ACKNOWLEDGMENTS

- Prof. Rajesh Prasad (Applied Mechanics, IITD) has been the source of knowledge for many a ‘fundas’ in this book and I have been fortunate to have learnt a lot of teaching skills from him.

REFERENCES

Few major references are included here. Other references may be found in individual chapters.


ONLINE

http://www.tf.uni-kiel.de/matwis/amat/def_en/overview_main.html

Caution Note: In any chapter, amongst the first few pages (say 5 pages) there will be some ‘big picture’ overview information. This may lead to ‘overloading’ and readers who find this ‘uncomfortable’ may skip particular slides in the first reading and come back to them later.
The contents of the current book will deviate markedly from the treatment of ‘usual’ textbooks.

- **Fresh perspective** will be presented on all topics. (Students are requested to consult other references keeping this in mind—i.e. there might be considerable differences in some places)

- Effort will be made to present *as much visual information as possible* → students should spend time over the figures/videos/etc. for effective learning.

- Lengthy paragraphs have been replaced with bulleted points.

- Most of the detailed material (for inquisitive / advanced students) appear as hyperlinks to the main chapters. However, if some advanced material *does* appear in the main chapter it is marked with a **Red Box** in one of the corners of the slide (e.g. as below) (students may choose to skip these in the first reading).

- Important slides are marked with a **Green Box** in one of the corners of the slide (e.g. as below).

- The entire book is intended for learning and understanding of the subject matter (and not merely for ‘exams’ or ‘syllabus coverage’ points of view).
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?

(We will list the important points which will put the issues involved in perspective)

The full implication of the aspects presented in this introductory chapter will only become clear after the student has covered major portions of this course. Hence, students are encouraged to return to this chapter many times during his/her progress through the course.
We shall start with a broad overview of .. well...almost everything! (the next slide)

The typical domain of materials science is enclosed in the ellipse. (next slide)

Traditionally materials were developed keeping in view a certain set of properties and were used for making components and structures.

With the advancement of materials science, materials are expected to perform the role of an ‘intelligent’ structure or a mechanism.

A good example of this would be applications of shape memory alloys:

- they can be used to make deployable antennas (STRUCTURE) or
- actuators (MECHANISM).

Though it will not be practical to explain all aspects of the diagram (presented in the next slide) in this elementary course, the overall perspective should be kept at the back of one’s mind while comprehending the subject.

A point to be noted is that one way of classification does not clash with another. E.g. from a state perspective we could have a liquid which is a metal from the band structure perspective. Or we could have a metal (band structure viewpoint) which is amorphous (structural viewpoint).
Strange?
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!
Based on **state** (phase) a given material can be **Gas**, **Liquid** or **Solid** (based on the thermodynamic variables: $P, T,...$).

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: **Slide 7**).

* Though these other terms are misnomers.
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 perspective
  \( \text{Hg is liquid metal at room temperature.} \)

- Or we could have a metal (band structure viewpoint), which is amorphous (structural viewpoint)
  \( \text{ZrTiCuNiBe bulk metallic glass.} \)

- Or we could have a ferromagnetic material (from spontaneous spin alignment point of view- a physical property), which is amorphous (e.g.) (structural viewpoint)
  \( \text{amorphous Co-Au alloys are ferromagnetic.} \)
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 a 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
Monolithic Materials

- Metals (& Alloys)
- Ceramics & Glasses
- Polymers (& Elastomers)

Hybrids

- Composite
- Sandwich
- Lattice
- Segment

Composites: have two (or more) solid components; usually one is a matrix and other is a reinforcement.

Sandwich structures: have a material on the surface (one or more sides) of a core material.

Lattice* Structures: typically a combination of material and space (e.g. metallic or ceramic forms, aerogels etc.).

Segmented Structures: are divided in 1D, 2D or 3D (may consist of one or more materials).

Hybrids are designed to improve certain properties of monolithic materials.

*Note: this use of the word 'lattice' should not be confused with the use of the word in connection with crystallography.
Common materials: *with various ‘viewpoints’*

- Glass: amorphous
- Ceramics
- Crystal
- Graphite
- Metals
- Polymers
Common materials: *examples*

- **Metals and alloys**: Cu, Ni, Fe, NiAl (intermetallic compound), Brass (Cu-Zn alloys)
- **Ceramics & glasses**: (usually oxides, nitrides, carbides) Alumina ($\text{Al}_2\text{O}_3$), Zirconia ($\text{Zr}_2\text{O}_3$)
- **Polymers** (thermoplasts, thermosets) (Elastomers): Polythene, Polyvinyl chloride, Polypropylene

**Based on Electrical Conduction**

- **Conductors**: Cu, Al, NiAl
- **Semiconductors**: Ge, Si, GaAs
- **Insulators**: Alumina, Polythene*

**Based on Ductility**

- **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.
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 length scales*) 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!
  - 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.

* 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
Materials Science

Atom Structure Crystal

Crystal Structure Microstructure

Electro-magnetic

Thermo-mechanical Treatments

Phases + Defects + Residual Stress

& their distributions

Component

- Casting
- Metal Forming
- Welding
- Powder Processing
- Machining

- Vacancies
- Dislocations
- Twins
- Stacking Faults
- Grain Boundaries
- Voids
- Cracks

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

* Including aspects like morphology of phases
What determines the properties of materials?

- There are microstructure ‘sensitive’ properties (often called structure sensitive properties) and microstructure insensitive properties (note the word is sensitive and not dependent).
- Microstructure ‘sensitive’ properties → Yield stress, hardness, Magnetic coercivity…
- Microstructure insensitive properties → Density, Elastic modulus…
- Hence, one has to keep in focus:
  - Atomic structure
  - Electromagnetic structure/Bonding
  - Microstructure to understand the properties.

- 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.
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.

### Effect of Bonding on properties: a broad flavour

<table>
<thead>
<tr>
<th>Bond</th>
<th>Bond Energy eV</th>
<th>Melting point</th>
<th>Hardness (Ductility)</th>
<th>Electrical Conductivity</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Covalent</td>
<td>5 (8×10⁻¹⁹ J)</td>
<td>High</td>
<td>Hard (poor)</td>
<td>Usually Low</td>
<td>Diamond, Graphite, Ge, Si</td>
</tr>
<tr>
<td>Ionic</td>
<td>1-3</td>
<td>High</td>
<td>Hard (poor)</td>
<td>Low</td>
<td>NaCl, ZnS, CsCl</td>
</tr>
<tr>
<td>Metallic</td>
<td>0.5</td>
<td>Varies</td>
<td>Varies</td>
<td>High</td>
<td>Fe, Cu, Ag</td>
</tr>
<tr>
<td>Van der Waals</td>
<td>0.001-0.1</td>
<td>Low</td>
<td>Soft (poor)</td>
<td>Low</td>
<td>Ne, Ar, Kr</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>Low</td>
<td>Soft (poor)</td>
<td>Usually Low</td>
<td></td>
<td>Ice</td>
</tr>
</tbody>
</table>

* For comparison thermal energy at RT (300K) is 0.03 eV
The four pillars of Materials Science and Engineering are:
(i) Physical structure → 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.
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).
- 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).

* Note: in a given situation, only one/some of these strategies may work.
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.

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).

The chapter technically ends here— but the inquisitive reader may continue to read the slides which follow.
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].
- For linear frequency (ν), there is angular frequency (ω = 2πν).

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).
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 like a particle or a wave (hence used in electron microscopy).
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 ‘residual stress’ and how can it arise in a material (/component)?

- The stress present in a material/component in the absence of external loading/forces or constraints (i.e. in a free-standing body) is called residual stress.
- Residual stress can ‘be’ in the macro-scale or micro-scale and can be deleterious or beneficial depending on the context (diagram below).
- Residual stress may have multiple origins as in the diagrams below.

**Based on scale**

- **Macro-scale**
  - Residual stress can be beneficial (+) or detrimental (–)
  - E.g.
    - – Stress corrosion cracking
    - + Residual Surface Stress in toughened glass

- **Micro-scale**
  - Due to a dislocation (a crystallographic defect)

**Origins/Related to**

- **Physical properties**
  - Thermal
  - Magnetic
  - Ferroelectric

- **Geometrical entities**

**Due to**

- **Defects**
  - Vacancies, Dislocations, Voids, Cracks

- **Phase Transformation & reactions**
  - Mismatch in coefficient of thermal expansion

- **Thermal origin**

**Residual Stress**

- Residual stresses due to an coherent precipitate
Thank You