about these in later chapters)

☐ Microstructure can be 'tailored' by thermo-mechanical treatments

A typical component/device could be a *hybrid* with many materials and having *multiple microstructures*

E.g. a pen cap can have plastic and metallic parts



- □ There are microstructure 'sensitive' properties (often called structure sensitive properties) and microstructure insensitive properties (*note the word is sensitive and not dependent*).
- $\square \succ \text{Microstructure 'sensitive' properties} \rightarrow \text{Yield stress, hardness, Magnetic coercivity...}$
 - > Microstructure insensitive properties \rightarrow Density, Elastic modulus...
- Hence, one has to keep in focus:



From an alternate perspective: Electronic interactions are responsible for most the material properties. From an understanding perspective this can be broken down into Bonding and Structure.

Effect of Bonding on properties: a broad flavour

- □ Two important contributing factors to the properties of materials is the nature of bonding and the atomic structure.
- □ Both of these are a result of electron interactions and resulting distribution in the material.

□ Note: the energies listed in the table below are approximate.

Bond	Bond Energy eV	Melting point	Hardness (Ductility)	Electrical Conductivity	Examples
Covalent	~1-10	High	Hard (poor)	Usually Low	Diamond, Graphite, Ge, Si
Ionic	~5-15	High	Hard (poor)	Low	NaCl, ZnS, CsCl
Metallic	~0.5-8	Varies	Varies	High	Fe, Cu, Ag
Van der Waals	~0.05-0.5	Low	Soft (poor)	Low	Ne, Ar, Kr
Hydrogen	~0.05-1.5	Low	Soft (poor)	Usually Low	Ice



What is the difference between 'structure level' and 'material level' properties?

- We come across terms like *stiffness* and *Young's modulus*. Or *Malleability* and *Ductility*.
- ❑ We have to consider three *components* to a general problem: Materials, Structures and Mechanisms. Structures have a specified geometry and are made of materials. Mechanisms are structures, which are designed to perform certain tasks (like change the direction of motion or derive a mechanical advantage). A building or a truss is a structure, while wood is a material (a composite). A lock is an example of a mechanism.
- Entities between these end-points of the triangle (the edges) can be envisaged; like Material-Structures and Compliant Mechanisms. Compliant mechanisms are structures which perform the role of a mechanism. A 'self unfolding' antenna, made of a shape memory alloy can be considered as a material-structure.
- ❑ A device or a 'machine' is usually made up of structures and mechanisms. In addition, the device may have functional parts like a magnetic material (for data storage). These functional parts/materials may be associated with motion (like in a piezo-actuator) or may not involve external motion (like the soft magnet core of a transformer).



- Elasticity is a property associated with a material, while stiffness is associated with a structure. Young's modulus and Poisson's ratio are two material properties which characterize the elastic behaviour of an isotropic material. E.g. Young's modulus is associated with a sample of steel, while the reversible deformation behaviour of a spring is characterized by stiffness. Young's modulus is a measure of the resistance of the material to deformation (in the reversible regime) and stiffness is the resistance of the *structure*. By making the geometry in the form of a helix in a spring, we obtain higher elongations for the same load (more 'springy') (and the deformation mode switches from tension to torsion). There is no counterpart of Poisson's ratio for a structure.
- □ In an actual test to determine some of the properties of a material, a standard test geometry may be specified. E.g. a uniaxial tension test may be performed on a specimen with a dogbone geometry to determine the Young's modulus (albeit the fact that the values determined by this method are often not very accurate).
- Often the geometry of the material is included (implicitly) in the definition of a property. E.g. in the determination of fracture toughness a geometry with a notch may be used and plane strain conditions (i.e. a thick enough sample) are assumed.
- Malleability is the ability to form a material into a particular shape. Ductility can be thought of a an inherent material property. Ductility is a measure of the ability of a material to undergo plastic deformation, which is usually characterized by percentage elongation or percentage reduction in area in a uniaxial tension test).





- The four pillars of Materials Science and Engineering are (a simplified view!!!):
 - (i) Physical structure \rightarrow Atomic structure (+ Microstructure)
 - (ii) Electromagnetic Structure→ Electronic and Magnetic structure
 - (iii) Thermodynamics
 - (iv) Kinetics
- If one gains understanding of these four pillars, one can comprehend most aspects of Material behaviour and engineer materials for applications.
- The subject of Materials Engineering can be envisaged as a confluence of Physics, Chemistry, Biology, Mechanical Engineering, etc.



Material usage strategies

- □ There are basically three strategies* available for the use of materials for specific purposes.
 - Design a material with better properties

(e.g. materials with better creep resistance at high temperatures).

 \succ Protect the material with surface coatings, cooling etc.

(e.g. paint the material to avoid corrosion).

➤ Use 'sacrificial materials' to protect the key component

(e.g. use of sacrificial anodes to prevent corrosion).

The obvious has not been stated above– i.e. use more "quantity" of material.

Also, we could do a better design of the component/mechanism/machine/... itself (so that the "load" on the material is not as much).

Modern material (/component) design: smart materials*

- Examples of smart materials, structures and 'components' (/organs) are abound in the biological world. Many of the 'stuff' found in the biological world have amazing design strategies, some of which we are just able to copy (biomimetic materials) and further use the 'inspiration' to design newer materials (biognostic materials). Some of the important qualities, which a smart material can have are listed below.
- Self reporting: lets us know of changes occurring in the material—e.g. damage accumulation can lead to magnetization.
- Responsive: responds to the environment and alters its properties (e.g. photochromatic lenses which darken on exposure to sun light).
- Responsive and self healing: responds to the environment or changes within the material and can heal any deleterious changes (e.g. if cracks grow material is released to heal the cracks).
- Self cleaning: this is like the 'gecko effect', where the surface cleans itself.
- Self lubricating: an old concept, wherein the material puts up a surface layer which acts like a lubricant (e.g. Al-graphite composites, wherein the graphite acts like a lubricant).
- Multi-functional: the material performs multiple roles in a single structure or component. E.g.: (i) the cover of a mobile can be its power cell too, (ii) an antenna made of shape memory alloy can be transported in collapsed form and extends itself on heating on-site (envisaged for space applications), (iii) ferroelectric and ferromagnetic.

Summary

- □ The goal of Materials Science and Engineering is to design materials with a certain set of properties, which gives a certain desired performance. Using suitable processing techniques the material can be synthesized and processed. The processing also determines the microstructure of the material.
- □ The material is expected to be used in a structure (e.g. bridge, truss, bolt) or a component (e.g. gear wheel, battery, computer chip, filament of a light bulb).
- □ To understand the microstructure the material scientist has to traverse across lengthscales and has to comprehend the defect structure in the material along with the phases and their distribution. The residual stress state in the material is also very important.
- Common types of materials available to an engineer are: Metals, Ceramics and Polymers. A hybrid made out of these materials may serve certain engineering goals better.
- Materials are also classified based on Band Structure (Metals, Semi-metals, Semiconductors, Insulators) or Atomic Structure (Crystals, Quasicrystals, Amorphous phases).

Some excursions into a broader picture

Basic Overview Fundas

- □ The coming slides puts together some '*Overview Fundas*'.
- □ These technically do not fit into any chapter or topic− hence they have been included in this chapter.
- Some of the concepts involved may be advanced for a beginner– however he/she may have a cursory look at these and recollect them when the appropriate topics have been understood.

Linear versus Angular

- □ For every linear (visualized as a straight arrow) entity there is usually an angular counterpart (visualized as a arc of a circle with an arrow).
- □ *Note: 'Proper perspective' is required to make the connection.*
- □ For *law of conservation of linear momentum*, there is the angular counterpart
 → the *law of conservation of angular momentum*.
- For the *edge dislocation*, there is the *screw dislocation*.
- □ For electric field, there is the magnetic field arising from 'spinning' (or revolving) charges. [Electron is associated charge and magnetic moment].
- Given For linear frequency (v), there is angular frequency ($\omega = 2\pi v$).

- □ We often want to convert linear 'stuff' to angular or vice-versa. Some examples are:
 - A solenoid 'converts' 'circular magnetic fields' to linear fields.
 - A spring converts linear loading into torsional loading of the material.
 - ➢ In Bragg's diffraction experiment (say XRD) linear information (d-spacing between atomic planes) is converted to angular information (the diffraction angle).
 - > The crank of a 'steam locomotive' converts linear motion of a piston to circular motion (of the wheel).

Ode to the electron

- Fundamental particles have important properties associated with them (not all have all the properties as below):
 - Size, Mass, Charge, Spin, Angular Momentum (arising from spin), Magnetic Moment (arising from spin of charged particles), etc.
- □ The electron in spite of being a familiar 'entity', is perhaps one of the most mysterious 'objects' around.
- □ It has no known size to less than about 10^{-15} m → it is as close as we can get to a geometrical point.
- □ Yet it has Mass, Charge and Spin (and hence angular and magnetic moments).
- □ It can behave a like a particle or a wave (hence used in electron microscopy).

Global versus local

- Often for an event to take place the necessary and sufficient conditions must be satisfied.
- ➡ For many processes taking place in materials science, one has to 'worry' about a picture involving a global criterion and a local criterion*. In many circumstances the global criterion is the necessary condition and local is a sufficient one.
- Let us take an example of a crack in a body loaded in tension (Fig. below). For the crack to grow, there must be sufficient elastic energy stored in the body (global, necessary condition), but this is not enough. The stresses at the crack tip (which depends on the crack tip radius or 'sharpness') must be sufficient to break the bonds at the crack tip (local, sufficient condition) and lead to the propagation of the crack.
- In many situations the global criterion is energy based, while the local is stress based.
- Other examples include: grain growth, formation of interfacial misfit dislocation during the growth of precipitate or epitaxial film, nucleation of second phase, etc.



* For now we assume that just one criterion needs to be satisfied.



What is the difference between homogeneous and isotropic?

0 & A

- In a homogeneous material the properties do not change from one position to another. A piece of Cu or an solid solution of Ni in Cu are examples of homogeneous materials, wherein the composition and structure is the same at each point in the material.
- On the other hand in heterogeneous material, the material composition or structure varies from one place to another, which further implies a change in the properties (from one place to another).
- □ From a practical standpoint, we usually consider a 'lengthscale' at which the homogeneity is considered. E.g. there might be some compositional variations (and hence local property variations) at the level of a few nanometers, but at the lengthscale of micrometers (microns) these heterogeneities even out and material can be considered homogeneous.
- □ In an isotropic material a given property is NOT direction dependent, while in an anisotropic a given property is direction dependent. A material could be isotropic w.r.t. to one property, while could be anisotropic with respect to another. E.g. A single crystal of Cu is isotropic w.r.t. electrical conductivity– a second order tensor property; while is anisotropic w.r.t. elastic modulus– a forth order tensor property. *Click here to know more*. (Also see next slide).

How can isotropy arise in a material? (or) How can a material be isotropic?

- A material can be isotropic (with respect to a property) in three ways.
- **These can arise from:**

0 & A

- ➢ (i) structure at the atomic level,
- ➤ (ii) structure at the microstructural level or
- (iii) tonsorial nature of the property in conjunction with the symmetry of structure (& Neumann's principle). These are explained below.
- (i) The material is disordered (amorphous/glass) and hence all directions are equivalent in the material (on an average). Such a material is truely isotropic.
- (ii) The may be crystalline, but the crystallites may be oriented randomly (like in a polycrystal) and hence at the lengthscale of the material (which is assumed to be much larger than the crystallite/grain size) the material *appears* to be isotropic.
- (iii) Even single crystals an be isotropic w.r.t. a given property. This depends on the tensorial nature of the property (i.e. is it a second order tensor or a higher order tensor), in conjunction with the symmetry of the crystal (& the Neumann's principle). This point is difficult to explain here and readers may click on the link at the bottom of the page.



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