MATERIALS SCIENCE AND ENGINEERING

An Introduction

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.

A Broad Overview

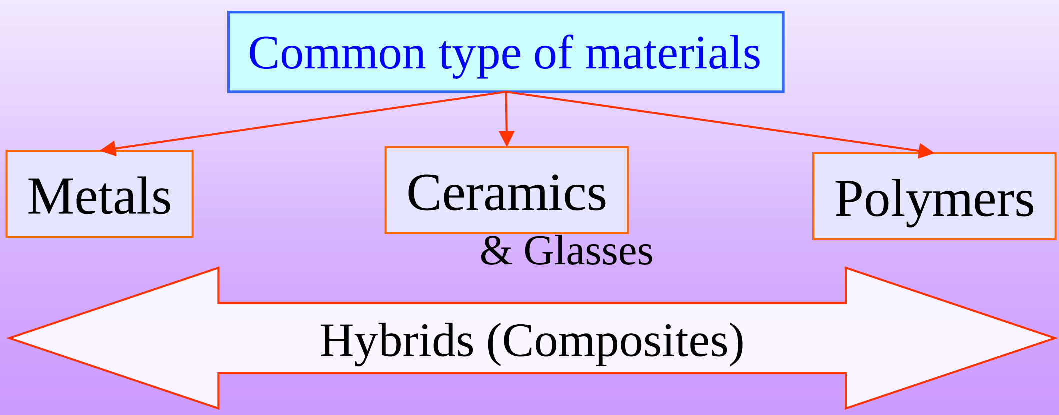
Skip the next slide if it makes you nervous!

- 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)*.

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.

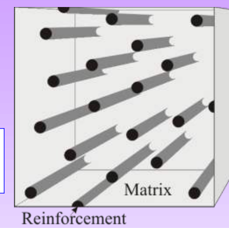
Bonding and structure are key factors in determining the properties of materials



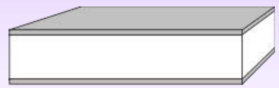
Diamond is poor electrical conductor but a good thermal conductor!! (phonons are responsible for this)

Materials

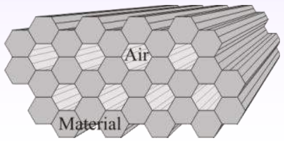
- **Monolithic**
  - Metals (& Metallic Alloys)
  - Ceramics and ceramic alloys & Glasses
  - Polymers (& Elastomers)
- **Hybrids**
  - Composite
  - Sandwich
  - Lattice
  - Segment



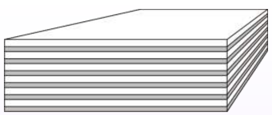
Composites: have two (or more) solid components; usually one is a matrix and other is a reinforcement

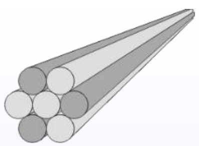


Sandwich structures: have a material on the surface (one or more sides) of a core material



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

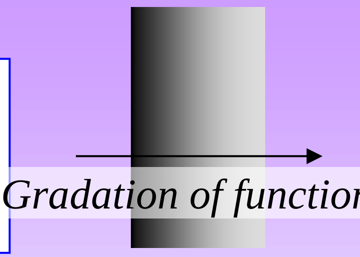
Classification of composites.

- 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).

Q & A

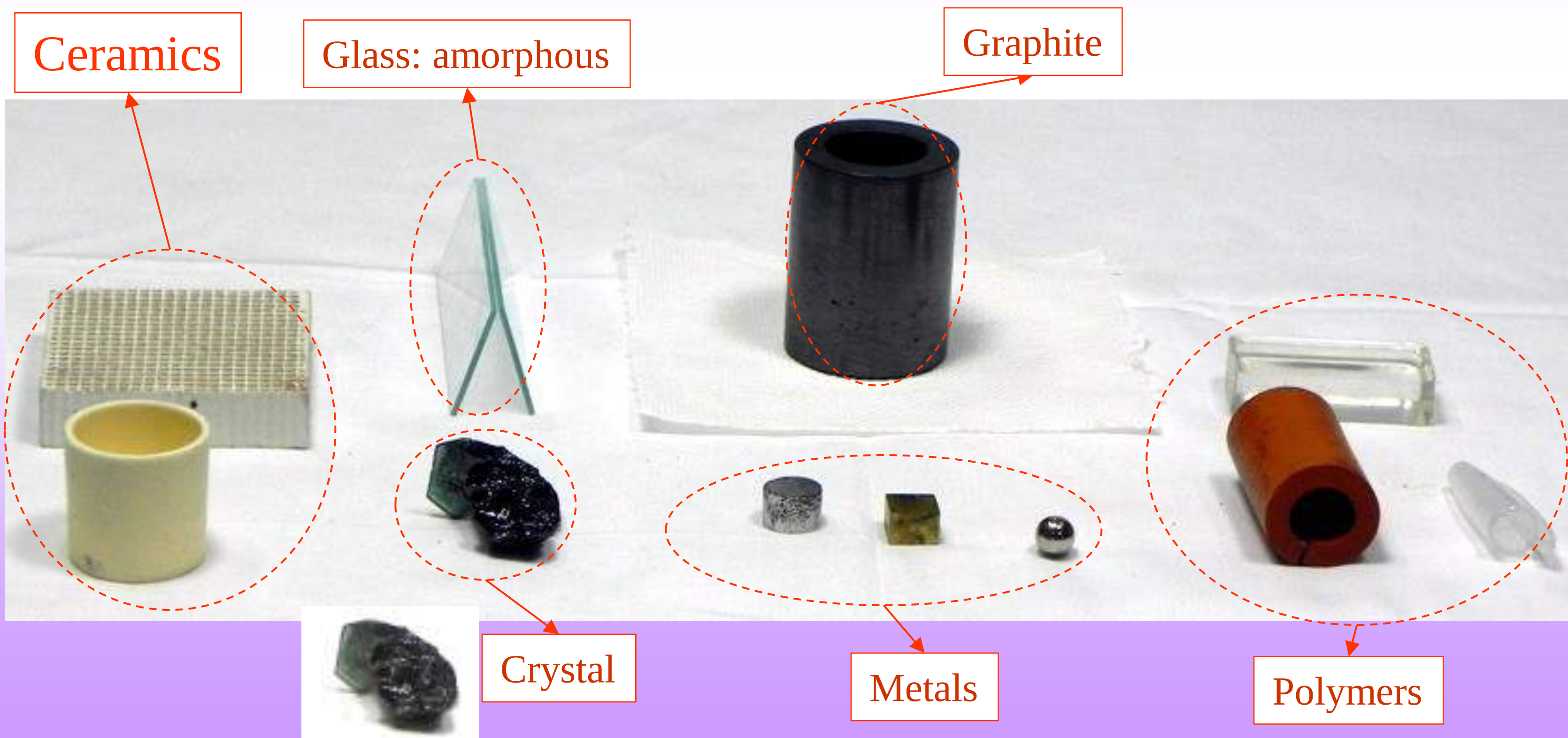
What are functionally graded materials?

- 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.



*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: *with various 'viewpoints'*



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 (Al_2O_3), Zirconia (Zr_2O_3)), Nitrides (Si_3N_4), Borides (MgB_2), Carbides (SiC)).
- Polymers (thermoplasts, thermosets) (Elastomers)
  - Polythene, Polyvinyl chloride, Polypropylene.

Based on Electrical Conduction

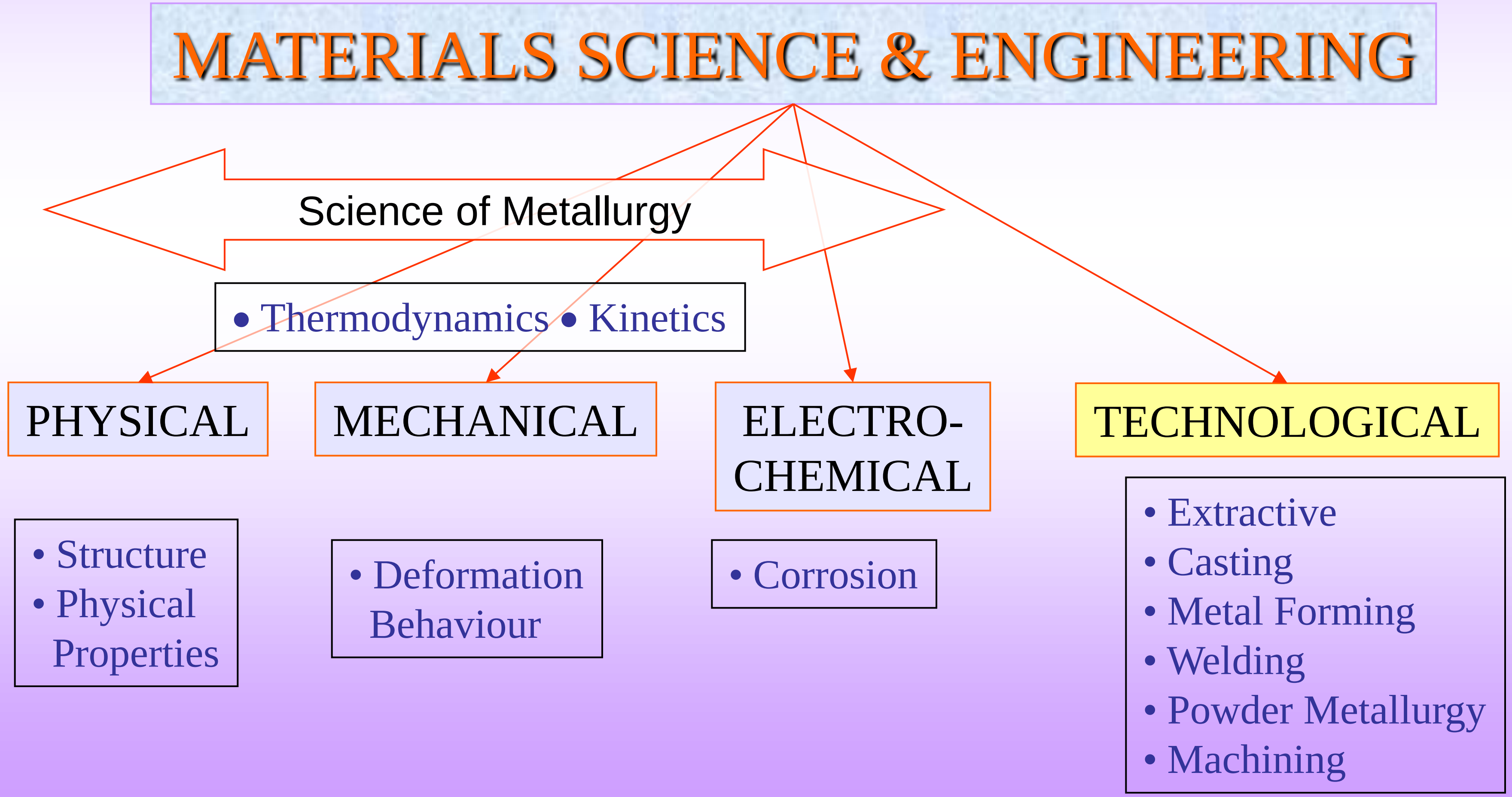
- Conductors ➢ Cu, Al, NiAl
- Semiconductors ➢ Ge, Si, GaAs
- Insulators ➢ Alumina, Polythene* *(also called 'dielectrics').*

Based on Ductility *(at room temperature ~25 ℃)*

- Ductile ➢ Metals, Alloys.
- Brittle ➢ Ceramics, Inorganic Glasses, Ge, Si.

** Some special polymers could be conducting.*

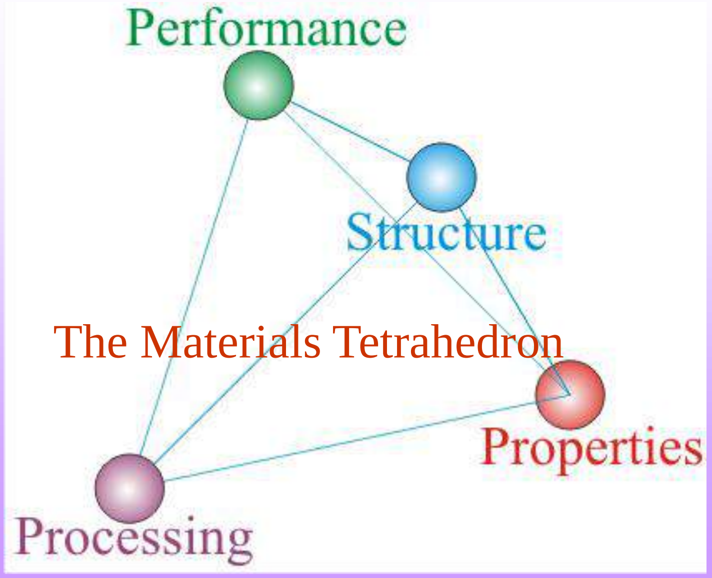
- The broad scientific and technological segments of Materials Science are shown in the diagram below.
- To gain a comprehensive understanding of materials science, all these aspects have to be studied.



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 lengthscales*) 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.

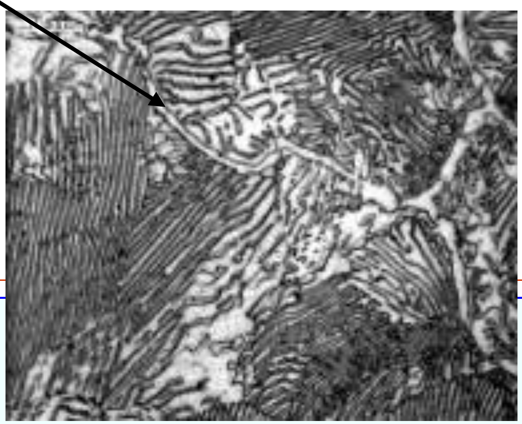
The broad goal of Materials Science & Engineering is to understand and 'engineer' this tetrahedron



* 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.

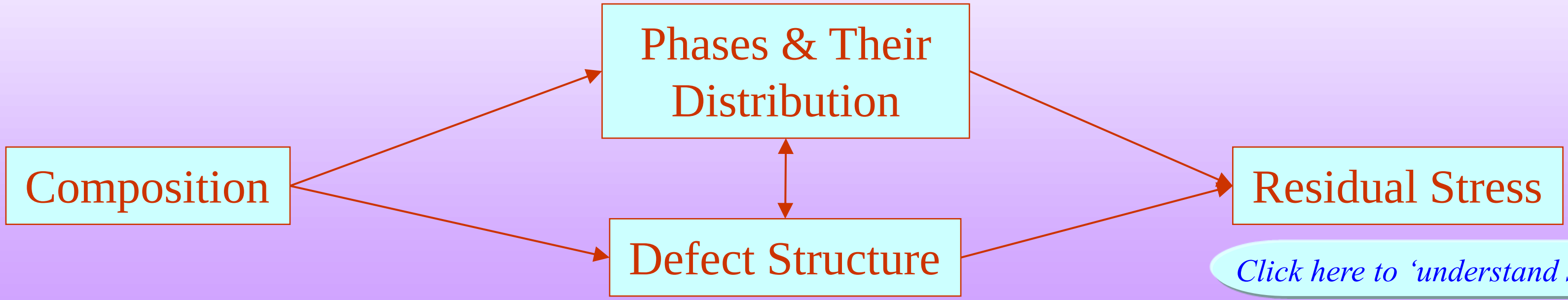


- Cannot just be the distribution of phases!
  - ➔ Dislocations can severely weaken a crystal.
- Cannot just be the defect structure in the phases present!
  - ➔ The presence of surface compressive stress toughens glass.

❑ 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).*



Click here to 'understand stress'

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.*

Properties influenced by → Atomic structure

Properties influenced by → Electromagnetic structure (Bonding characteristics)

- This implies that a change in the crystal structure due to a phase transformation (e.g. Fe BCC goes to Fe FCC), is also accompanied by a change in the bonding character and concomitantly a change in the properties.

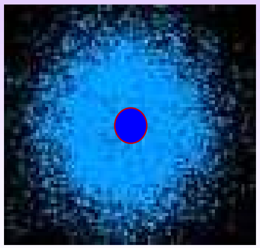
Note: the nuclear structure (at its interactions) is usually ignored in such considerations.

"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.



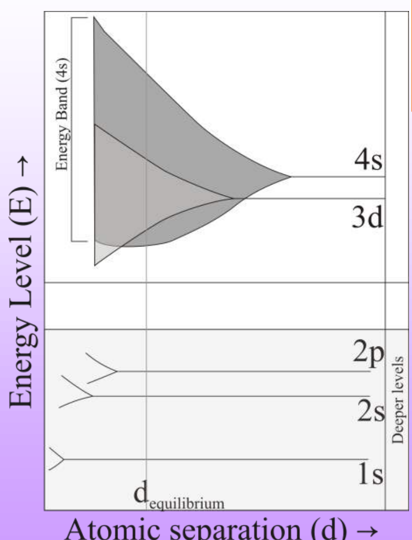
Crystal

Atom → Structure → Microstructure → Component

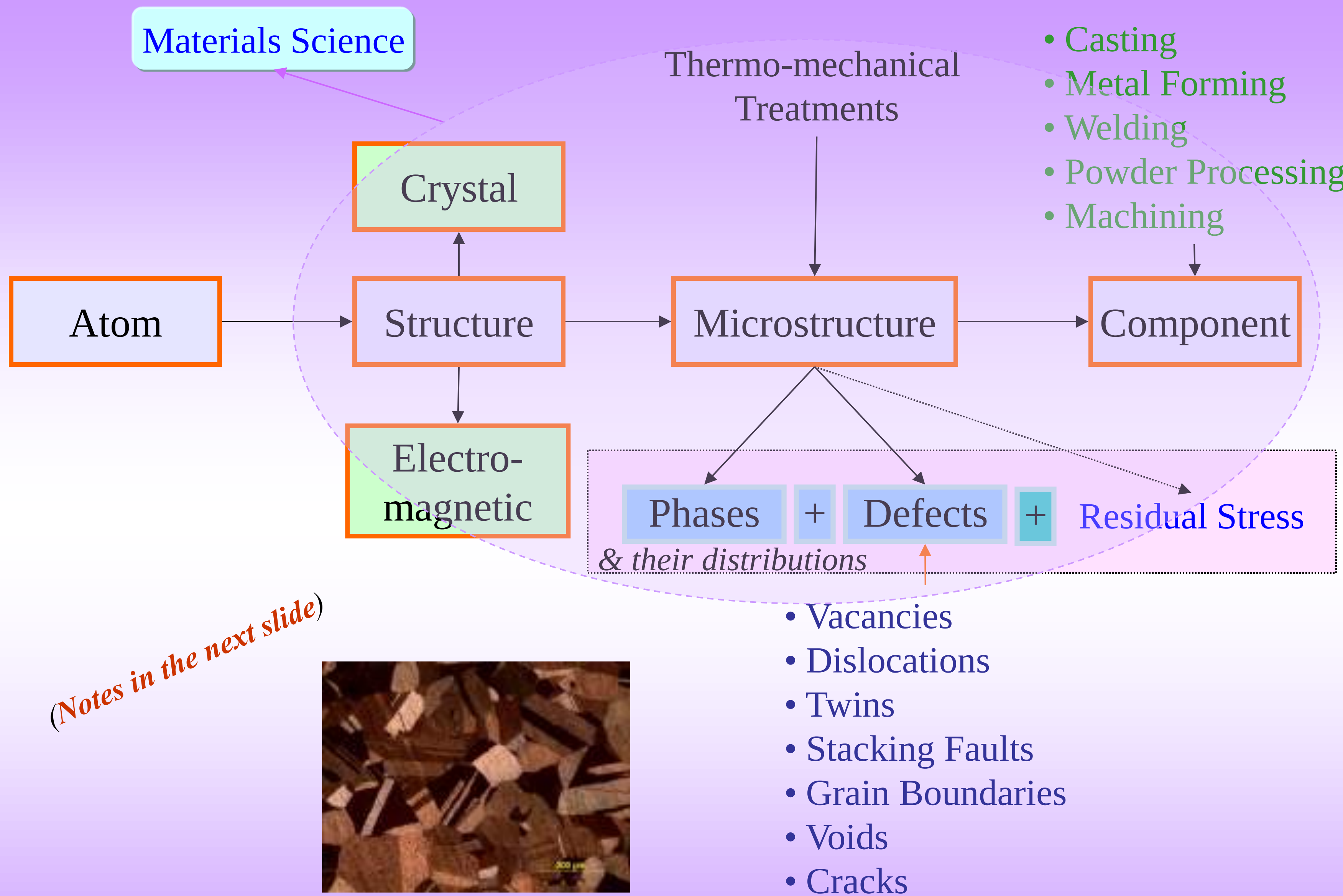
Electro-magnetic

Thermo-mechanical Treatments

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



Processing determines shape and microstructure of a 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

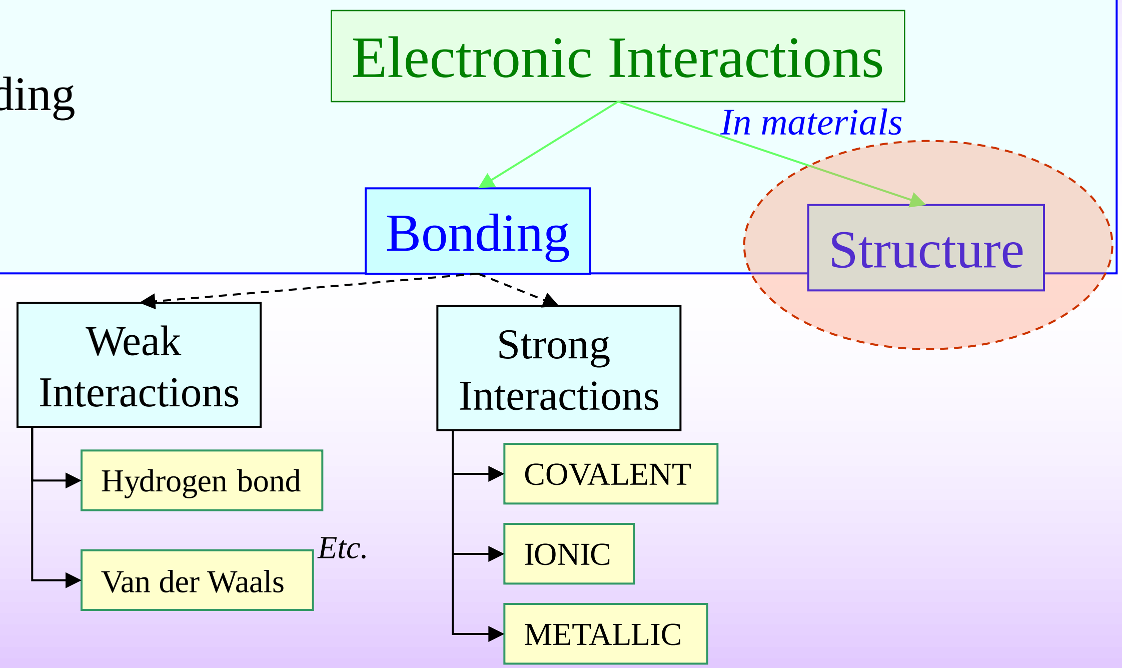
Click here to know more about microstructures

* *Including aspects like morphology of phases*

Funda Check

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.

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

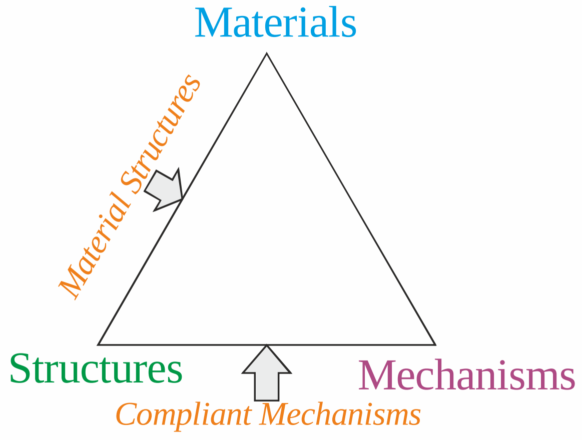
* *For comparison thermal energy at RT (300K) is 0.03 eV*

(Note: 1eV = 1.602×10^{-19})

Q & A

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).



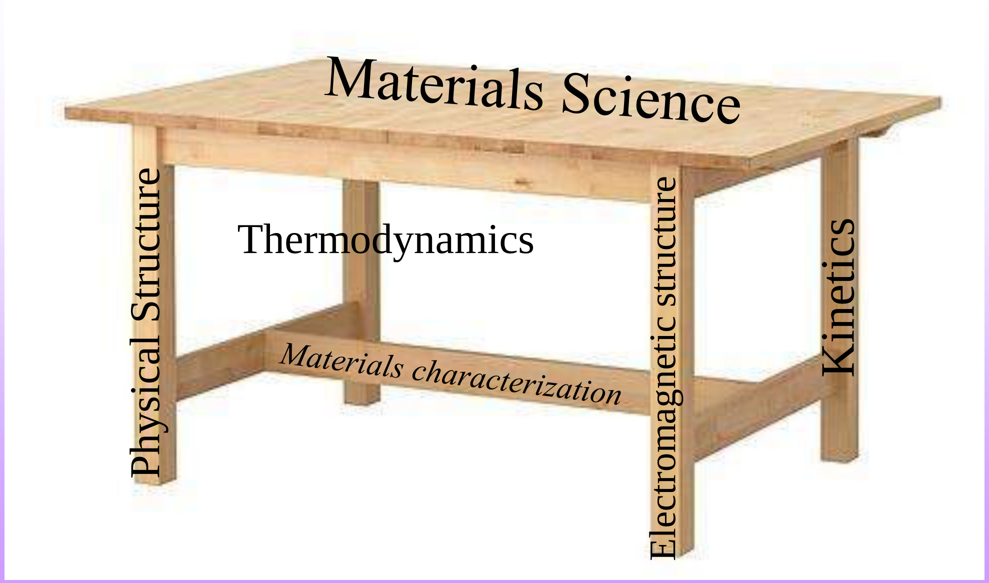
Continued…

- 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 dog-bone 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).

Funda Check

What are the four founding pillars of materials science?

- The four pillars of Materials Science and Engineering are *(a simplified view!!!)*:
  (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.
- The subject of Materials Engineering can be envisaged as a confluence of Physics, Chemistry, Biology, Mechanical Engineering, etc.



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