

# 1 Lecture 1

## Question 1 *Material Science vs Materials Engineering ?*

**Materials Science** involves investigating relationships between structures and properties of materials. While **Materials Engineering** involves designing/engineering the structure of a material to produce a predetermined set of properties using relations of structure-body. So a material scientist develops/synthesizes new materials whereas the engineer creates products using those existing materials and/or develop techniques for processing materials.

## Question 2 *What is the structure of a material.*

**Structure** in general refers to the arrangement of material's internal components .

**Subatomic Structure** involves electrons within the individual atoms and other particles inside the nuclei.

**Atomic:** Organization of atoms or molecules relative to one another.

**Microscopic:** Groups of atoms that are normally agglomerated together

**Macroscopic:** seen using the naked eye.

## Question 3 *What is a Property of a material ?*

It's a material's trait in terms of the kind and magnitude of a response to a specific imposed stimulus.

## Question 4 *What are Mechanical Properties of a material ?*

It's the response or deformation of a material due to an applied load or force.

## Question 5 *Mechanical Properties Standards ?*

Mechanical properties are measured using standardized testing techniques coordinated by professional societies such as the ASTM American Society for Testing and Materials.

## Question 6 *Processing and Performance?*

**Processing** refers to the methodology or techniques by which a material is prepared.

**Performance** indicates how good the materials will do its function.

## Question 7 *Processing and Performance and so on relations.*

The **structure** of a material depends on how it is **processed** , and material's **performance** is a function of its **properties** . And the properties is affected by the structure.

## Question 8 *Classification of Materials*

C-MPC

- Metals
  - Dense atomic packing (Metallic bonding)
  - Non localized electrons (good conductors)
  - Metals are dense because they are made of heavy atoms, packed densely together (iron, for instance, has an atomic weight of 56).
- Ceramics
  - Compounds of metallic and non metallic elements
  - Brittle
  - Ceramics, for the most part, have lower densities than metals because they contain light nonmetals like O, N or C atoms.
- Polymers
  - Most are organic compounds based on C and H
  - Low Density, and Ductile.
  - Polymers have low densities because they are largely made of light carbon (atomic weight: 12) and hydrogen (atomic weight: 1)
- Composites

- Physical binding between materials from other classes to get intermediate properties.

#### Question 9 *What does Failure mean ?*

The end goal of studying property structure and processing relationships is that a product or component can perform its function and not fail in service.

Failure does not necessarily mean fracture. Failure to perform a function can be due to

- **Excessive Elastic deformation:** excessive deflection of closely mating parts can result in interference and damage to the parts, this type of failure is controlled by the modulus of elasticity, not by the strength of the material. Generally, little metallurgical control can be exercised over the elastic modulus. The most effective way to increase the stiffness of a member is usually by changing its shape and increasing the dimensions of its cross section.
- **Yielding and excessive plastic deformation:** occurs when the elastic limit of the metal has been exceeded. Yielding produces permanent change of shape, which may prevent the part from
- **Fracture:** The formation of a crack which can result in complete disruption of continuity of the member constitutes fracture. A part made from a ductile metal which is loaded statically rarely fractures because it will first fail by excessive plastic deformation. Fracture could be a combined effect of stress and other factors such as corrosion for example.

## 2 Lecture 2

#### Question 10 *Types of bonding ?*

- **Ionic:** Compounds that consist of Metallic + non-metallic elements. Atoms of a metallic element easily give up their valence electrons to the nonmetallic atoms. In the process all the atoms acquire stable or inert gas configurations and, in addition, an electrical charge; that is, they become ions. identical to that of argon. In sodium chloride, all the sodium and chlorine exist as ions. The attractive bonding forces are coulombic; that is, positive and negative ions attract each other.
- **Covalent:** In covalent bonding stable electron configurations are assumed by **the sharing** of electrons between adjacent atoms.
- **Metallic:** is found in metals and their alloys. With this model, these valence electrons are not bound to any particular atom in the solid and are more or less free to drift throughout the entire metal. They may be thought of as belonging to the metal as a whole, or forming a “**sea of electrons**” or an “**electron cloud**.”. The remaining nonvalence electrons and atomic nuclei form what are called ion cores, which possess a net positive charge equal in magnitude to the total valence

#### Question 11 *What are types of Crystal Structures?*

- **Single Crystalline:** Atoms are arranged in regular repetitive manner having long range order (long range periodic structure)
- **Polycrystalline:** Many individual crystals (local periodicity)
- **Amorphous:** Atomic arrangement does not have any order

#### Question 12 *How to describe a crystal structure ?*

Using a lattice and a motif;

- **lattice:** Description of the pattern of motifs/basis. (The whole pattern)
- **motif:** the basis that is being repeated. (an atom or a group of atoms)

#### Question 13 *What is a Bravais Lattice ?*

It is an infinite arrangement of points or atoms in space that has the following property: The lattice looks exactly the same when viewed from any lattice point.

#### Question 14 *How to represent a space lattice ?*

using three translational vectors and three angles between each pair of these lattice vectors (**Lattice parameters**).

#### Question 15 *How is a unit cell defined ?*

Using these vectors and angles we represent the smallest unit of the crystal structure that is when repeated along the three translational axes will produce the crystal structure.

**Question 16** *How many Bravais lattices there exist ?*

14. There are only 14 unique [patterns that are mathematically proven to fill a 3D space that possess translational symmetry.

**Question 17** *How many crystal systems there exist ?*

7 and are Cubic, Hexagonal, Tetragonal, Rhombohedral, Orthorhombic, Monoclinic and Triclinic.

**Question 18** *Define the Correspondence principle.*

Usually the external shape of a material is influenced by the internal structure (crystal system). Snow flakes is a good example of this principle.

**Question 19** *What are our unit cells of interest in this course ?*

The seven crystal systems give up 14 different unit cells, we will focus on only four of them; SC - BCC - FCC - HCP.

**Question 20** *What is the coordination number in a unit cell?*

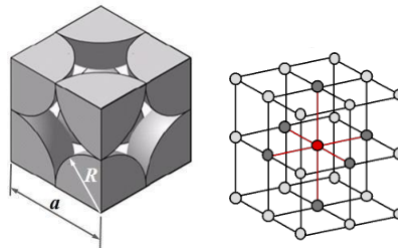
The number of each atom's nearest neighbours.

**Question 21** *What is the atomic packing factor in a unit cell APF?*

represents the total volume of the unit cell that is occupied by atoms. APF of 0.7 means the unit cell is 70% fill with atoms.

**Question 22** *Number of atoms per unit cell in Simple Cubic unit cell?*

$$N = 8\text{corners} * \frac{1}{8} = 1\text{atom}.$$



**Question 23** *Examples of Simple cubic?*

Polonium (PO)

**Question 24** *What is the relationship between  $r$  and  $a$  in Simple Cubic unit cell?*

$a = 2R$ .

**Question 25** *Coordination number in Simple Cubic unit cell?*

$$CN = 6.$$

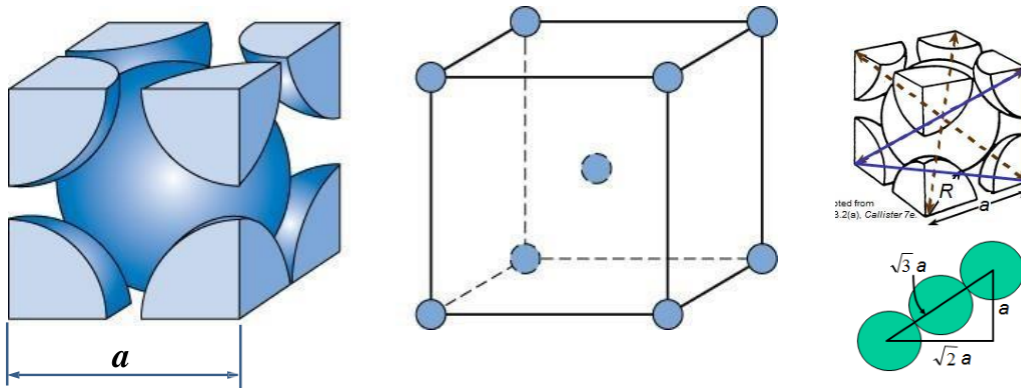
**Question 26** *The atomic packing factor in Simple Cubic unit cell?*

$$APF = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{1 * \frac{4}{3} * \pi R^3}{a^3} = \frac{1 * \frac{4}{3} * \pi R^3}{(2R)^3} = 0.523.$$

52% of it is filled with atoms.

**Question 27** *Number of atoms per unit cell in Body Centred Cube unit cell?*

$$N = 8\text{corners} * \frac{1}{8} + 1\text{centered} = 2\text{atom}.$$



**Question 28** *Examples of BCC ?*

alpha-iron (α-Fe), Tungsten (W), Chromium (Cr), Tantalum (Ta), Molybdenum (Mo)

**Question 29** *What is the relationship between  $r$  and  $a$  in Body Centred Cube unit cell?*

$$a = \frac{4R}{\sqrt{3}}$$

**Question 30** *Coordination number in Body Centred Cube unit cell?*

$$CN = 8.$$

**Question 31** *The atomic packing factor in Body Centred Cube unit cell?*

$$APF = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{2 * \frac{4}{3} * \pi R^3}{a^3} = \frac{1 * \frac{4}{3} * \pi R^3}{(4R/\sqrt{3})^3} = 0.68.$$

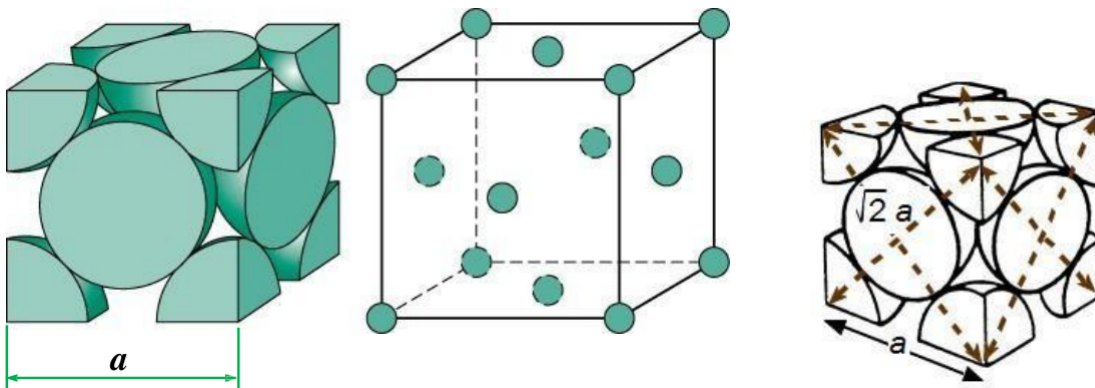
68 % of it is filled with atoms.

**Question 32** *Number of atoms per unit cell in Face Centred Cubic (FCC) unit cell?*

**Question 33** *Examples of FCC?*

Gamma iron (γ-Fe), aluminium (Al), Gold (Au), Nickel (Ni), Silver (Ag), Copper (Cu), Platinum (Pt), Lead (Pb).

$$N = 8 \text{ corners} * \frac{1}{8} + 6 * \frac{1}{2} = 4 \text{ atom}.$$



**Question 34** *What is the relationship between  $r$  and  $a$  in Face Centred Cubic (FCC) unit cell?*

$$a = \frac{4R}{\sqrt{2}}.$$

**Question 35** *Coordination number in Face Centred Cubic (FCC) unit cell?*

$$CN = 12.$$

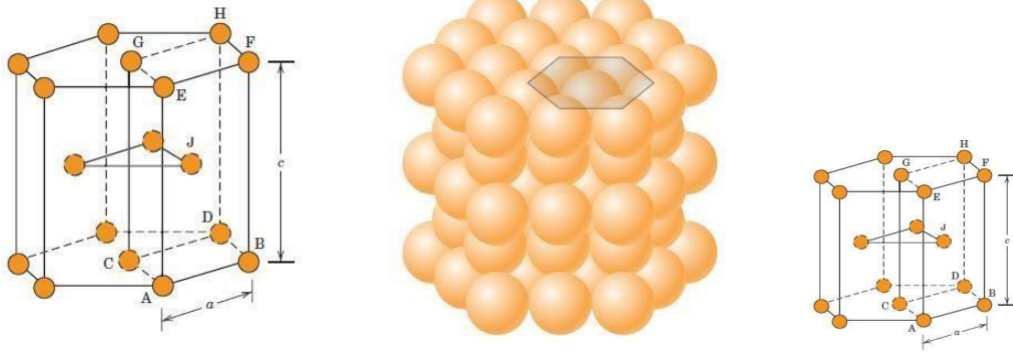
**Question 36** The atomic packing factor in Face Centred Cubic (FCC) unit cell?

$$APF = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{4 * \frac{4}{3} * \pi R^3}{a^3} = \frac{4 * \frac{4}{3} * \pi R^3}{(4R/\sqrt{2})^3} = 0.74.$$

74% of it is filled with atoms.

**Question 37** Number of atoms per unit cell in Hexagonal Close Packed (HCP) unit cell?

$$N = 12 * \frac{1}{6} + 2 * \frac{1}{2} + 3 = 6 \text{ atoms.}$$



**Question 38** Examples of HCP ?

Magnesium (Mg), Zinc (Zn), Cadmium (Cd), Titanium (Ti).

**Question 39** What is the relationship between  $r$  and  $a$  in Hexagonal Close Packed (HCP) unit cell?

$$a = 2R.$$

**Question 40** Coordination number in Hexagonal Close Packed (HCP) unit cell?

$$CN = 12.$$

**Question 41** The atomic packing factor in Hexagonal Close Packed (HCP) unit cell?

$$APF = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{6 * \frac{4}{3} * \pi R^3}{0.5 * c * a^2 * \sin(60)} = \frac{6 * \frac{4}{3} * \pi R^3}{\frac{\sqrt{3}}{4} * \sqrt{\frac{8}{3}} * (2R)^3} = 0.74.$$

74% of it is filled with atoms.

$c$  is the height and  $a$  is the side length

**Question 42** What is theoretical density ?

Density of a unit cell.

$$\rho = \frac{\text{mass of unit cell}}{\text{volume of unit cell}}.$$

$$\rho = \frac{nA}{N_A V_C}.$$

Where:  $n$ : number of atoms in a unit cell.

$A$ : molecular weight. mass of one mole of a substance in gm/mole

$N_A$ : Avogadro's no. =  $6.023 * 10^{23}$

$V_C$ : volume of unit cell.

### 3 Lecture 3

**Question 43** What is *Polymorphism/Allotropy*?

Two or more distinct crystal structures for the same material.

**Question 44** Examples of Polymorphism?

Carbon can be Graphite, Diamond and Graphene.

**Question 45** Define Grain Boundaries ?

The zone of crystalline mismatch between adjacent grains. The lattice has different orientation on either side of the grain boundary.

**Question 46** Compare single crystal (GRAIN) and polycrystalline materials in terms of properties.

- Single
  - Properties vary with direction: **anisotropic**.
  - such as the modulus of elasticity(E) in BCC iron.
- Poly crystal
  - may or may not vary with direction.
  - if the grains are randomly oriented then it is **isotropic** .

**Question 47** What is the relationship between grain size and strength of materials ?

the **Hall-Petch** Relationship: When the grain size decreases the strength of the material increases . Inverse Relation.

**Question 48** How to measure the Grain Size ?

The Linear Intercept method where

$$d_x = \frac{L * z}{V * n_x}.$$

Where L: length of each line (The longer the better)

z: number of lines

V: magnification

n: number of intercepts.

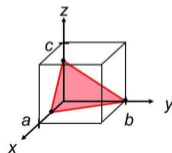
**Question 49** What are Miller Indices/Planes ?

The reciprocals of the fractional intercepts with the crystallographic axes. Indices are represented in (hkl) parentheses

**Question 50** How to calculate Millers ?

Identify the plane intercepts, take the reciprocal, reduce any fraction by multiplication.

example	a	b	c
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/1/2	1/1	1/3/4
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



Note that not all planes are that easy, some planes need you to change the origin, you can avoid this origin changing thing by getting the equation of the plane itself using simple math.

**Question 51** What are structure directions ?

it's simply the direction :) (end point - start point). [uvw]

**Question 52** How to find directions ?

Get the vector direction (end-start), remove any fraction by multiplication, put the result in square brackets and convert any negative to a bar.

**Question 53** When is a Direction  $[uvw]$  is normal to a Plan  $(hkl)$  ?

When  $u=h$ ,  $v=k$ , and  $w=l$  in a cubic system.

**Question 54** Linear Density?

The number of atoms per unit length whose centres lie on the direction vector for a specific crystallographic direction. = no. of atoms centred on the direction vector/length of the vector

**Question 55** Planar Density ?

number of atoms per unit area that are centred on particular crystallographic plane. = no. of atoms centred on a plane/area of the plane.

**Question 56** Why are Miller Indices important ?

Those planes and directions influence;

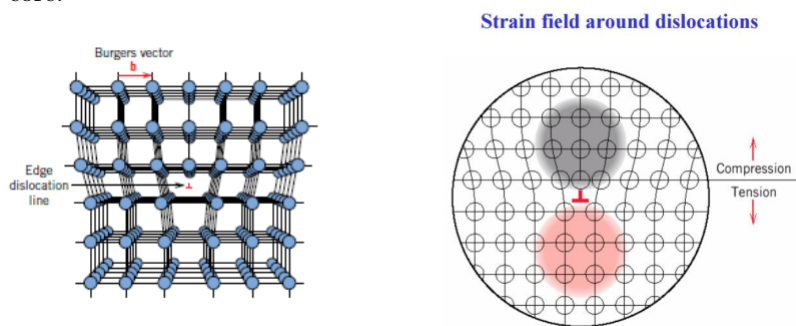
- Optical Properties
- Chemical Reactivity
- Surface Tension

**Question 57** What do defects affect ?

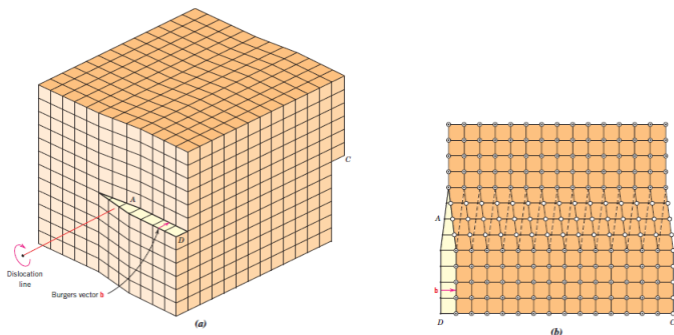
Defects are the reason why materials show lower strength than they could.

**Question 58** What are types of defects or imperfections in a crystal structure ?

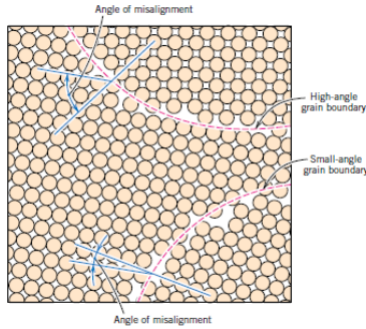
- **Point defect:** such as
  - **Vacancy:** vacant lattice site, one that is normally occupied but now missing.
  - **self-interstitial:** a one that is crowded. Opposite of a vacancy.
  - **small substitutional atoms:** one that is smaller than normal
  - **large substitutional atoms:** of course you know.
- **Linear defects:**
  - **Edge dislocation** : an extra plane of atoms present in the lattice. The atoms above the dislocation line are squeezed together while those below are pulled apart. (Compression and Tension). The magnitude and direction of the lattice distortion is represented by a **Burgers Vector** ( $b$ ). And this dislocation have some strain fields (vector field) that arises at their cores. And of course the strain drops rapidly with distance from the dislocation core.



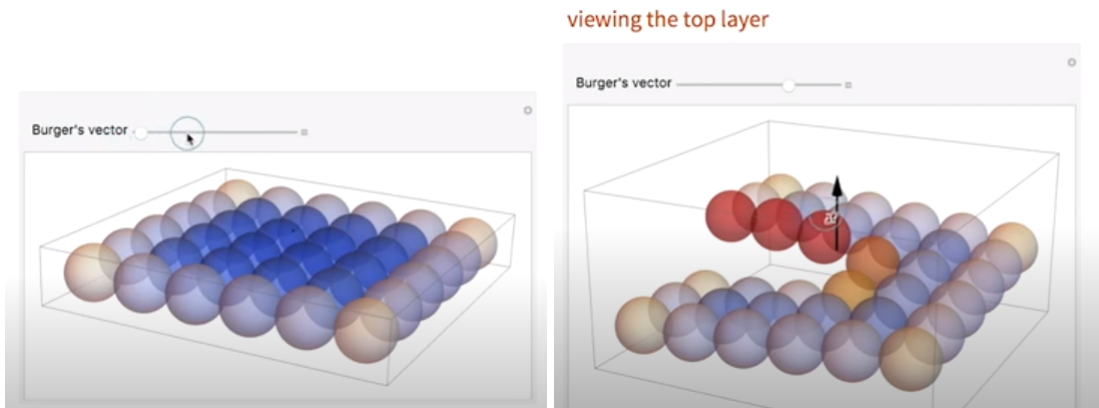
- **Screw dislocations.** Atoms at one side are higher than the other, this spiral shape forms some kind of a crew



- **Planar defect:** Interracial defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations. Grain Boundaries are a result of that defect. Various degrees of crystallographic misalignment between adjacent grains are possible.



**Question 59** *How does a screw dislocation look like ?*



**Question 60** *Why defects are important ?*

Because they affect the

- Conductivity: specially in semi-conductors
- Hardness/Ductility
- Diffusion coefficient