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MATERIALS SCIENCE FOR ENGINEERS – ME232AT

Presented by,

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The Fundamentals of Materials

The electronic structure of atoms, Types of atomic and molecular bonds; ionic bonding; covalent bonding; metallic bonding; secondary bonding; mixed bonding; hybridization.

Energy bands in metals, insulators, and semiconductors.

Basic crystallography. Defects and dislocations.

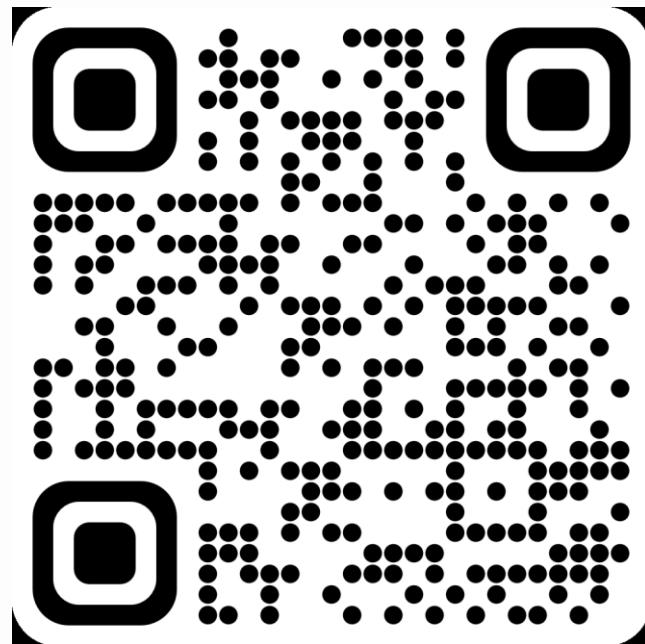
Types of Materials: Polymers, metals and alloys, semiconductors, ceramics, composites

- Types of Materials –
- Properties of Materials –
- Microstructure – internal arrangement of atoms and/or molecules

- Matter – Solids
 - Crystalline -
 - Amorphous -
- Repetition = Symmetry

Types of repetition: Rotation and Translation

The electronic structure of atoms



The Shells, Subshells and Orbitals

<https://youtu.be/Q0UEMXM5MTI?si=2MAW3ZRmsx7FH0-r>

The electronic structure of atoms refers to the **distribution of electrons within an atom**, specifying the arrangement of these subatomic particles in various energy levels or shells. This organization is governed by principles such as the ***Pauli Exclusion Principle, Hund's Rule, and the Aufbau Principle***.

Principle. The electronic structure is crucial in understanding an element's chemical behavior and its placement in the periodic table.

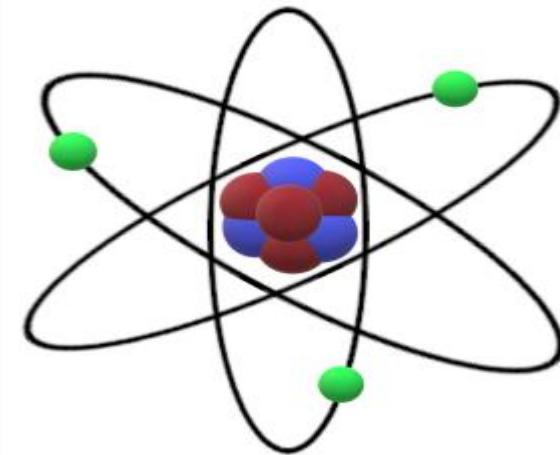


Fig. 1.1 Electronic configuration

Green-coloured spears are subatomic particles that carry a negative charge and orbit around the nucleus of an atom. The nucleus of an atom consists of a proton (positive charge particle, red spheres) and a neutron (neutral charge particle, blue spheres).

Electron Shells: Electrons are arranged in energy levels or shells, labelled numerically as $n = 1, 2, 3$, and so on. Electrons in higher energy levels are farther from the nucleus and possess more energy.

Subshells (or Orbitals): Each shell is further divided into subshells, which are designated as s, p, d, and f. These subshells have a specific number of orbitals: s has 1, p has 3, d has 5, and f has 7.

Shell No.	Shell Name	Sub Shell	Electrons	Total Electrons
1	K	1s	2	2
2	L	2s 2p	2 6	8
3	M	3s 3p 3d	2 6 10	18
4	N	4s 4p 4d 4f	2 6 10 14	32

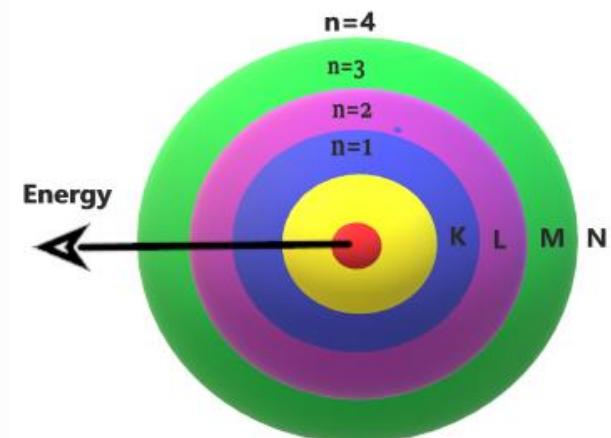
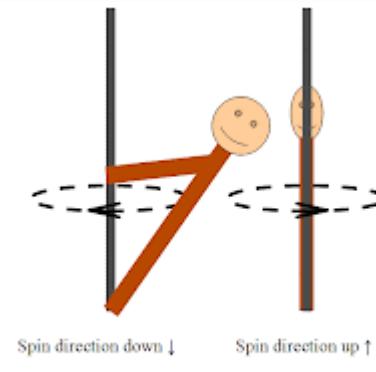
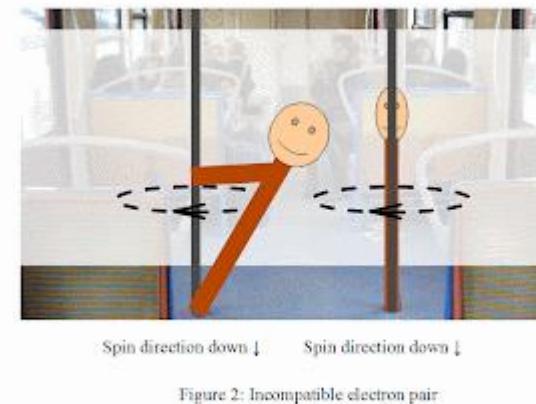


Fig. 1.2 Principle of quantum number (n)

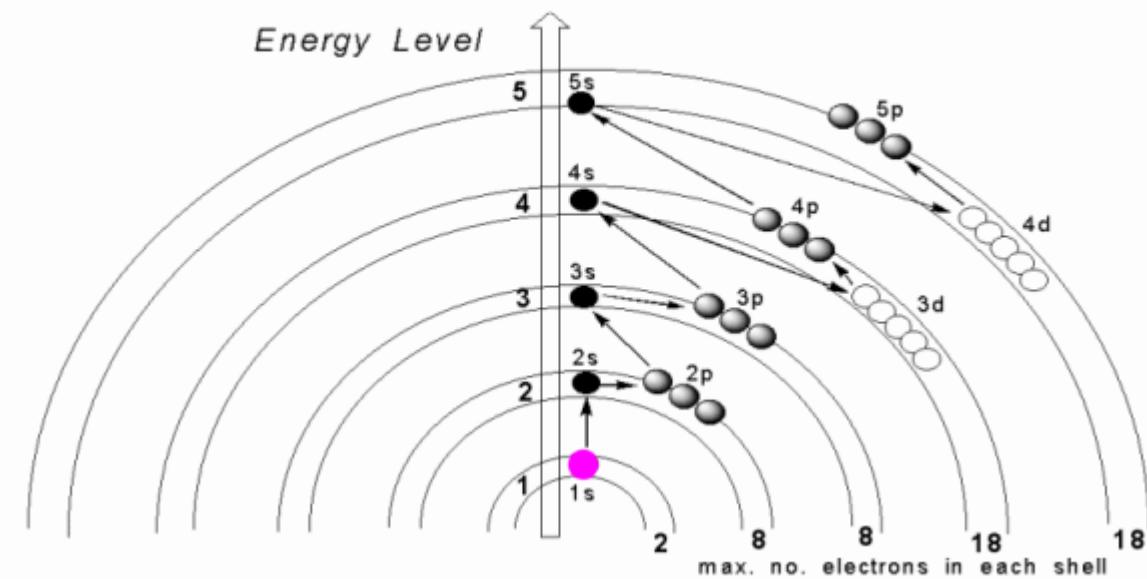
Pauli Exclusion Principle: No two electrons in an atom can have the same set of quantum numbers. This means that each orbital can hold a maximum of two electrons with opposite spins.

Aufbau Principle: Electrons fill the lowest energy orbitals first before moving to higher energy ones. This principle provides a sequence for filling orbitals based on increasing energy.



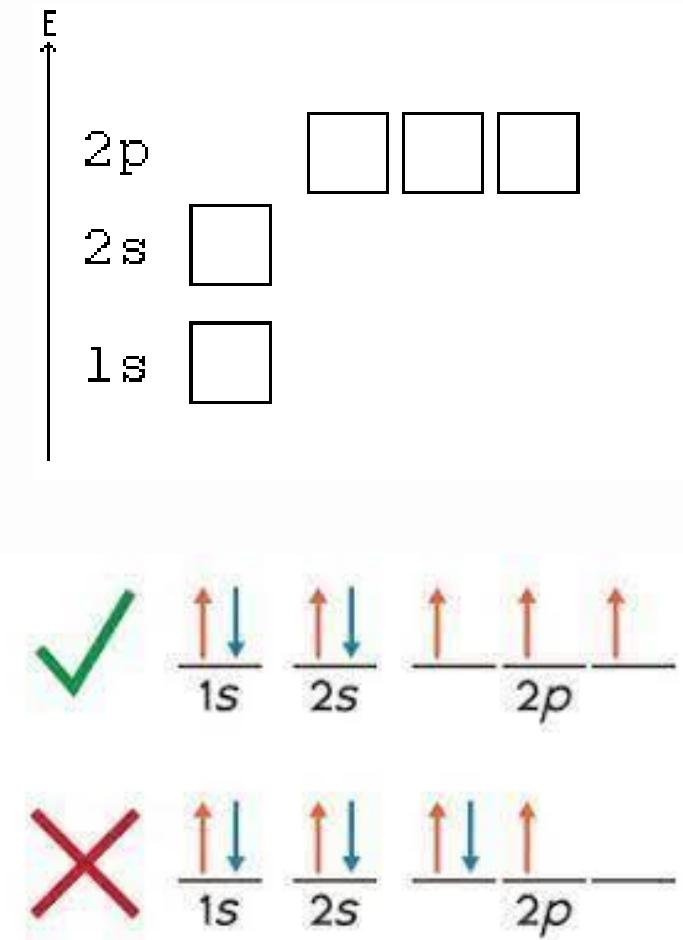
Adapted from: [CK-12.org](http://www.ck12.org) - October 2010

Aufbau Principle



Hund's Rule: When electrons occupy orbitals of equal energy (degenerate orbitals), they fill singly before pairing up. This results in the maximum spin alignment and minimizes the electron-electron repulsion.

Valence Electrons: Electrons in the outermost shell (valence shell) are called valence electrons. These electrons play a crucial role in determining an element's chemical properties and its ability to form bonds.



Atomic and molecular bonds are interactions that hold atoms and molecules together. There are several types of bonds, each characterized by the way electrons are shared, transferred, or attracted between atoms. Atomic bonding in solids may be considered in terms of attractive and repulsive forces and energies. The three types of **primary bond** in solids are **ionic, covalent, and metallic**. For *ionic* bonds, electrically charged ions are formed by the transference of valence electrons from one atom type to another; forces are coulombic. There is a sharing of valence electrons between adjacent atoms when bonding is *covalent*. With metallic bonding, the valence electrons form a “sea of electrons” that is uniformly dispersed around the metal ion cores and acts as a form of glue for them.

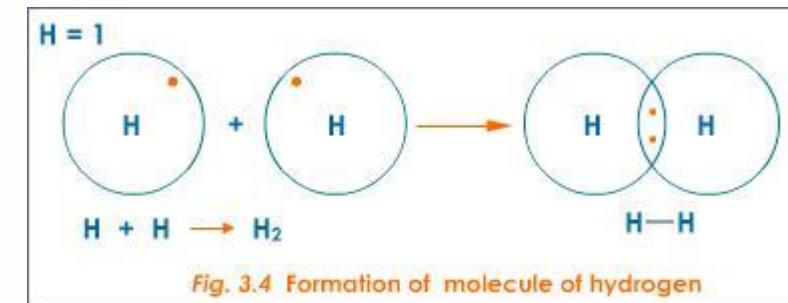
I. Primary Interatomic Bonds: (Covalent, Ionic, Metallic)

➤ Covalent Bonds:

Nature: Formed between non-metal atoms.

Electron Sharing: Electrons are shared between atoms to achieve a stable electron configuration.

Example: Hydrogen molecule (H_2).



➤ Ionic Bonds:

Nature: Formed between a metal and a non-metal.

Electron Transfer: Electrons are transferred from the metal atom (cation) to the non-metal atom (anion).

Example: Sodium chloride (NaCl), MgO.

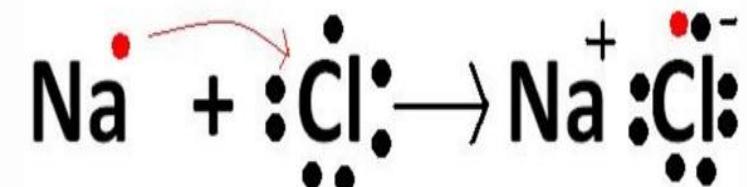


Fig 1.7 Example for Ionic Bonds

➤ Covalent Bonds:

In **covalent bonding**, stable electron configurations are assumed by the sharing of electrons between adjacent atoms.

Two atoms that are covalently bonded will each contribute at least one electron to the bond, and the shared electrons may be considered to belong to both atoms.

Covalent bonding is schematically illustrated in the figure for a molecule of methane.

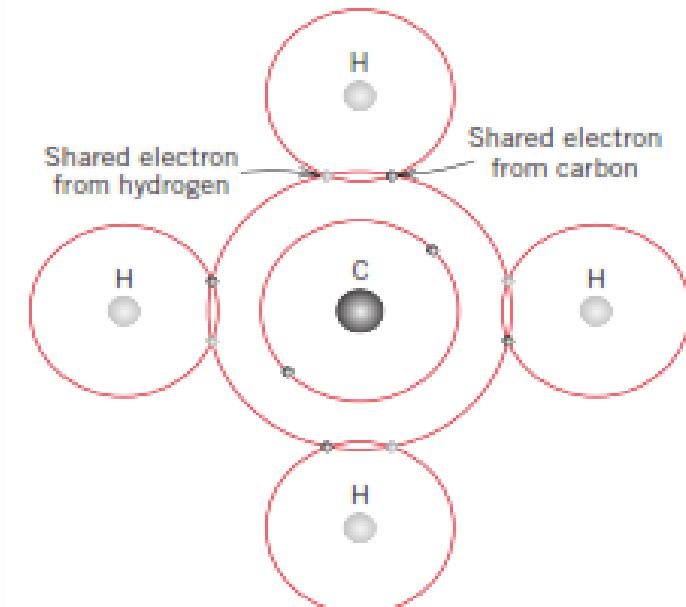
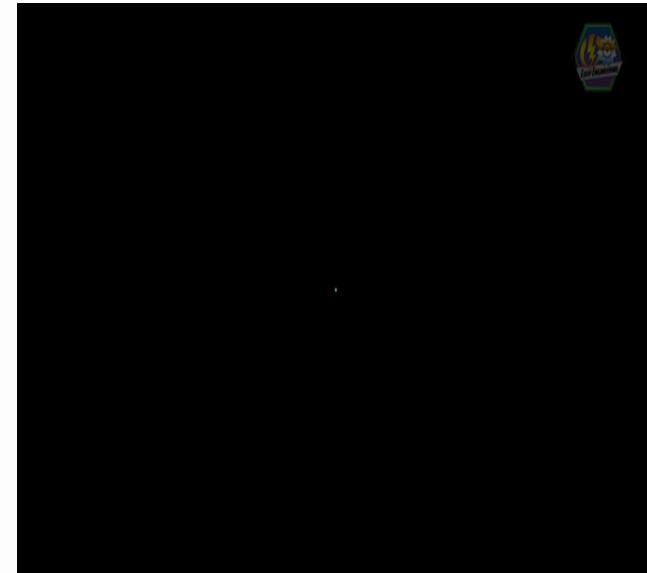
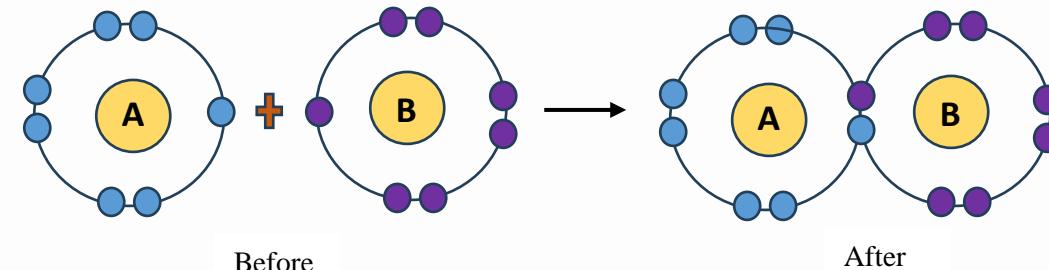


Figure 2.10 Schematic representation of covalent bonding in a molecule of methane (CH_4).



<https://www.youtube.com/watch?v=ttEBGT0CMsQ&list=PPSV>

Covalent Bonds Mechanism

Covalent Bonds:

1. Polar Covalent Bonds:

Nature: Similar to covalent bonds but with unequal sharing of electrons.

Electron Distribution: One atom attracts the shared electrons more strongly, creating a partial negative and partial positive charge.

Example: Water molecule (H_2O), HCl

2. Nonpolar Covalent Bonds:

Nature: Similar to covalent bonds with equal sharing of electrons.

Electron Distribution: Electrons are shared equally between atoms.

Example: Oxygen molecule (O_2), CH_4

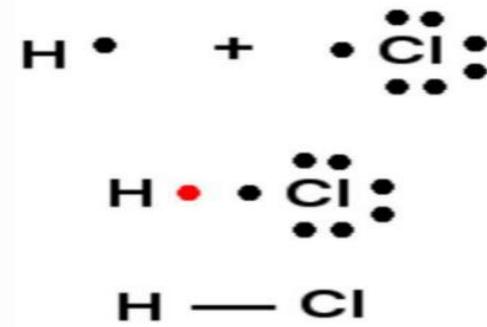


Fig 1.5 Example for polar Covalent Bonds

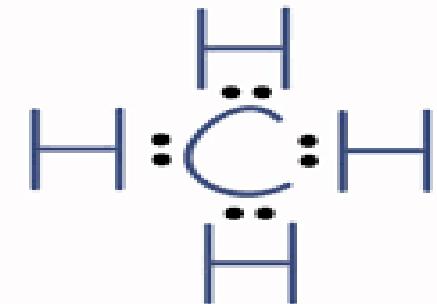


Fig 1.6 Example for Nonpolar Covalent Bonds

➤ Metallic Bonds:

Nature: Formed between metal atoms.

Electron Sea Model: Electrons are delocalized and move freely among metal cations, creating a "sea" of electrons.

Example: Copper (Cu) in a metallic structure.

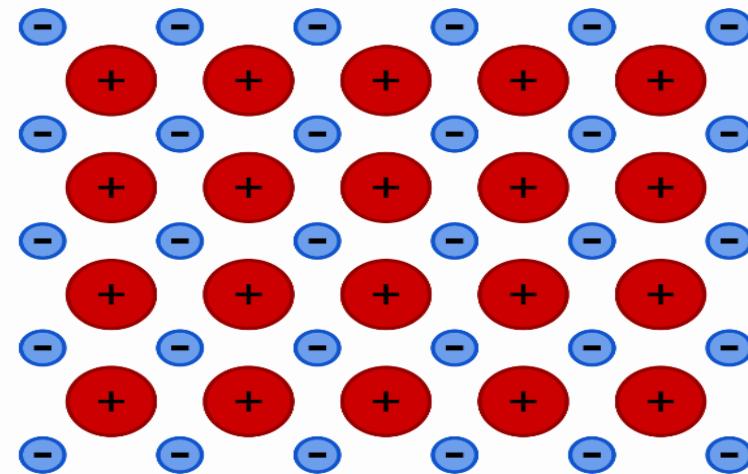


Fig 1.8 Example for Metal Bonds

II. Secondary Interatomic Bonds:

Secondary, van der Waals, or physical bonds are weak in comparison to the primary or chemical ones;

➤ Hydrogen Bonds:

Nature: A type of dipole-dipole interaction.

Bonding Elements: Involves hydrogen bonded to highly electronegative atoms (O, N, F).

Example: Hydrogen bonding in water (H_2O).

➤ Van der Waals Forces:

Nature: Weak attractive forces between molecules.

Types: Includes London dispersion forces, dipole-dipole interactions, and hydrogen bonding.

Example: Intermolecular forces between noble gases.

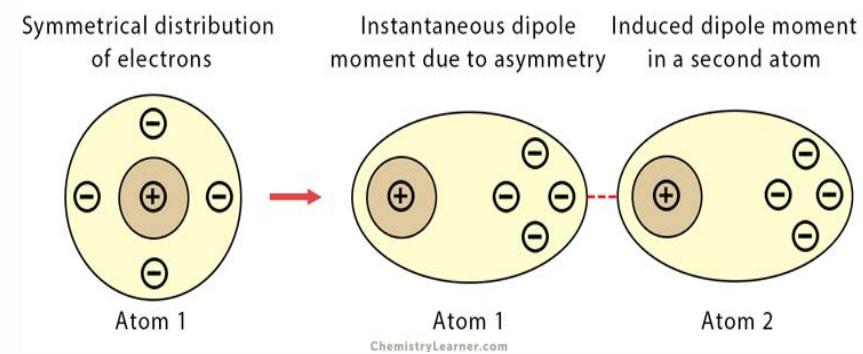


Fig. 1.11 Example for London Dispersion Forces (Van der Waals Forces)

❖ Coordinate (Dative) Bonds:

Nature: A special type of covalent bond where both electrons come from one atom.

Formation: One atom donates both electrons to form a bond.

Example: Formation of ammonium ion (NH_4^+).

❖ Salt Bridges:

Nature: An electrostatic attraction between positive and negative ions.

Common in: Ionic compounds in a solution.

Example: Formation of a salt bridge in electrolyte solutions.

Understanding these types of bonds is crucial for ***explaining the properties and behaviors*** of different substances in chemistry. The type of bond formed between atoms influences the ***structure, physical properties, and reactivity of molecules and compounds***.

Mixed Bonding: Mixed bonding refers to a type of chemical bonding that combines characteristics of different bonding types, such as ionic, covalent, metallic, or hydrogen bonding. It occurs when there is a partial sharing or transfer of electrons between atoms.

- Mixed bonding refers to the presence of both ionic and covalent bonding within a single compound or system. In such cases, part of the bonding between atoms involves the transfer of electrons (ionic bonding), while another part involves the sharing of electrons (covalent bonding). This results in a hybrid structure where both types of interactions contribute to the compound's overall stability and properties.
- **An example of mixed bonding is seen in the compound sodium hypochlorite (NaOCl)**, which is the active ingredient in household bleach. In NaOCl , the oxygen atom is more electronegative than the sodium atom. As a result, the oxygen atom attracts the shared electron pair in the covalent bond more strongly, creating a partial negative charge. The sodium atom, having lost an electron to oxygen, carries a partial positive charge. This partial transfer of electrons leads to an ionic character in the compound, while the sharing of the electron pair between oxygen and chlorine atoms contributes to the covalent character.
- **Calcium Carbonate (CaCO_3):** The bond between calcium (Ca^{2+}) and the carbonate ion (CO_3^{2-}) is ionic. However, within the carbonate ion (CO_3^{2-}), the carbon and oxygen atoms are bonded covalently.

hybridization bonding

Hybridization bonding refers to a concept in chemistry that involves the mixing of atomic orbitals to form new hybrid orbitals. These hybrid orbitals are then used to describe the bonding in molecules. It is a model that helps explain molecular shapes and the types of bonds formed between atoms.

The most commonly encountered hybridization types are sp, sp², and sp³ hybridizations. Each hybridization type corresponds to a specific arrangement of electron domains around the central atom in a molecule.

sp Hybridization: In sp hybridization, one 's' orbital and one p orbital from the central atom combine to form two sp hybrid orbitals. These hybrid orbitals are linearly oriented at an angle of 180° to each other. Examples of molecules that exhibit sp hybridization include linear molecules like BeCl₂ and linear carbon-containing molecules like acetylene (C₂H₂) shown in Fig.

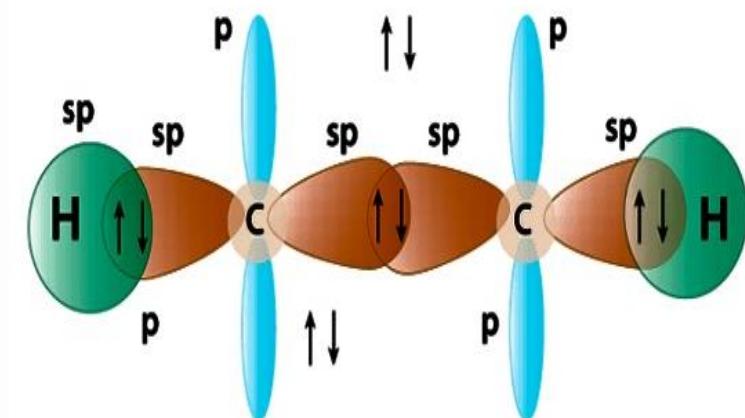


Fig. 1.12 C₂H₂ sp hybridization

sp² Hybridization: In sp² hybridization, one ‘s’ orbital and two p orbitals from the central atom combine to form three sp² hybrid orbitals. These hybrid orbitals are trigonally oriented in a plane, with angles of 120° between them. This type of hybridization is commonly observed in molecules with a trigonal planar geometry, such as boron trichloride (BCl₃) and molecules containing a carbon-carbon double bond, like ethylene (C₂H₄) shown in Fig. 1.13.

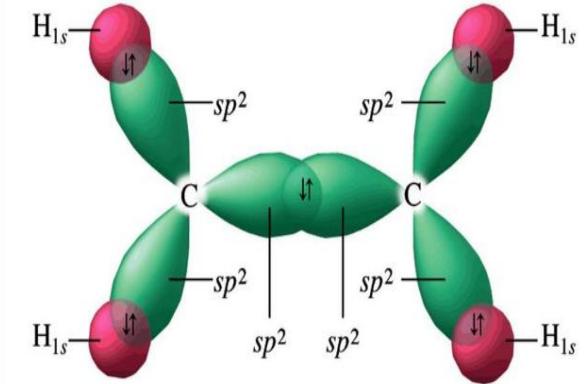


Fig. 1.13 C₂H₄ sp² hybridization

Sp³ Hybridization: In sp³ hybridization, one ‘s’ orbital and three p orbitals from the central atom combine to form four sp³ hybrid orbitals. These hybrid orbitals are tetrahedrally oriented, with angles of approximately 109.5° between them. Examples of molecules exhibiting sp³ hybridization include methane (CH₄) as shown in Fig. 1.14 and other molecules with a tetrahedral geometry.

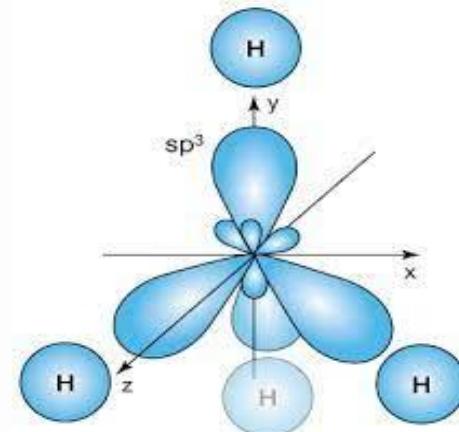
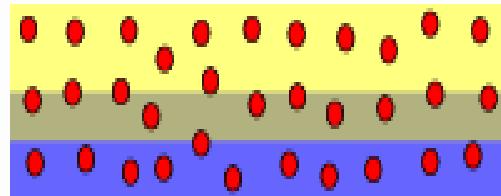


Fig. 1.14 C₂H₄ sp³ hybridization

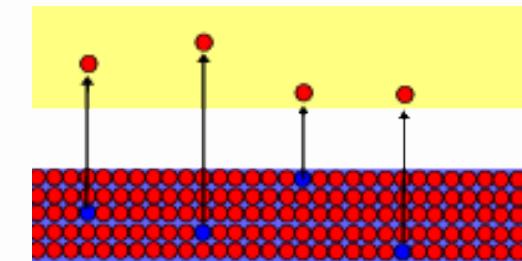
Metals

In a metal the conduction and valence bands overlap so electrons can easily pass into the conduction band. This means that the number density of free charge carriers will be very high.



Semiconductors

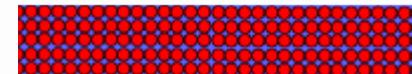
In semiconductors there is a gap between the valence band and conduction band, also the valence band is completely full. If some electrons in the valence band are provided with the right level of energy they can jump the gap into the conduction band. This energy can be provided by thermal energy. However the number of free electrons in the conduction band is still much less than that of a conductor.



Note some conduction can take place in the valence band provided it is not completely full. For every electron that moves into the conduction band it creates the equivalent of one mobile charge carrier in the valence band.

Insulators

In an insulator the energy gap between the valence band and the conduction band is much larger and a large amount of energy would be needed for electrons to jump into the conduction band. For this reason there are far fewer electrons in the conduction band of an insulator than that of a semiconductor.



Solids can be categorized into three main groups on the basis of band gaps as

- A. Insulators**
- B. Semiconductor**
- C. Conductor.**

A. Insulators

- The forbidden energy gap (E_g) is greater than 3eV
- do not conduct electricity
- number of electrons is just enough to completely fill a number of allowed energy bands.
- Above these bands there exists a series of completely empty bands.
- At ordinary temperatures electron can't be thermally excited across this gap from the valence band to the conduction band.
- As the bands are either completely filled or empty, no electric current flow.

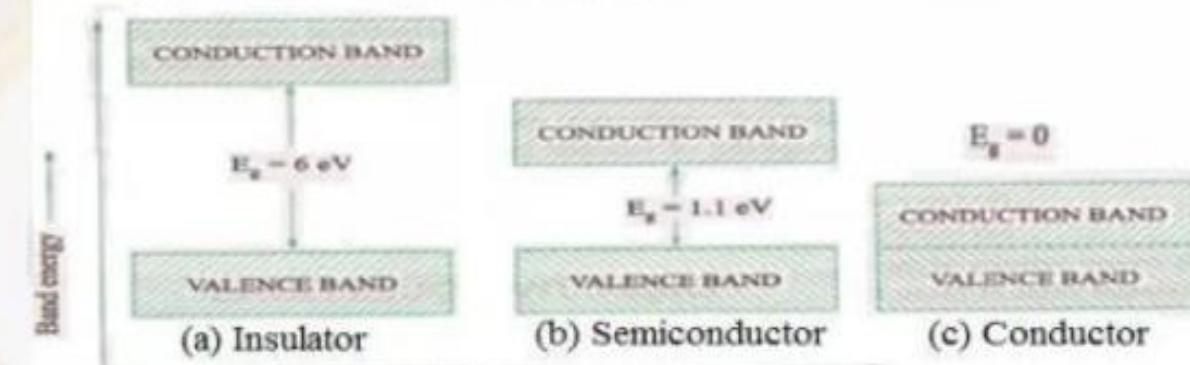


Fig. 1 Energy band diagram of (a) Insulator, (b) Semiconductor and (c) Conductor

- The topmost filled band is known as the valence band
- The lowermost empty band known as the conduction band
- The gap between valence band and conduction band is known as forbidden energy gap (E_g)

Semiconductor

- semiconductor exhibits an electrical conductivity intermediate between that of metal and insulators
- the energy gap E_g is relatively small (of the order of 1eV).
- an appreciable number of electrons can be thermally excited across the gap from the states near the top of the valence band to states the bottom of the conduction band.
- As the temperature approaches absolute zero, the thermal excitation becomes vanishingly small and therefore all semiconductors behave as insulators at such temperatures.

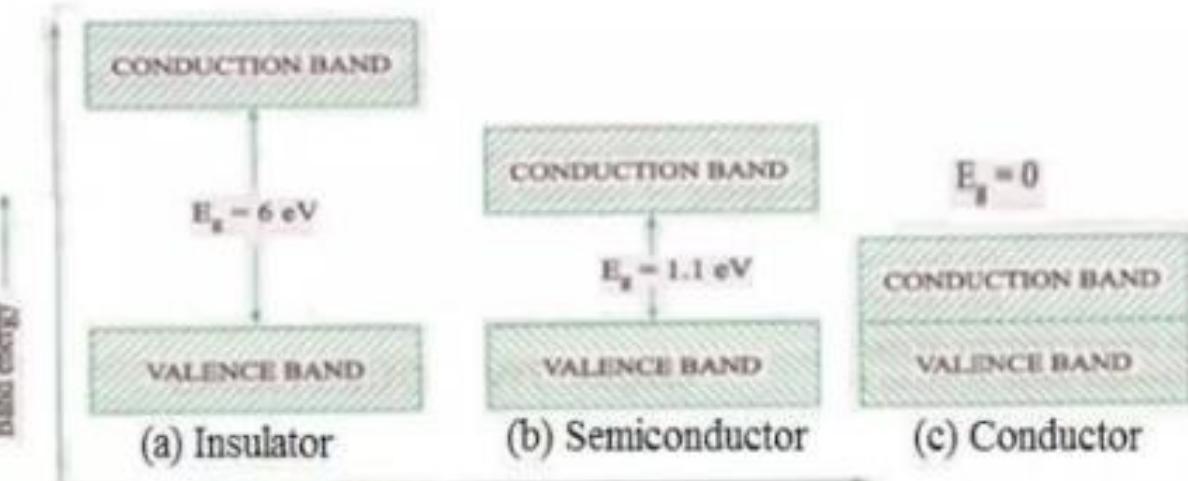


Fig. 1 Energy band diagram of (a) Insulator, (b) Semiconductor and (c) Conductor

Conductor

- Upper most energy band is partially filled or if the uppermost filled band and the next unoccupied band overlap in energy, the crystal is known as conductors (metal).
- the electron in the uppermost band find adjacent vacant states to move into, by absorbing energy from an applied electric field. These electrons thus behave as free electrons and conduct electric currents.
- The electrical conductivity of a metal, at room temperature, is of order of 10^6 mho/cm , that of semiconductor lies in the range 10^3 mho/cm to 10^6 mho/cm , and that of a good insulator is of order of 10^{-12} mho/cm .

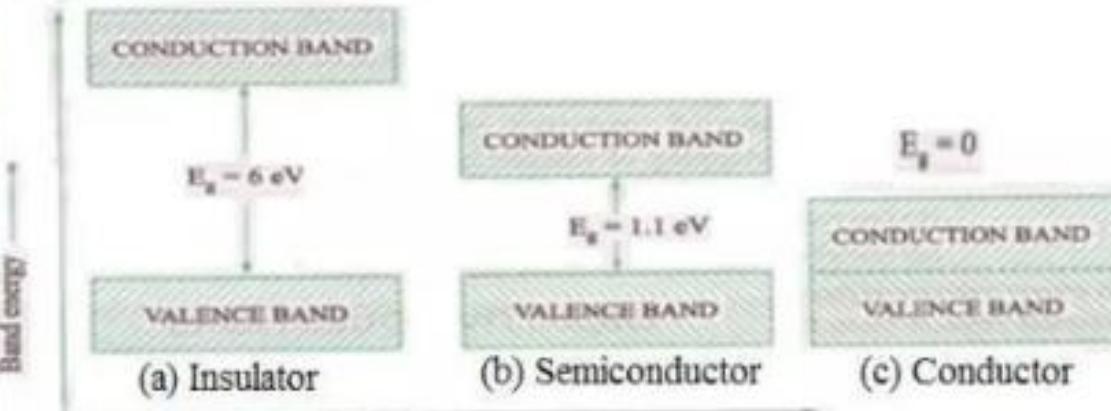
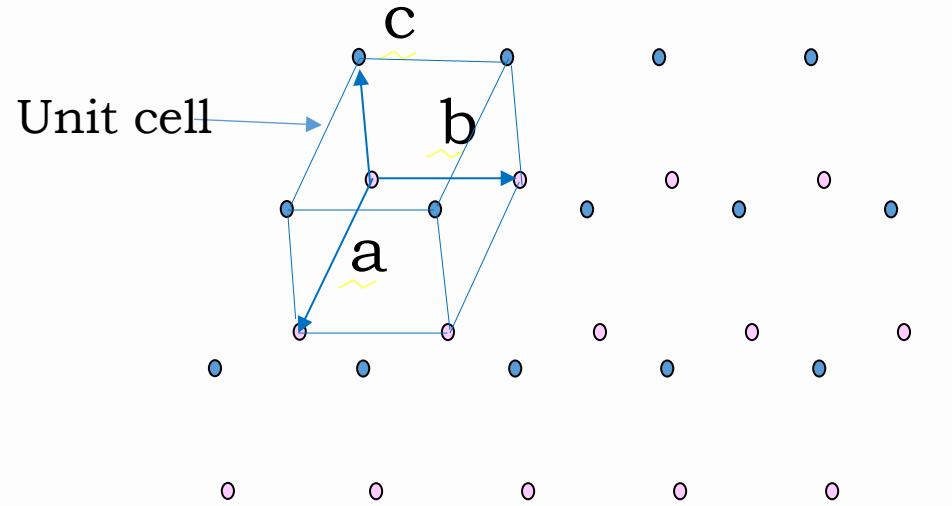


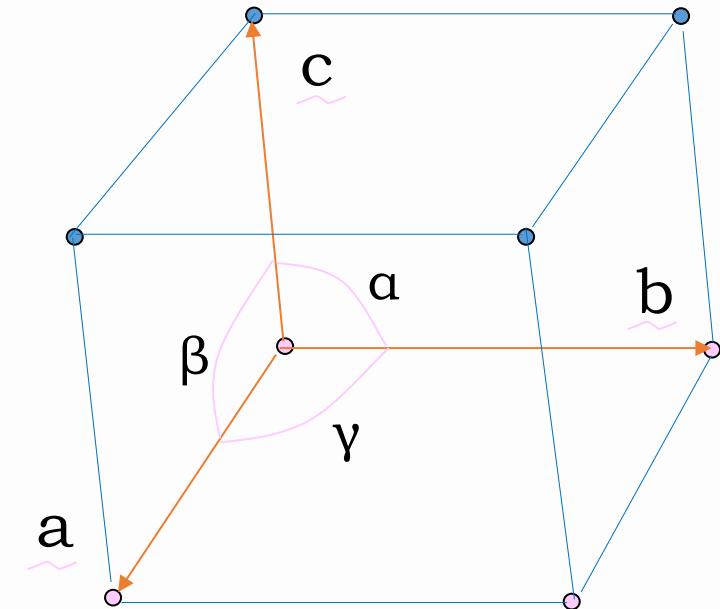
Fig. 1 Energy band diagram of (a) Insulator, (b) Semiconductor and (c) Conductor

- The band gap E_g of a typical insulator, such as diamond is about 6eV while that of semiconductors lies in the range of 2 eV to 2.5eV and in conductor it is zero

Space Lattice: An infinite array of points in 3D space in which each point is identically located with respect to other

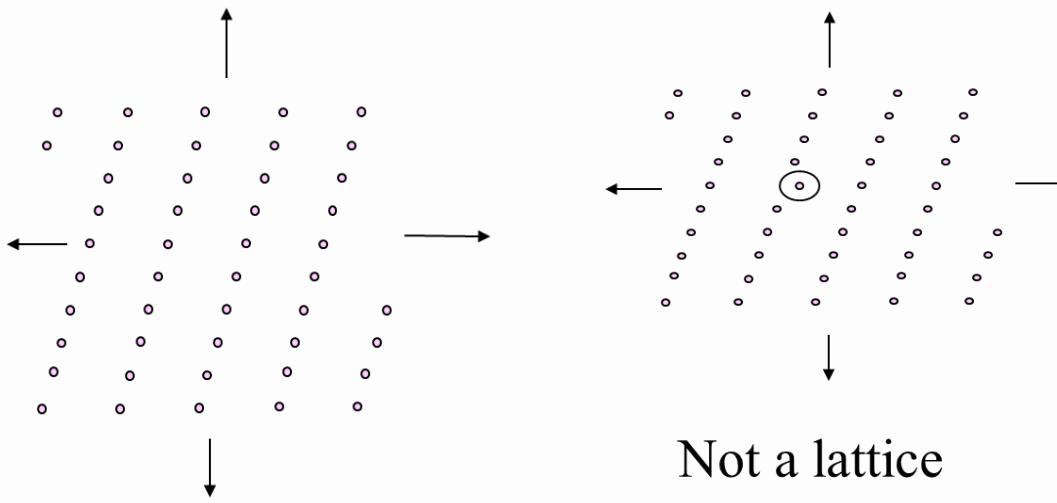


a, b, and c are the basis vectors for the lattice

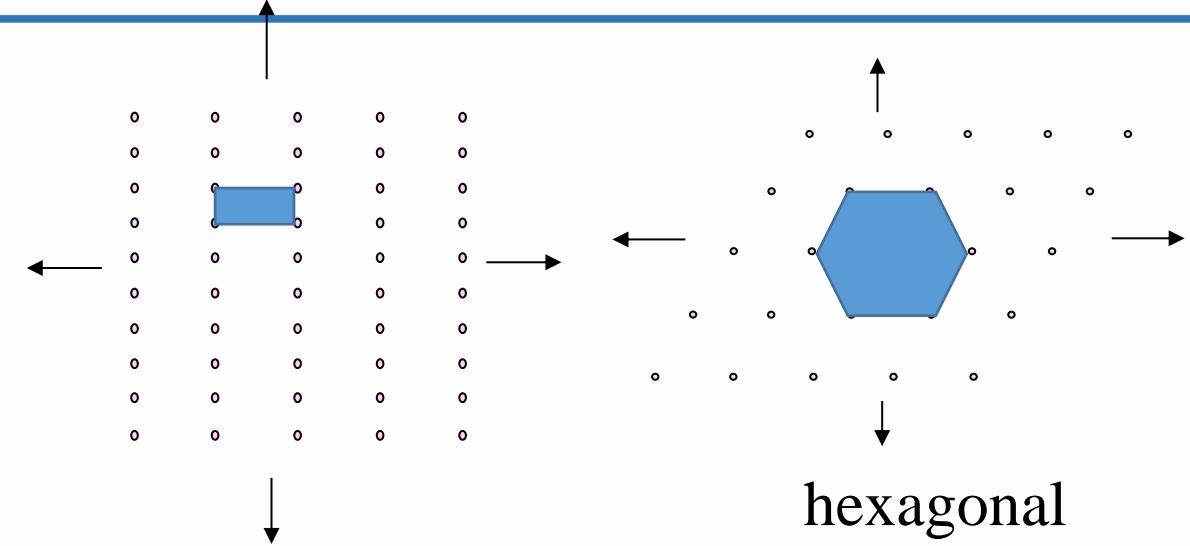


Lattice parameters:

Lattice - infinite, perfectly periodic array of points in a space

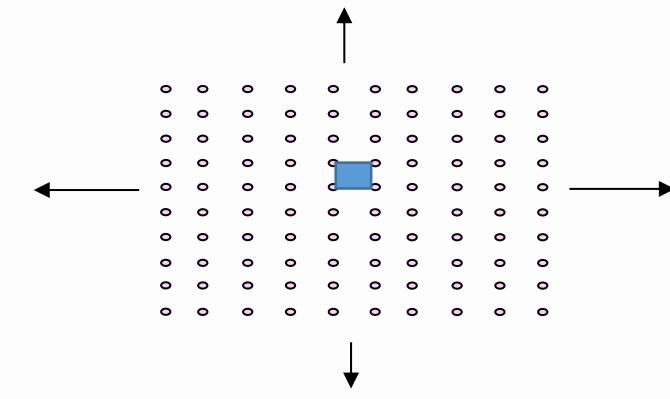


Not a lattice



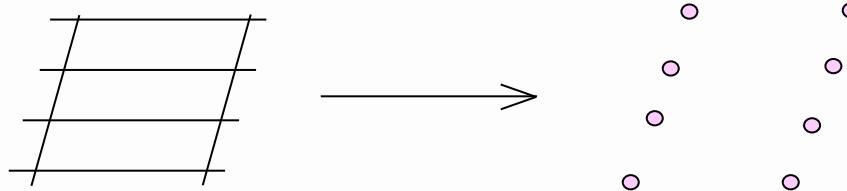
rectangular

hexagonal



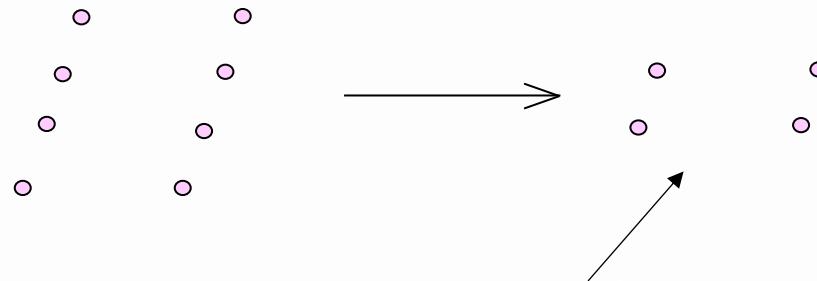
square

We abstracted points from the shape:



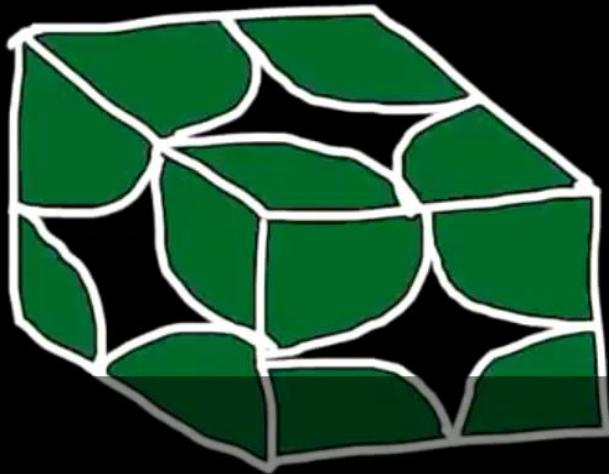
Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.

Now we abstract further:



This is a UNIT CELL
Represented by two lengths and an angle

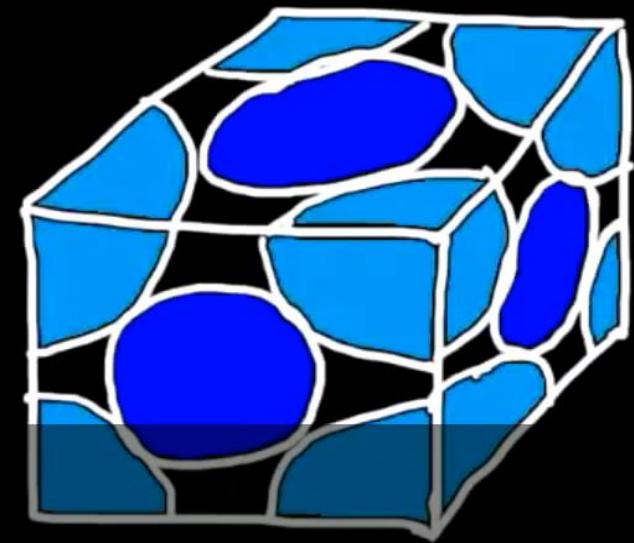
Simple Cubic



Body Centered Cubic



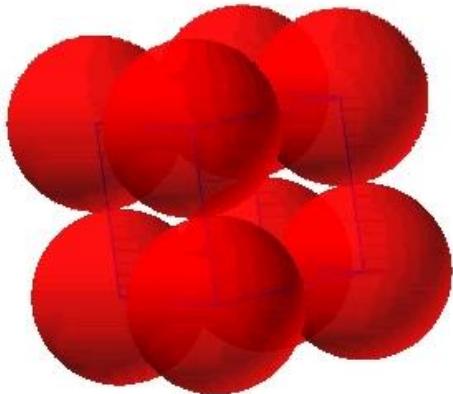
Face Centered Cubic



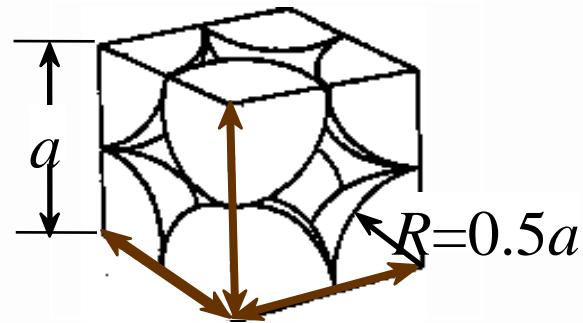
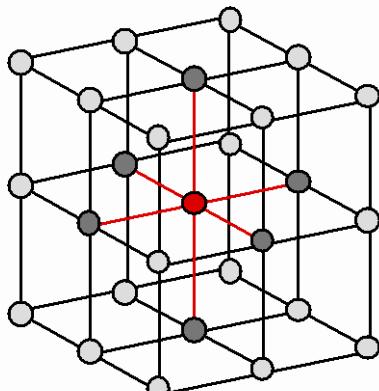
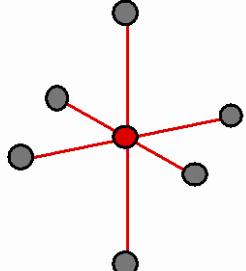
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Simple Cubic Structure (SC)

Atomic Packing Factor (APF)



- **Coordination No. = 6**
(# nearest neighbors) for each atom as seen



close-packed directions
contains $(8 \times 1/8) =$
1 atom/unit cell

Adapted from Fig. 3.23, *Callister 7e*.

$$\text{APF} = \frac{\text{Volume of atoms in unit cell}^*}{\text{Volume of unit cell}}$$

*assume hard spheres

$$\text{APF} = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{4}{3} \pi (0.5a)^3}{a^3}$$

volume
atom

volume
unit cell

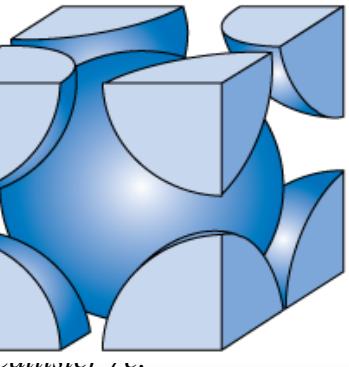
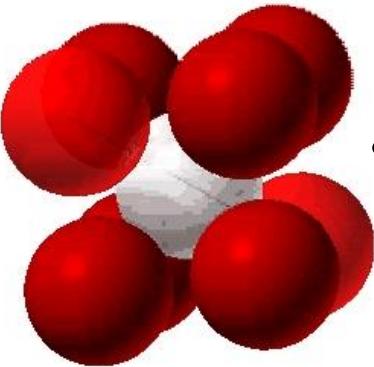
Here: $a = R_{\text{at}} * 2$

Where R_{at} is the 'handbook' atomic radius

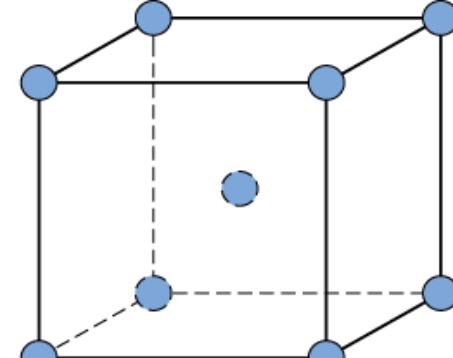
- APF for a simple cubic structure = $0.52 = 52\%$

- Atoms touch each other along *cube diagonals within a unit cell.* ex: Cr, W, Fe (α), Tantalum, Molybdenum

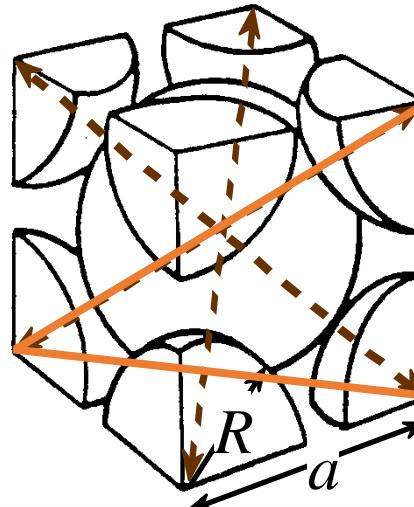
--Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.



- Coordination # = 8



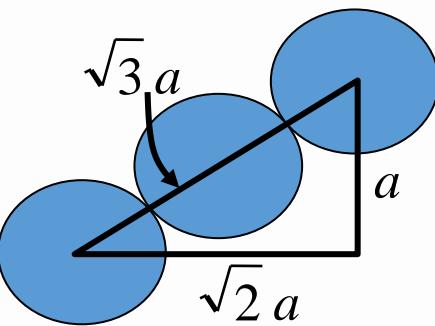
$$(\text{Solid diagonal})^2 = \text{Sum of squares of all three diagonals}$$



$$\text{APF} = \frac{\frac{atoms}{unit\ cell}}{\frac{volume}{unit\ cell}} = \frac{2 \cdot \frac{4}{3} \pi (\sqrt{3}a/4)^3}{a^3}$$

← $\frac{volume}{atom}$

← $\frac{volume}{unit\ cell}$



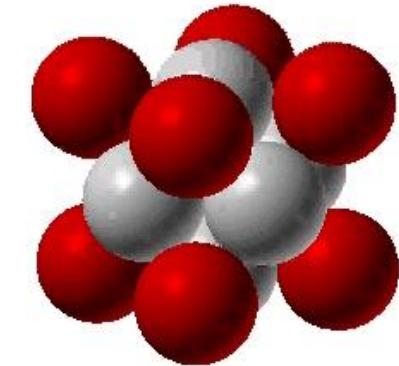
Close-packed directions:
length = $4R = \sqrt{3}a$

2 atoms/unit cell: (1 center) + (8 corners \times 1/8)

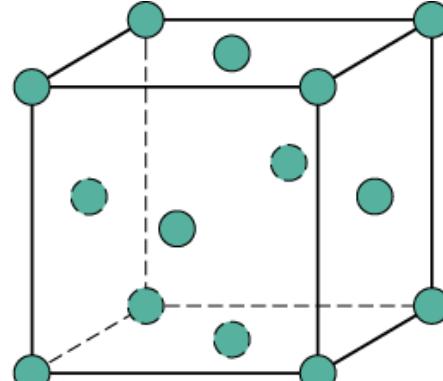
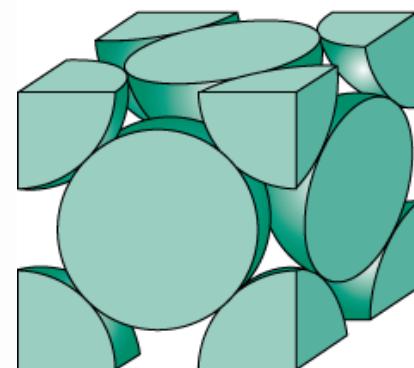
• APF for a body-centered cubic structure = 0.68 = 68%

- Atoms touch each other along *face diagonals*. ex: Al, Cu, Au, Pb, Ni, Pt, Ag

--Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of

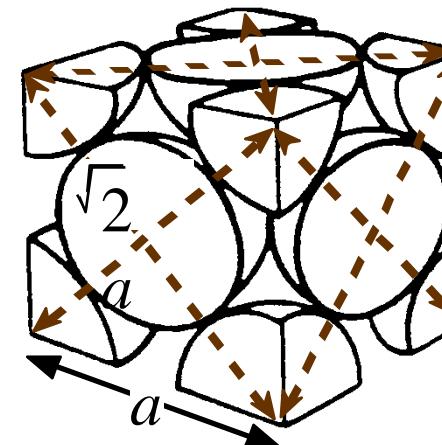


- Coordination # = 12



$$4 \text{ atoms/unit cell: } (6 \text{ face} \times \frac{1}{2}) + (8 \text{ corners} \times \frac{1}{8})$$

(Courtesy P.M. Anderson)



The maximum achievable APF!

Close-packed directions:
length = $4R = \sqrt{2} a$
($a = 2\sqrt{2}^*R$)

$$\text{APF} = \frac{\frac{\text{atoms}}{\text{unit cell}} \cdot \frac{4}{3} \pi (\sqrt{2}a/4)^3}{a^3}$$

volume atom volume unit cell

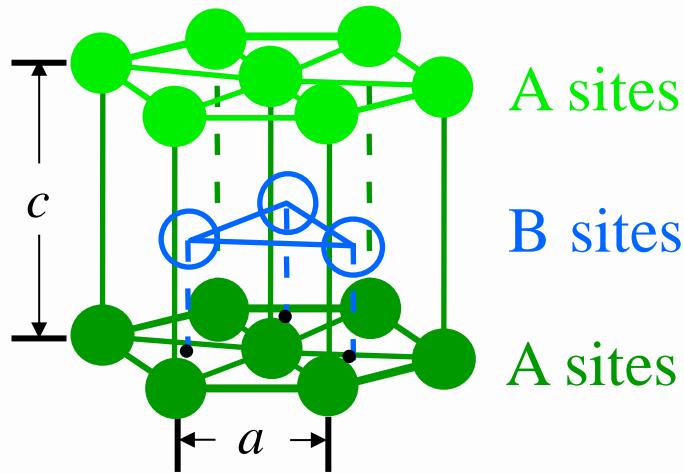
- APF for a face-centered cubic structure = $0.74 = 74\%$

Adapted from Fig. 3.1, Callister 7e.

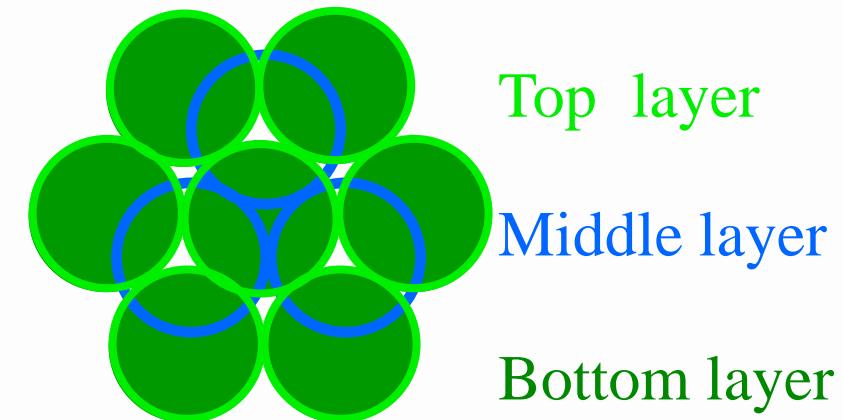
- ABAB... Stacking Sequence

ex: Cd, Mg, Ti, Zn

- 3D Projection



- 2D Projection



- Coordination # = 12

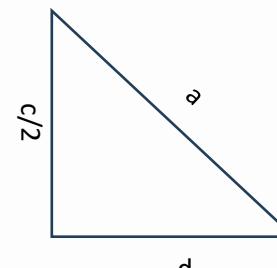
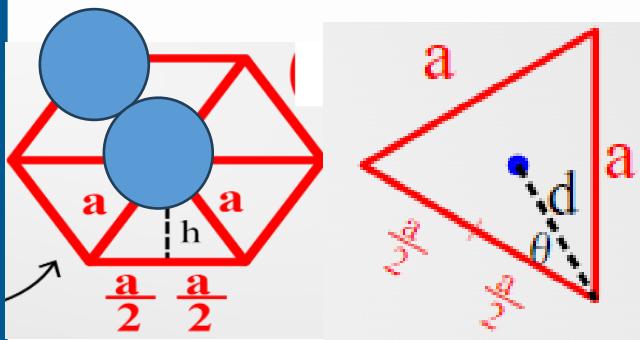
6 atoms/unit cell

- $c/a = 1.633$ (ideal)

- $\text{APF} = 0.74$

Hexagonal Close-Packed Structure (HCP)

Go, change the world



12 atoms on the corners with $1/6$ of their volume inside the unit cell = $12 \times 1/6 = 2$ atoms

3 atoms inside the cell, with 100 % of their volume inside the unit cell = 3 atoms

2 atoms on the faces, with $\frac{1}{2}$ of their volume inside the unit cell = $2 \times \frac{1}{2} = 1$ atom

Total atoms = 6 atoms per cell

Volume of the 6 atoms = $6 \times 4/3 \pi r^3 = 8 \pi r^3$

Volume of the HCP = Area of the hexagon x height of the prism

$$\text{Area of triangle} = \frac{1}{2} \text{Base} * \text{height} = \frac{1}{2} a \times h$$

$$h = \sqrt{a^2 - \frac{a^2}{4}} = \frac{\sqrt{3}}{2} a$$

$$\text{Area of triangle} = \frac{1}{2} a \frac{\sqrt{3}}{2} a = \frac{\sqrt{3}}{4} a^2$$

$$\text{Area of Hexagon} = \text{Hexagon made of 6 triangle} = 6 \times \frac{\sqrt{3}}{4} a^2 = \frac{3\sqrt{3}}{2} a^2$$

$$\theta = 30^\circ$$

$$d = \frac{a}{2 \cos \theta} = \frac{a}{\sqrt{3}}$$

$$c = \sqrt{\frac{8}{3}} a \text{ or } 4 \sqrt{\frac{2}{3}} r$$

$$\frac{c}{2} = a^2 - d^2 = a^2 - \frac{a}{\sqrt{3}}$$

$$\text{Volume of unit cell} = \text{area of hexagon} \times c = \frac{3\sqrt{3}}{2} a^2 \times \sqrt{\frac{8}{3}} a$$

$$\text{Volume of unit cell} = 24 \sqrt{2} r^3$$

$$\text{Atomic packing factor} = \frac{\text{volume of atoms}}{\text{volume of unit cell}} = \frac{8 \pi r^3}{24 \sqrt{2} r^3} = \frac{\pi}{3\sqrt{2}} = 74\%$$

There is no such thing as a perfect crystal.

- What are these imperfections?
- Why are they important?

Many of the important properties of materials are due to the presence of imperfections.

The study of imperfections has a two-fold purpose, namely,

- A better understanding of crystals and how they affect the properties of metals.
- Exploration of possibilities of minimizing or eliminating these defects.

The term “**defect**” or “**imperfection**” is generally used to describe any deviation from the perfect periodic array of atoms in the crystal.

- Vacancy atoms
- Interstitial atoms
- impurities- Interstitial, Substitutional, Frenkel and Schottky
- Dislocations - Edge and Screw dislocations
- Grain Boundaries, stacking fault, tilt, and twin boundaries
- Voids, porosity, cracks, inclusions

Point defects / 0D defects

Line defects /1D defects

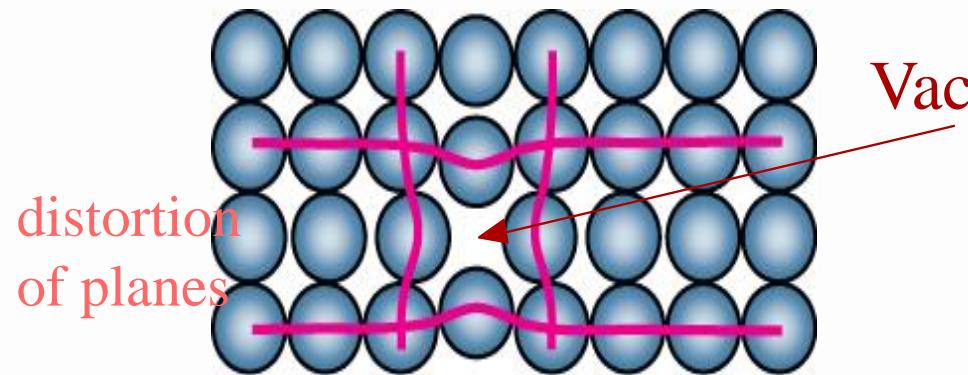
Area/surface/Plane defects / 2D defects

Volume defects / 3D defects

Point Defects in Metals

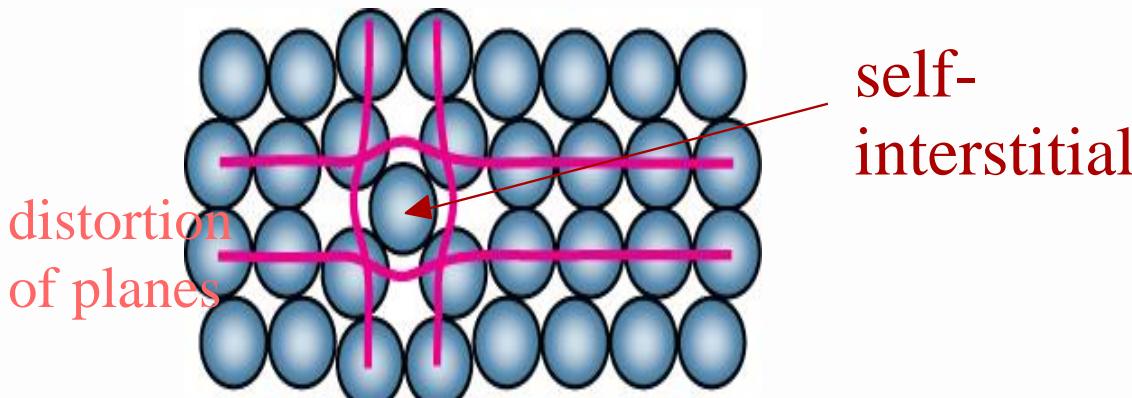
- **Vacancies:**

-vacant atomic sites in a structure.



- **Self-Interstitials:**

-"extra" atoms positioned between atomic sites.



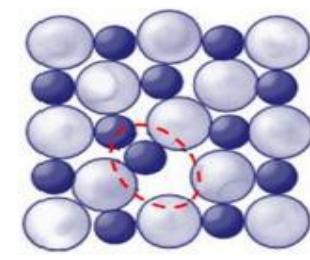
They are imperfect point-like regions, one or two atomic diameters in size and hence referred to as 'zero dimensional imperfections'.

There are different kinds of point imperfections.

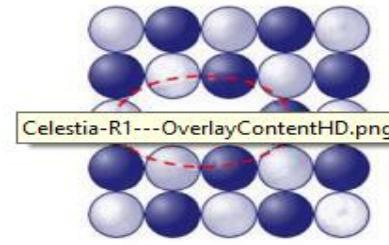
Vacancy VACANCIES

If an atom is missing from its normal site in the matrix, the defect is called a *vacancy defect*.

It may be a single vacancy, divacancy or a trivacancy.



Frenkel defect



Schottky defect

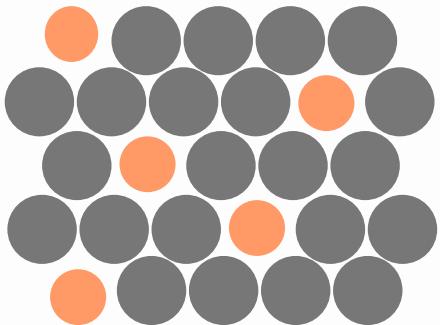
In ceramic materials point defects occur in pair to maintain the electroneutrality.

A cation-vacancy and a cation-interstitial pair is known as **Frenkel defect**.

A cation vacancy-anion vacancy pair is known as a **Schottky defect**.

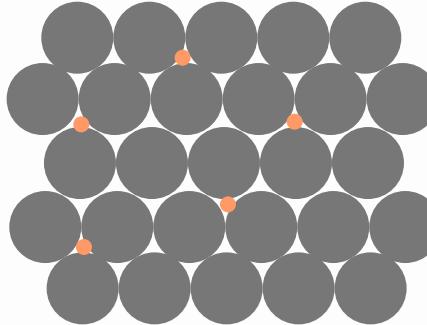
Two outcomes if impurity (B) added to host (A):

- Solid solution of B in A (i.e., random dist. of point defects)



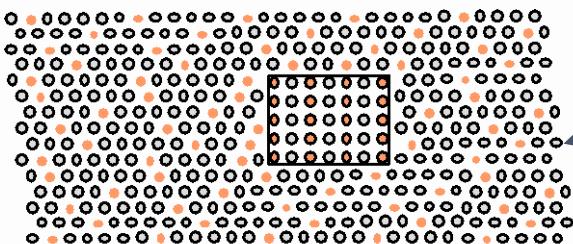
Substitutional solid soln.
(e.g., Cu in Ni)

OR

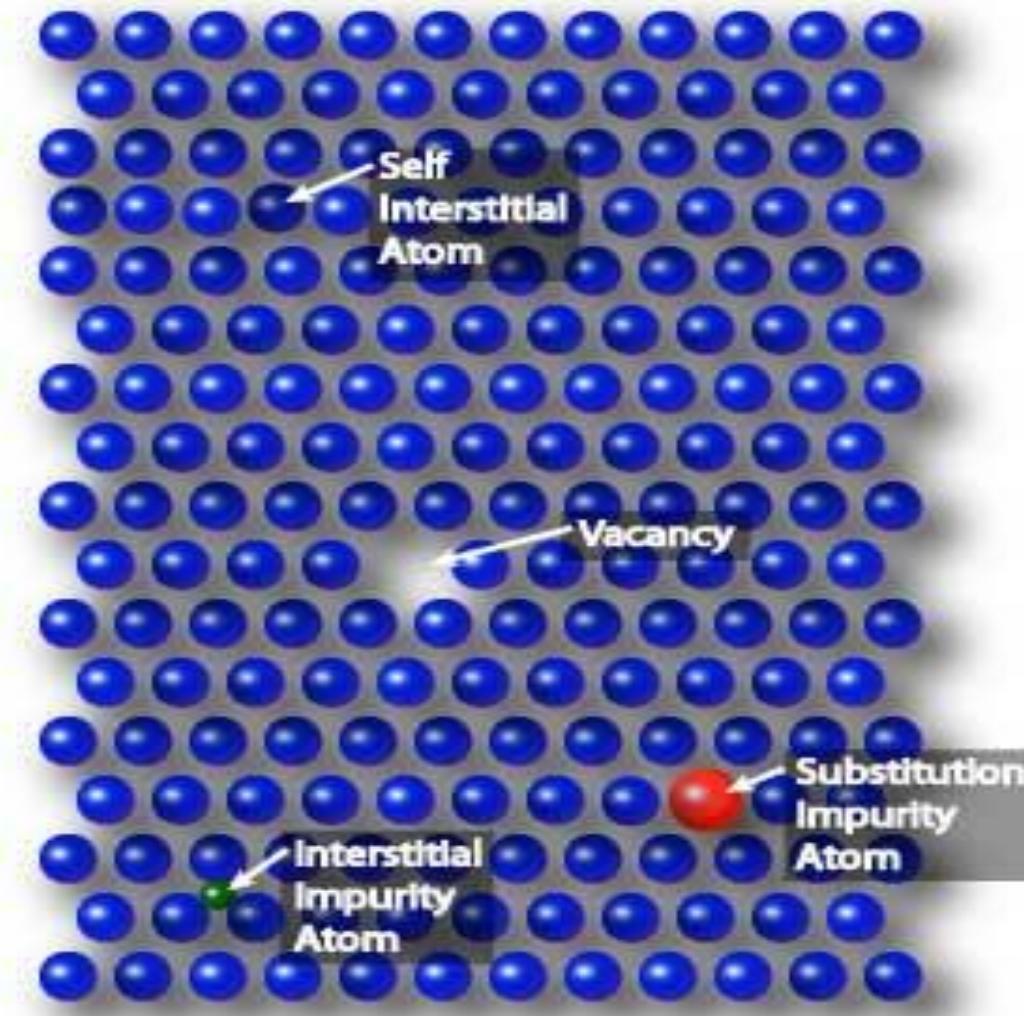


Interstitial solid soln.
(e.g., C in Fe)

- Solid solution of B in A plus particles of a new phase (usually for a larger amount of B)



Second phase particle
-- different composition
-- often different structure.



• Line Defects (Dislocations)

- Are one-dimensional defects around which atoms are misaligned
- slip between crystal planes result when dislocations move,
- produce permanent (plastic) deformation.

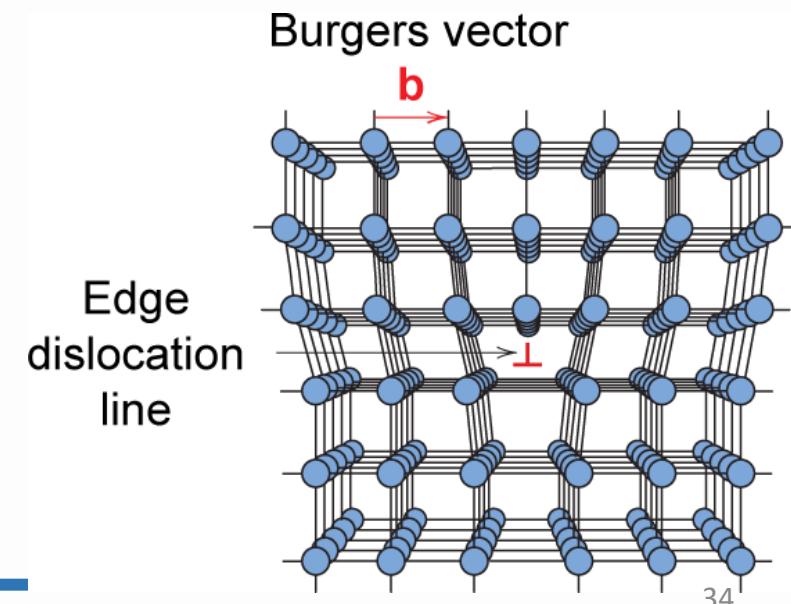
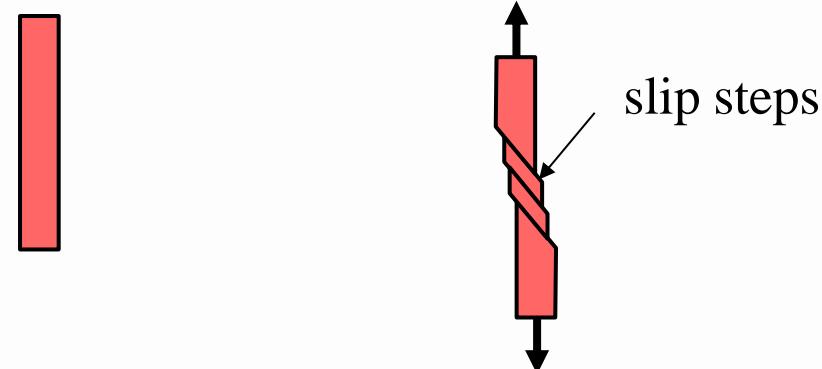
Edge dislocation: extra half-plane of atoms inserted in a crystal structure. **b** perpendicular (\perp) to dislocation line

- Edge dislocations are represented by ‘ \perp ’ or ‘T’ depending on whether the incomplete plane starts from the top or from the bottom of the crystal.
- These two configurations are referred to as positive and negative edge dislocations respectively.

Burger's vector, **b:** measure of lattice distortion

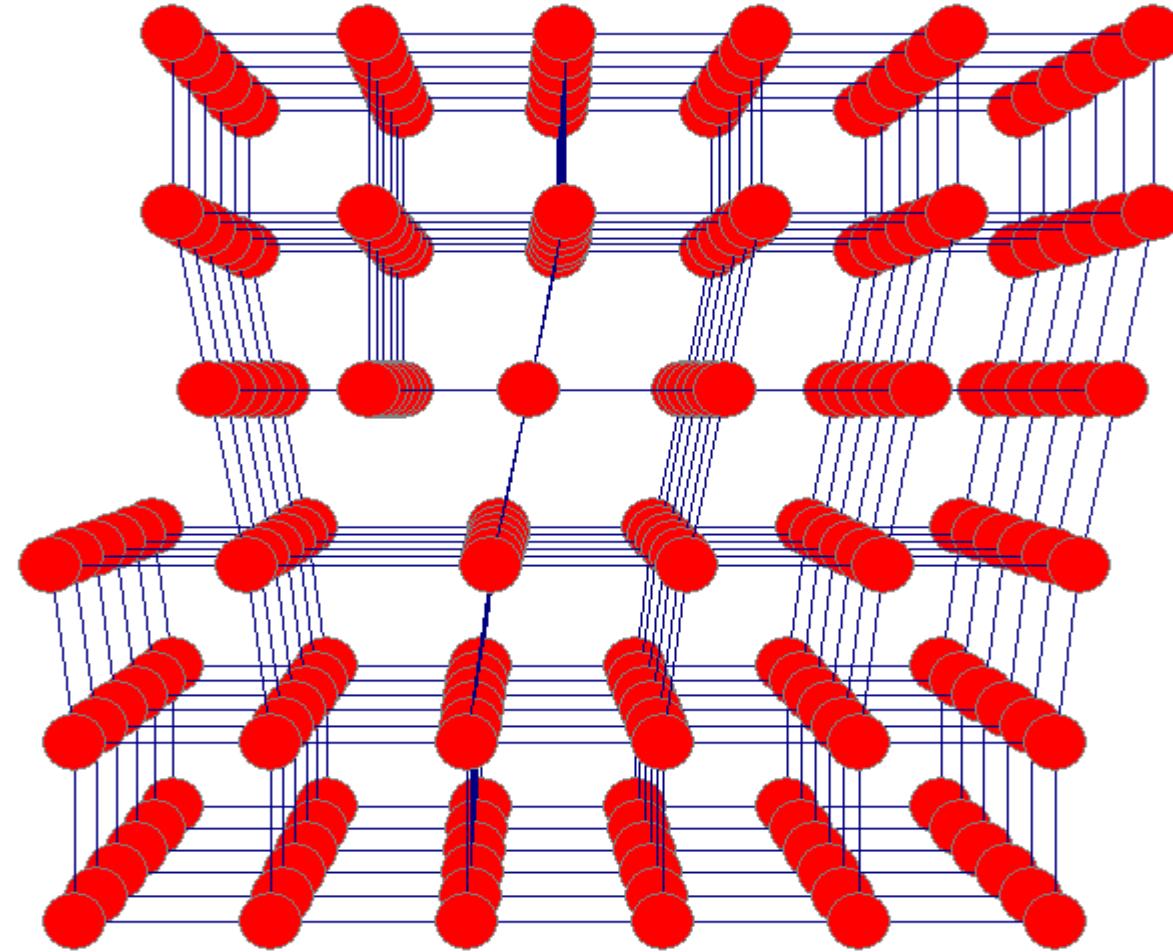
Schematic of Zinc (HCP):

- before deformation
- after tensile elongation



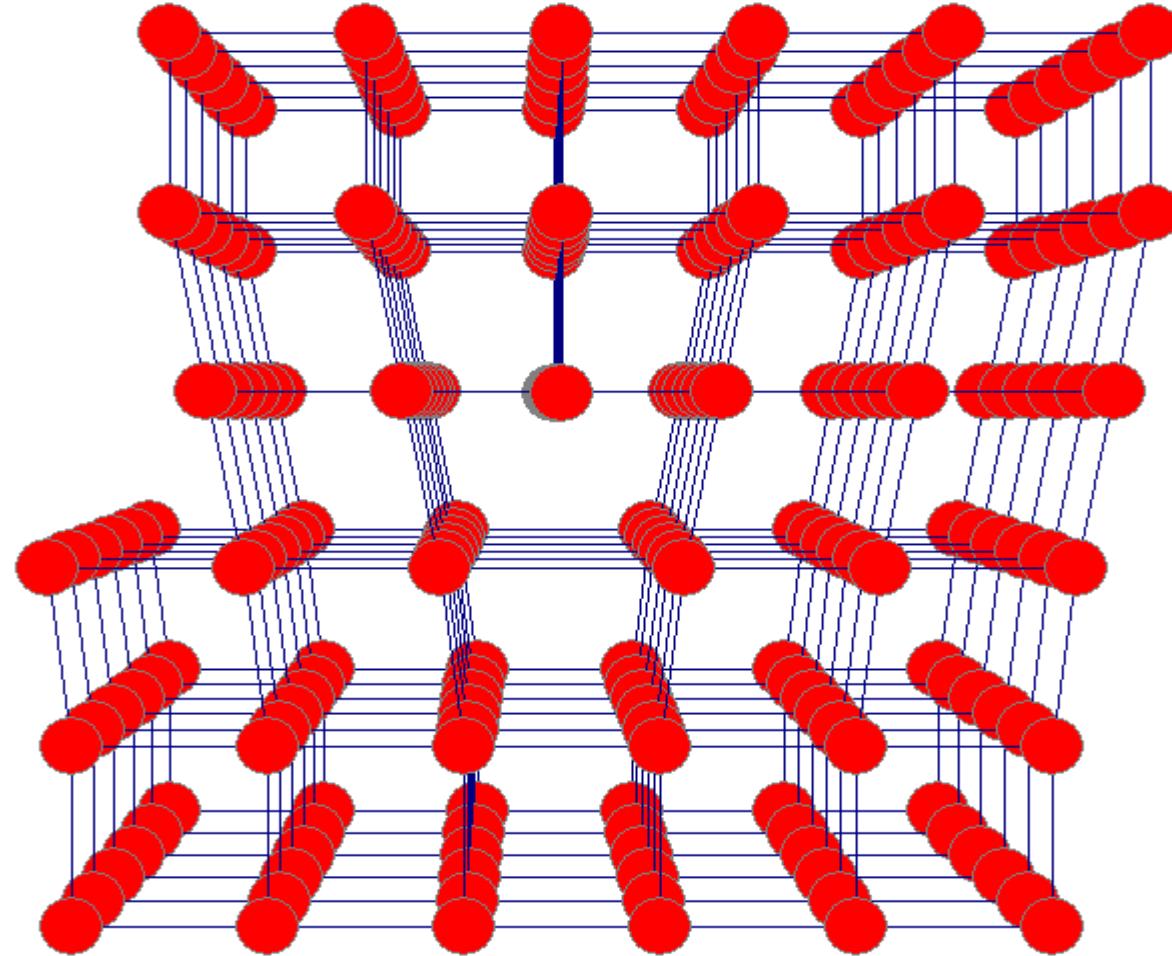
Edge dislocation

Go, change the world



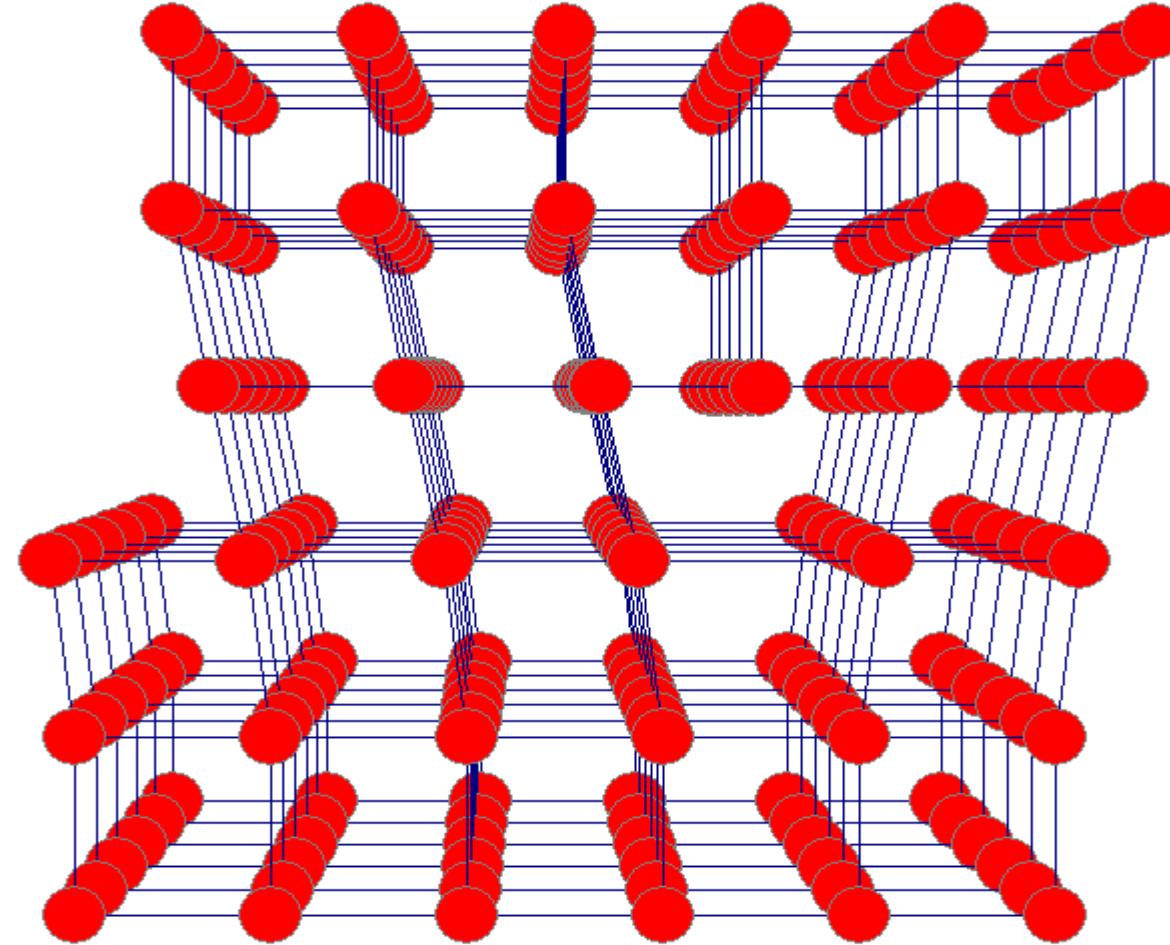
Edge dislocation

Go, change the world



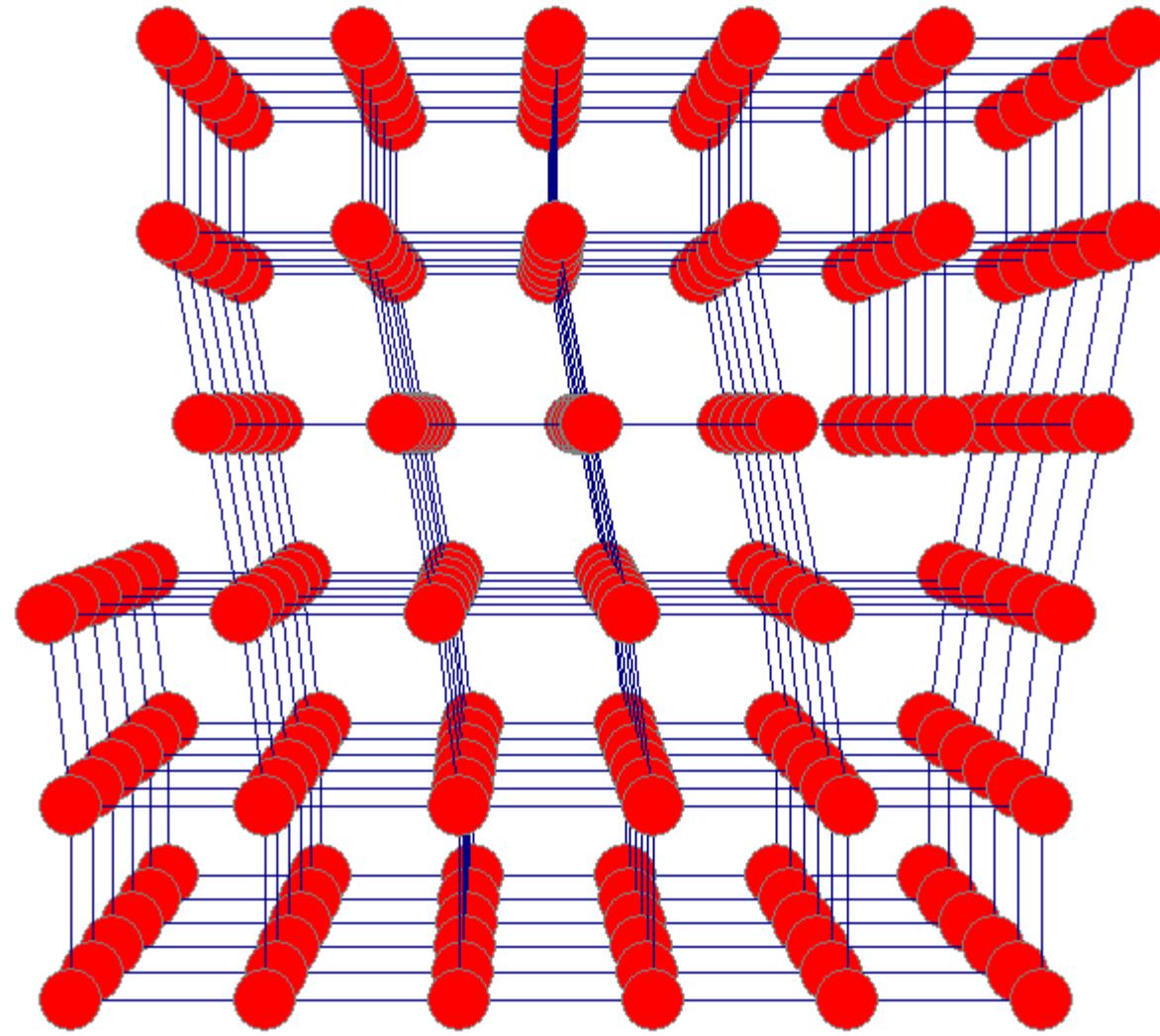
Edge dislocation

Go, change the world



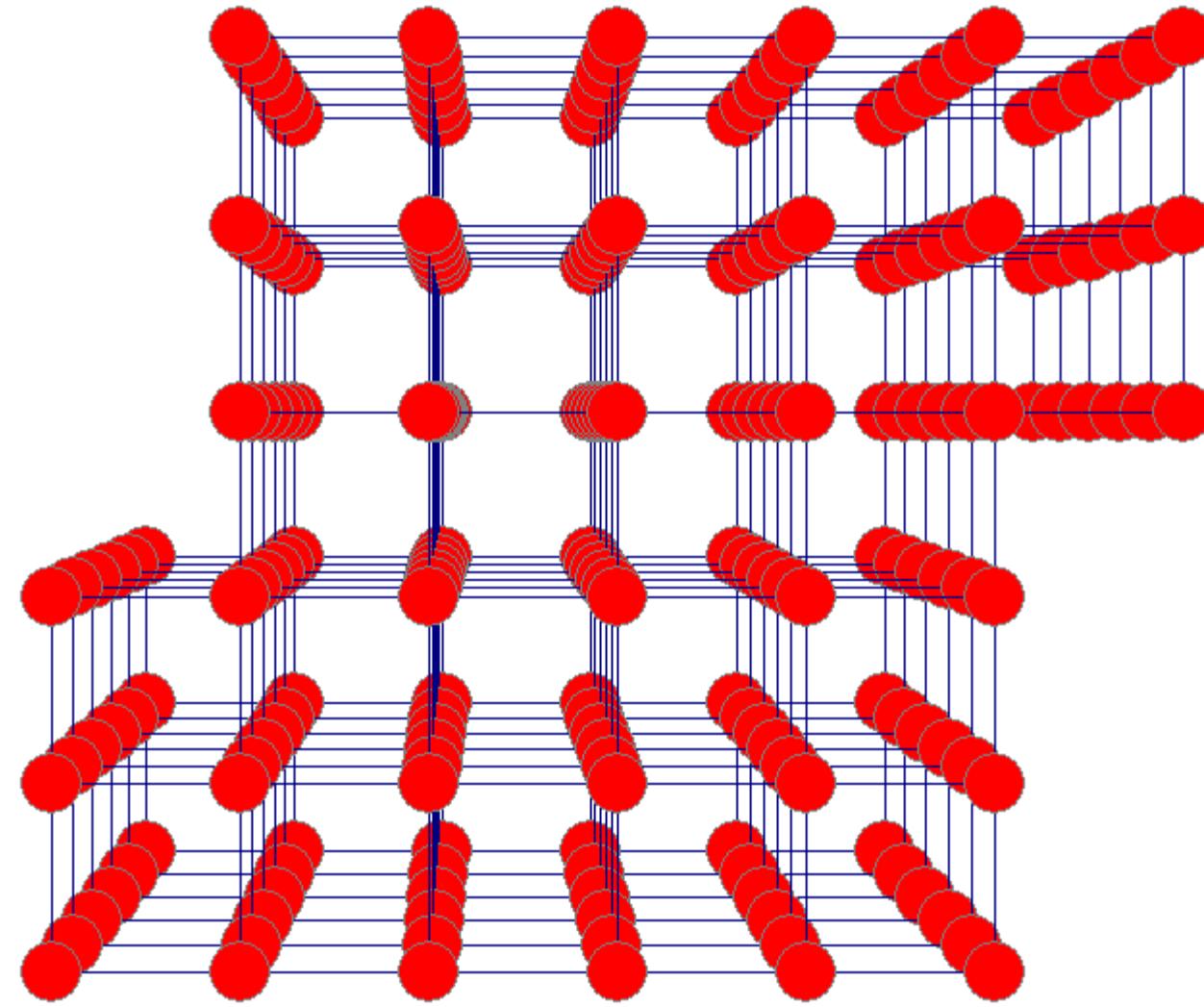
Edge dislocation

Go, change the world



Edge dislocation

Go, change the world



Movement of an Edge Dislocation

Go, change the world

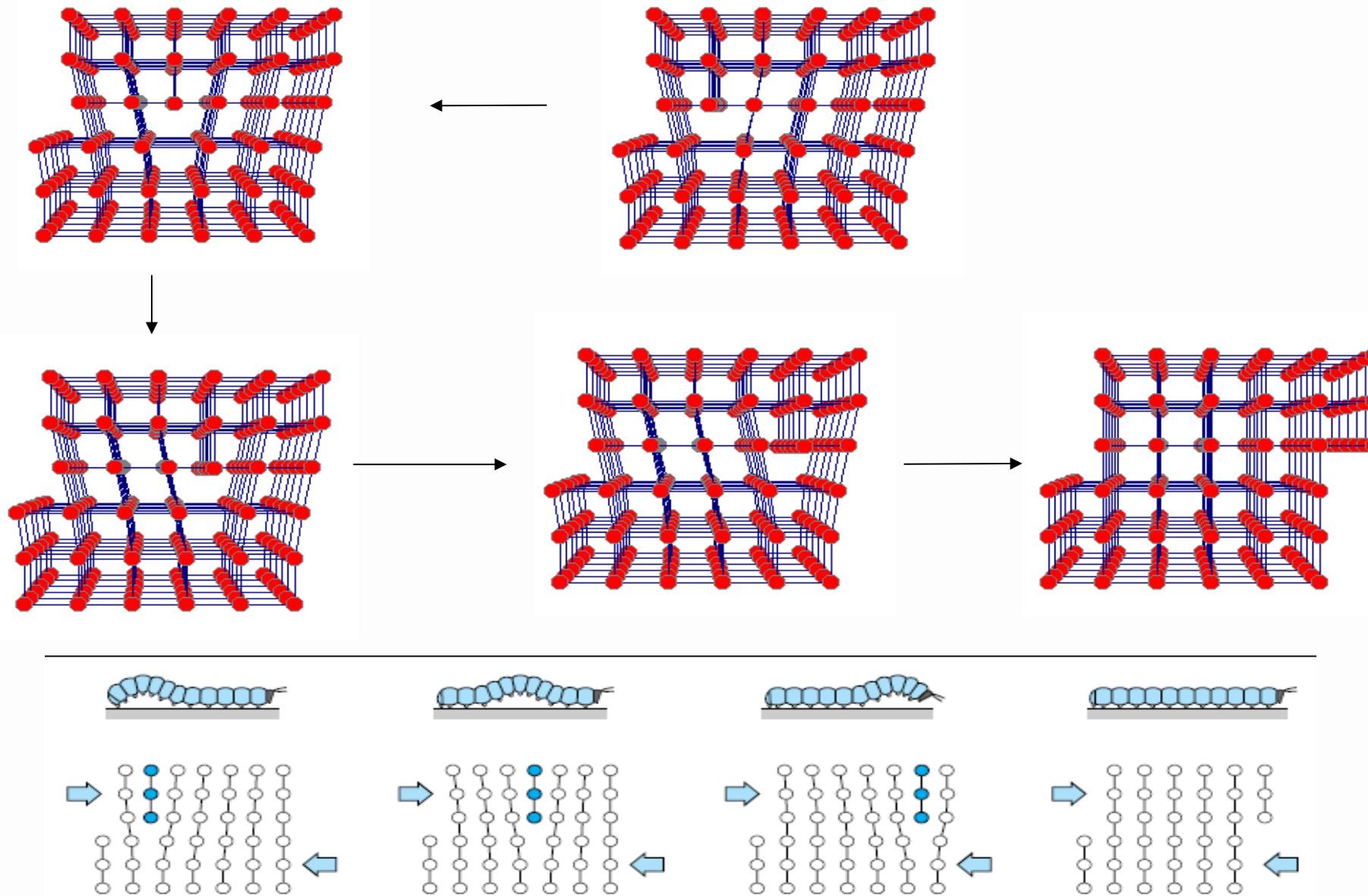
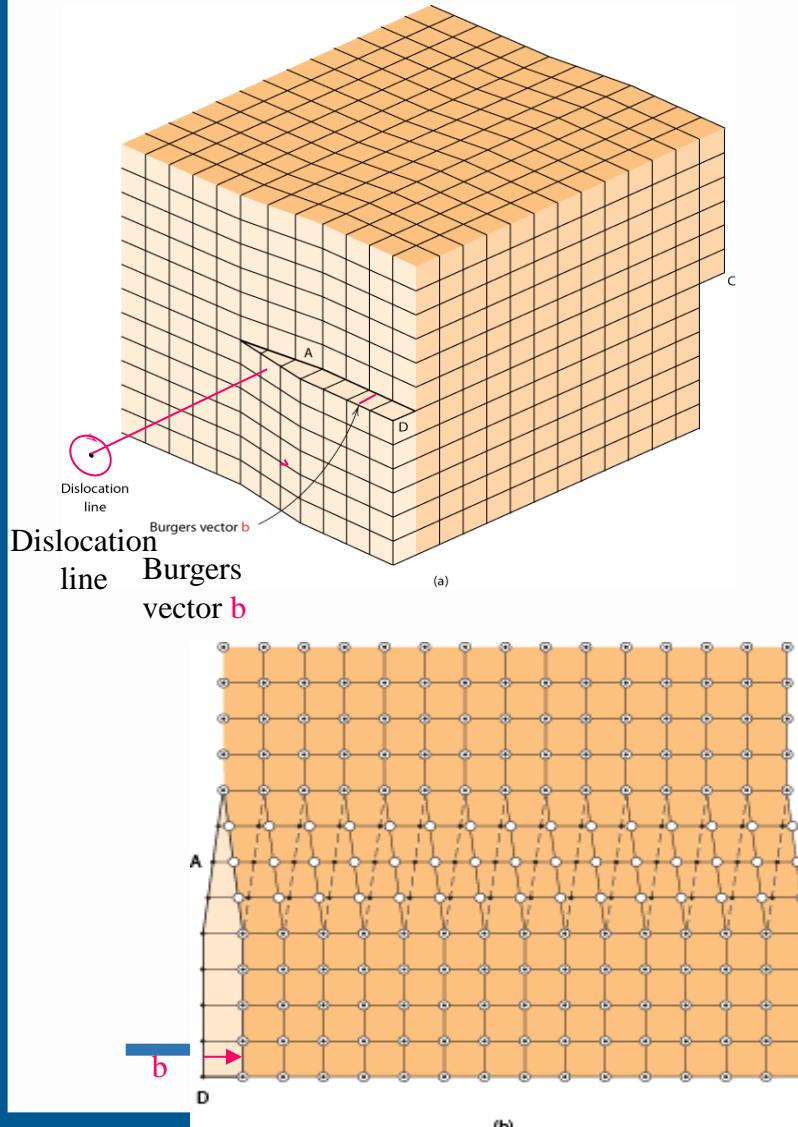


FIGURE 7.3 Representation of the analogy between caterpillar and dislocation motion.

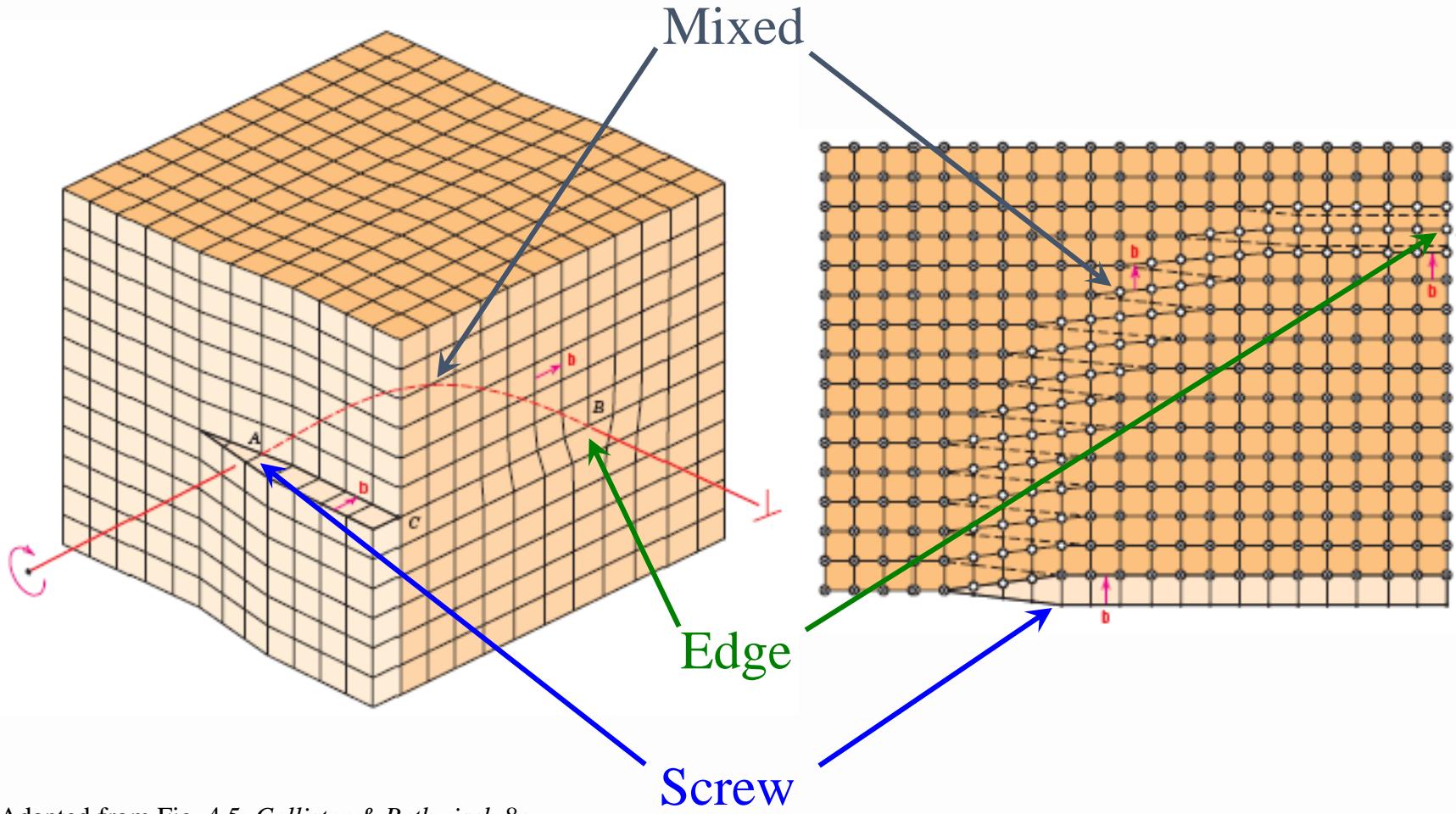
Screw Dislocation



- In this dislocation, the atoms are displaced in two separate planes perpendicular to each other.
- It forms a spiral ramp around the dislocation.
- The Burgers Vector is parallel to the screw dislocation line.
- Speed of movement of a screw dislocation is lesser compared to edge dislocation. Normally, the real dislocations in the crystals are the mixtures of edge and screw dislocation.

Edge, Screw, and Mixed Dislocations

Go, change the world



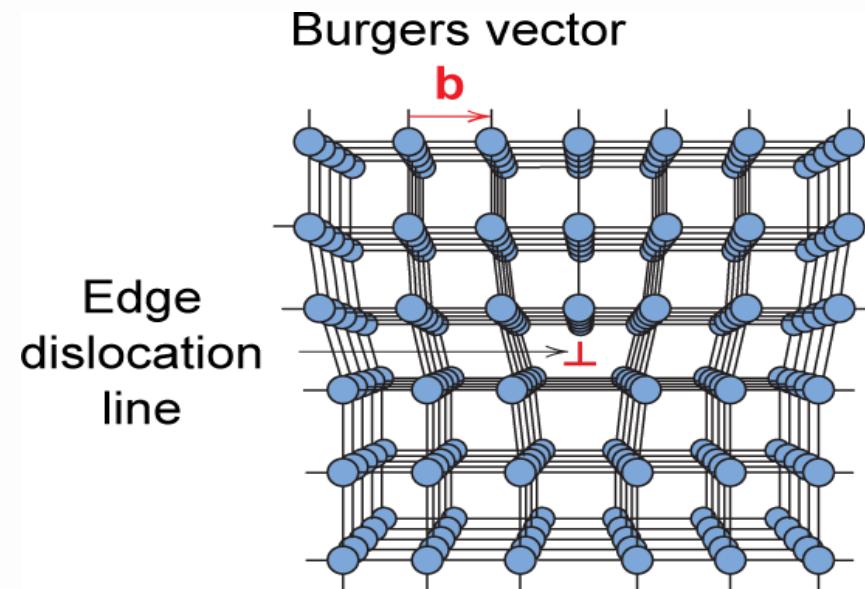
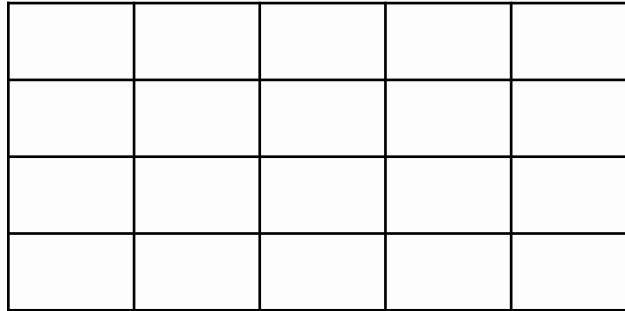
Adapted from Fig. 4.5, Callister & Rethwisch 8e.

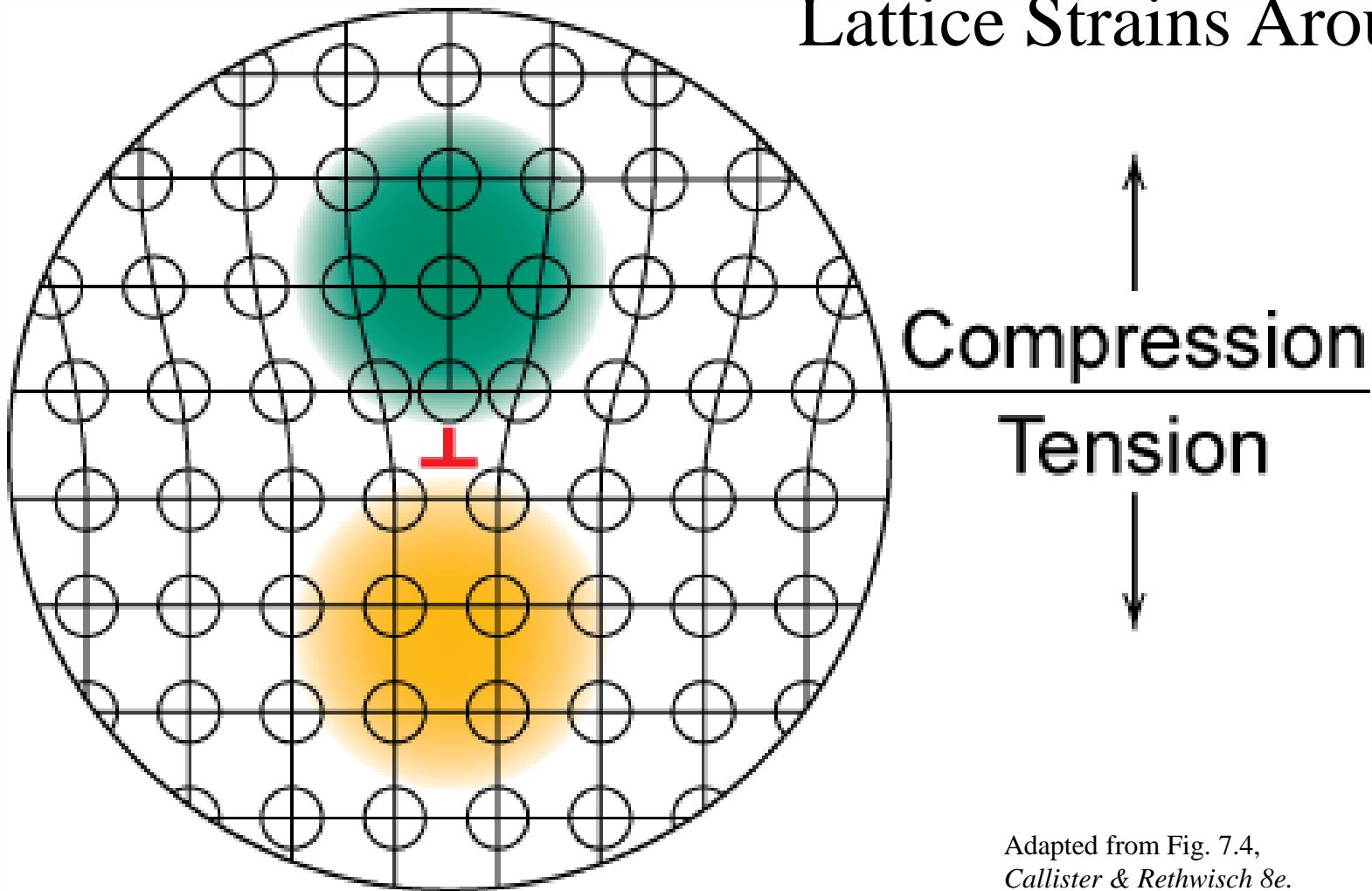
Comparison between edge & screw dislocations

Though both the edge and screw dislocations are line defects, they differ in many aspects. The main comparisons are listed below.

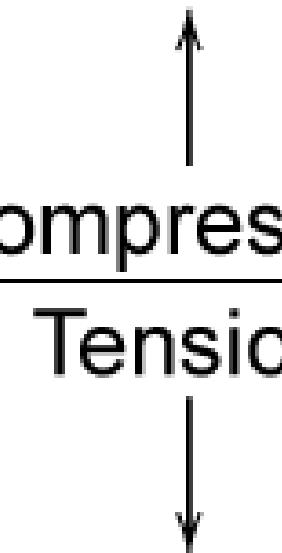
Edge dislocation	Screw dislocation
1. An edge dislocation is formed by the linear movement of a complete set of atomic planes, with the insertion of one extra half plane of atoms.	1. A screw dislocation is formed by the angular movement of a partial set of atomic planes on one side along a line.
2. The movement of the set of atoms occurs on a slip line that is perpendicular to the movement.	2. The movement of the set of atoms occurs along a line (dislocation line) that is parallel to the movement.
3. The Burger vector is <i>perpendicular</i> to the edge dislocation line.	3. The Burger vector is <i>parallel</i> to the screw dislocation line.
4. The displaced atomic planes are arranged in steps like a staircase manner.	4. The displaced atomic planes are arranged in a spiral staircase or screw manner.
5. Above the slip line with the extra half plane of atoms it has region of compressive strain, while the bottom part has a region of tensile strain.	5. Around the screw dislocation there is a region of shear strain (with stored energy).
6. An edge dislocation is denoted by the symbol " \perp ".	6. A screw dislocation is denoted by the symbol " \curvearrowleft ".

Dislocations play an important role in plastic deformation of crystalline solids. Their importance in plastic deformation is *relevant to their characteristic nature of motion* in specific directions (slip-directions) on specific planes (slip-planes), where edge dislocation move by *slip and climb* while screw dislocation can be moved by *slip and cross-slip*.



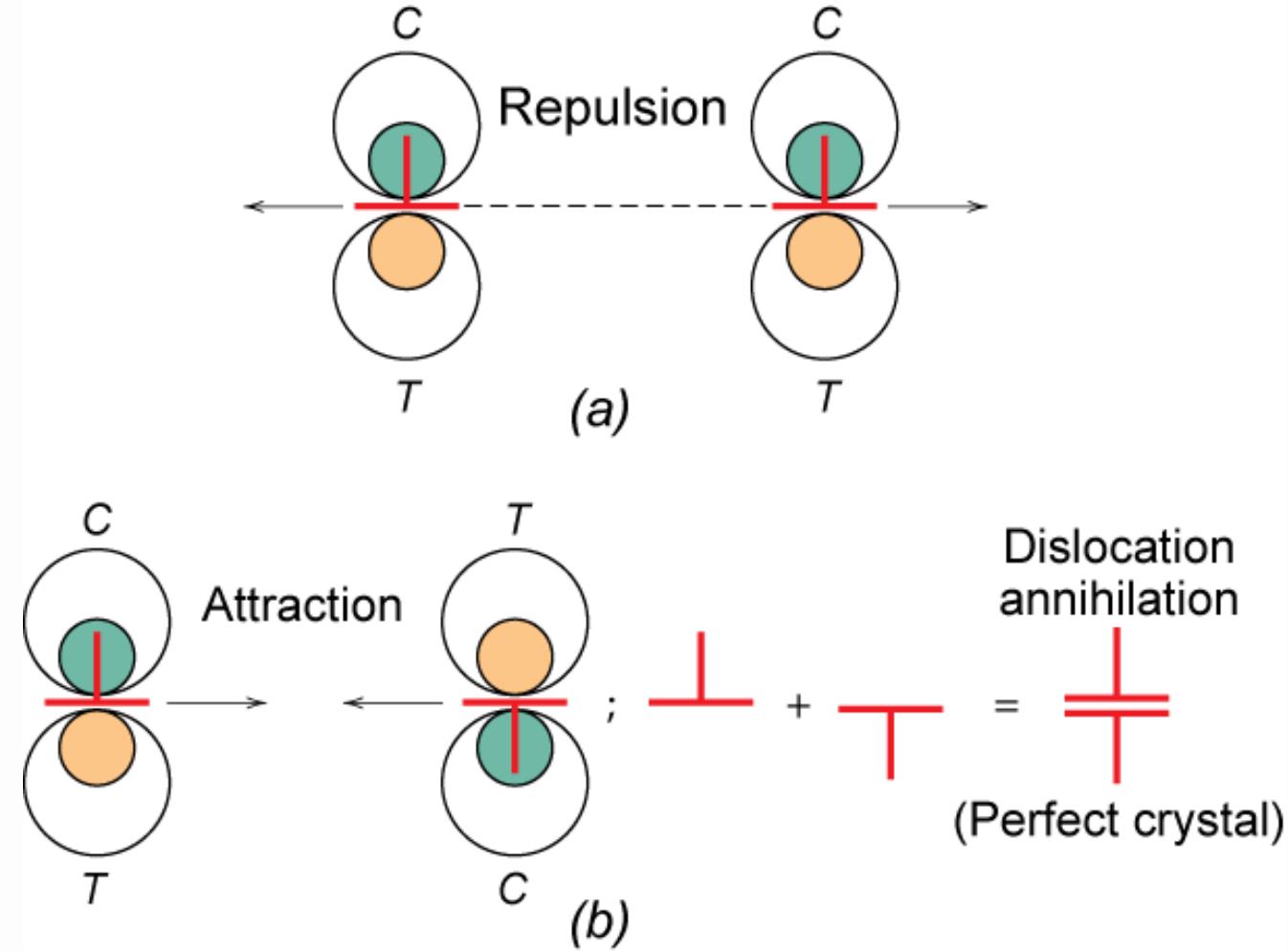


Lattice Strains Around Dislocations

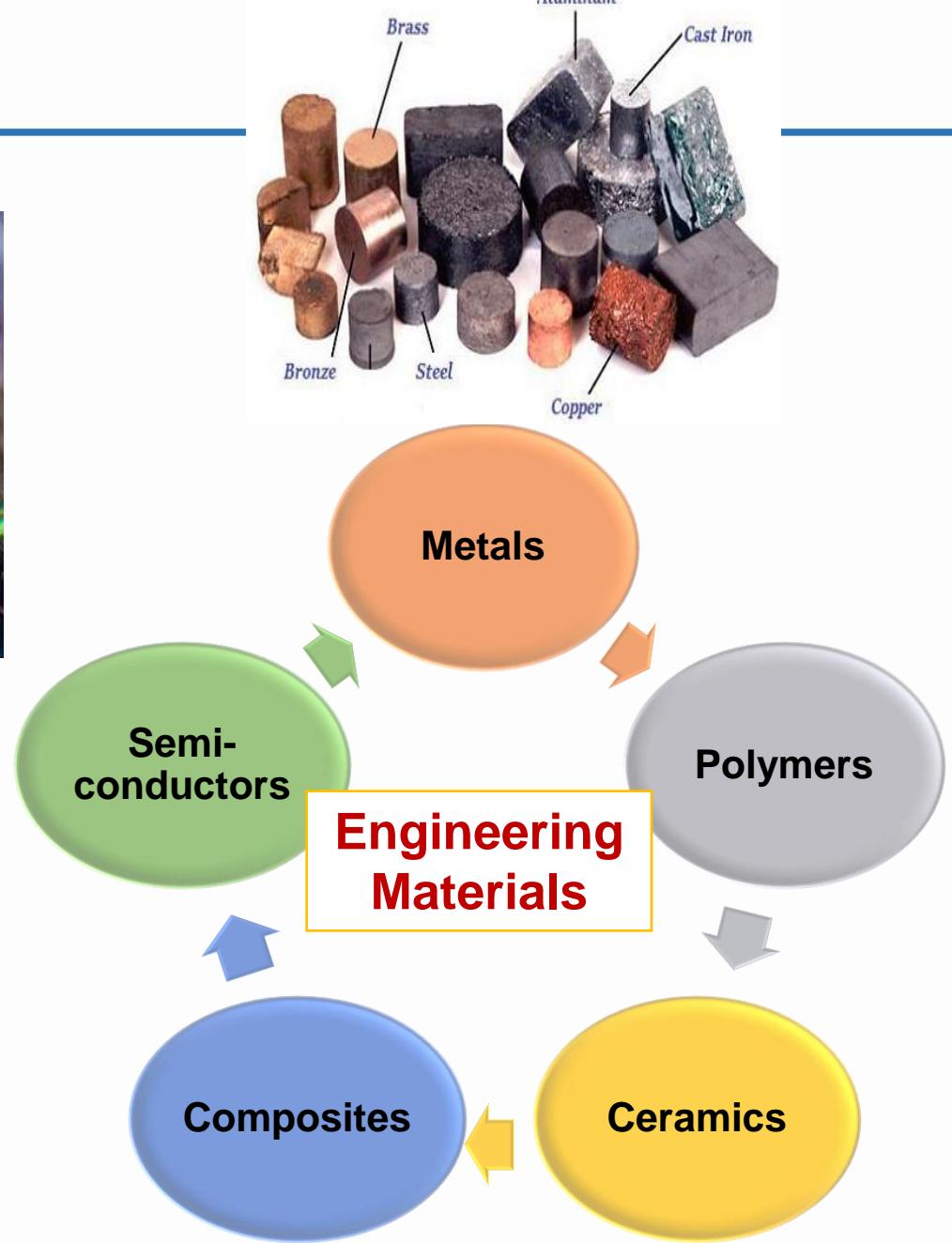
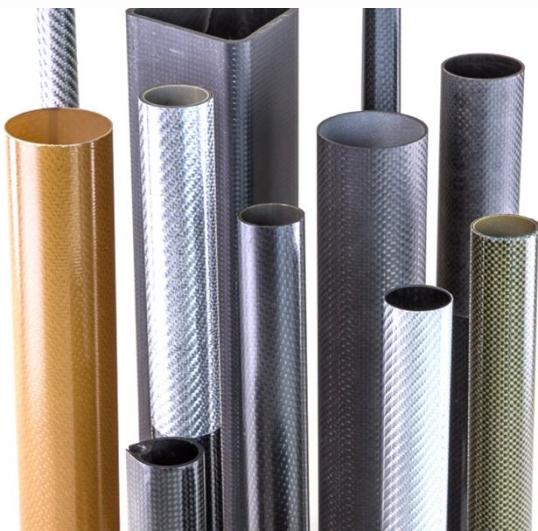
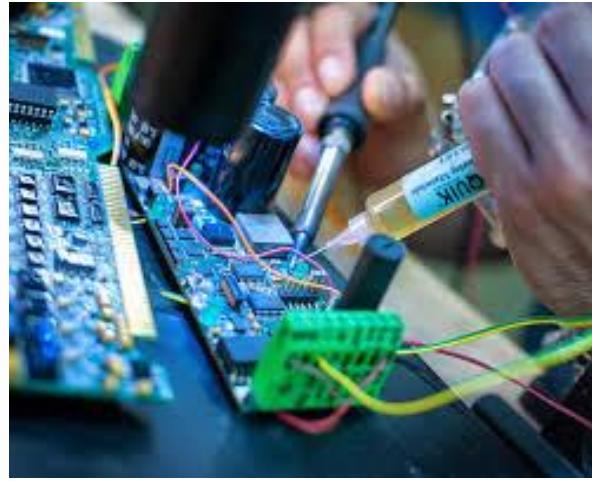


Adapted from Fig. 7.4,
Callister & Rethwisch 8e.

Lattice Strain Interactions Between Dislocations



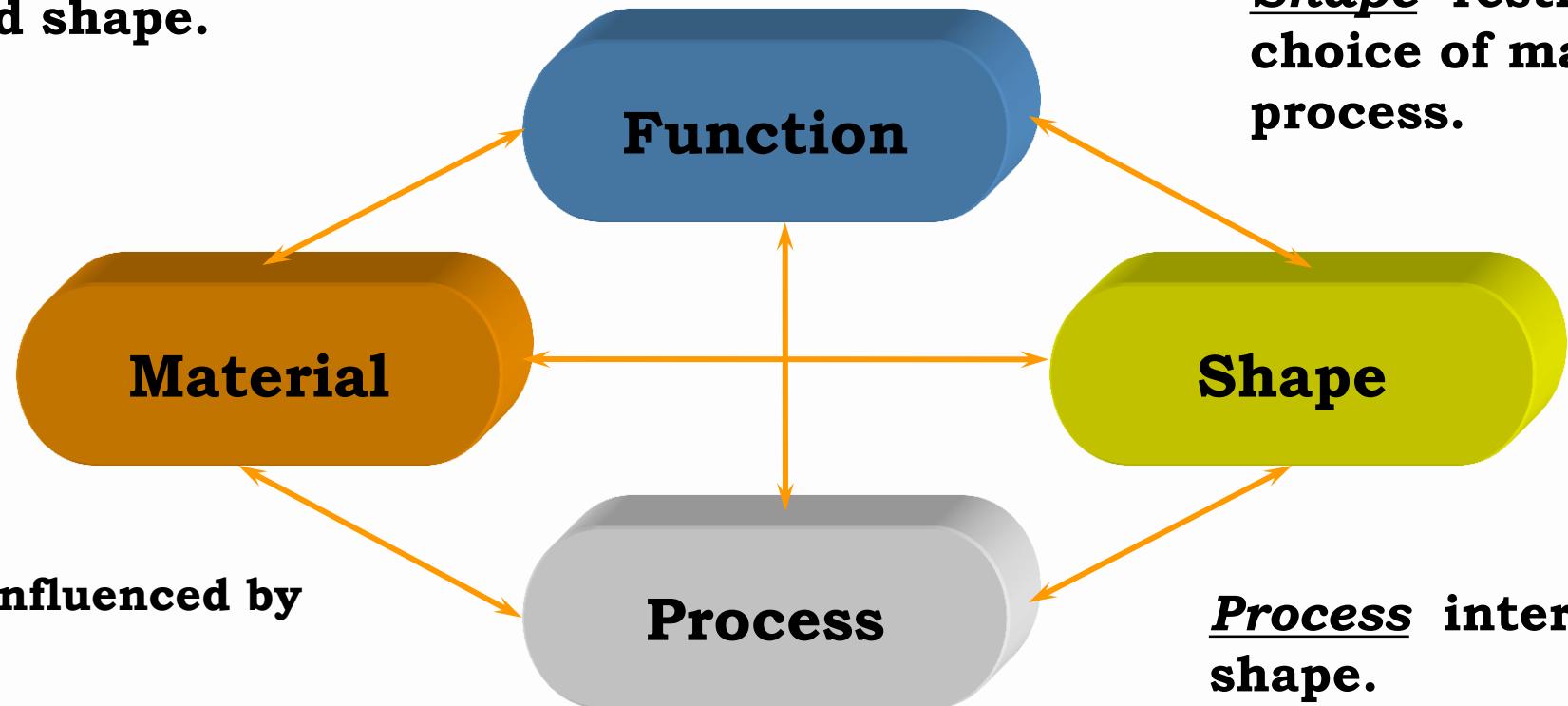
Adapted from Fig. 7.5,
Callister & Rethwisch
 8e.



8



Function dictates the choice of material and shape.



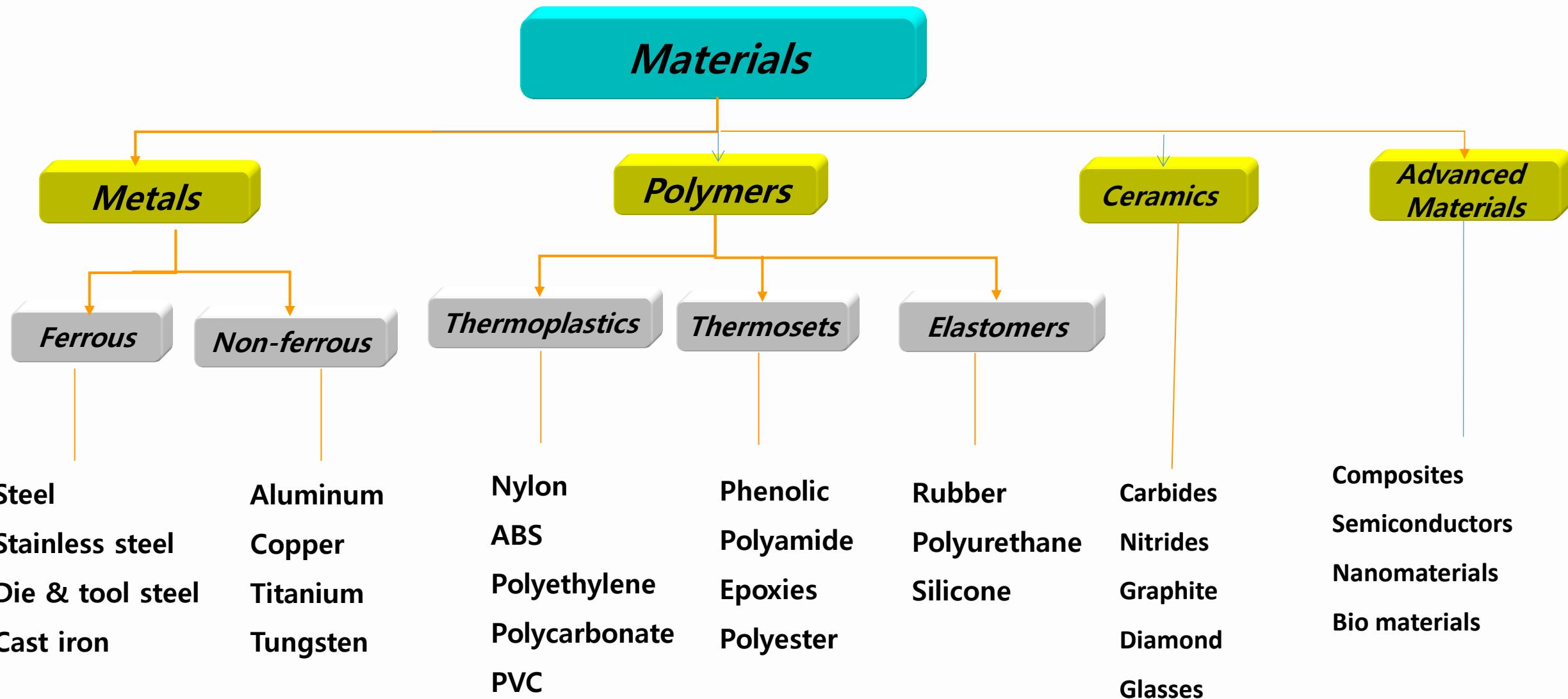
Shape restricts the choice of material and process.



Process is influenced by **material**

Process interacts with shape.

Material selection and process cannot be separated from the shape and the function of the product, two way interaction.



Classification of Engineering Materials



Thermoplastics



Nylon

ABS

Polyethylene

Polycarbonate

PVC



Polymers

Thermosets

Phenolic

Polyamide

Epoxy

Polyester



Elastomers



Rubber

Polyurethane

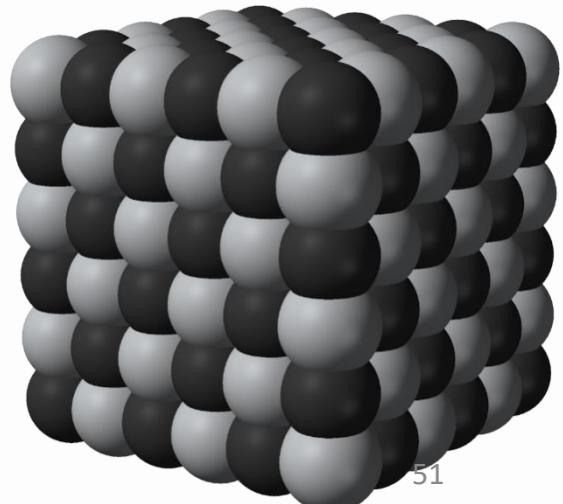
Silicone

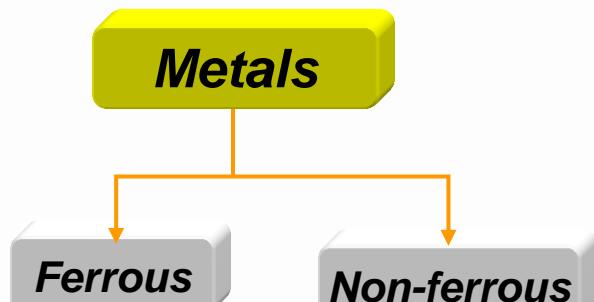


- A solid material which is typically hard, shiny, malleable, fusible, and ductile, with good electrical and thermal conductivity (e.g. iron, gold, silver, and aluminum, and alloys such as steel).



The atoms of metallic substances are closely positioned to neighboring atoms in one of two common arrangements.





Has iron as main constituent

Steel
Stainless steel
Die & tool steel
Cast iron

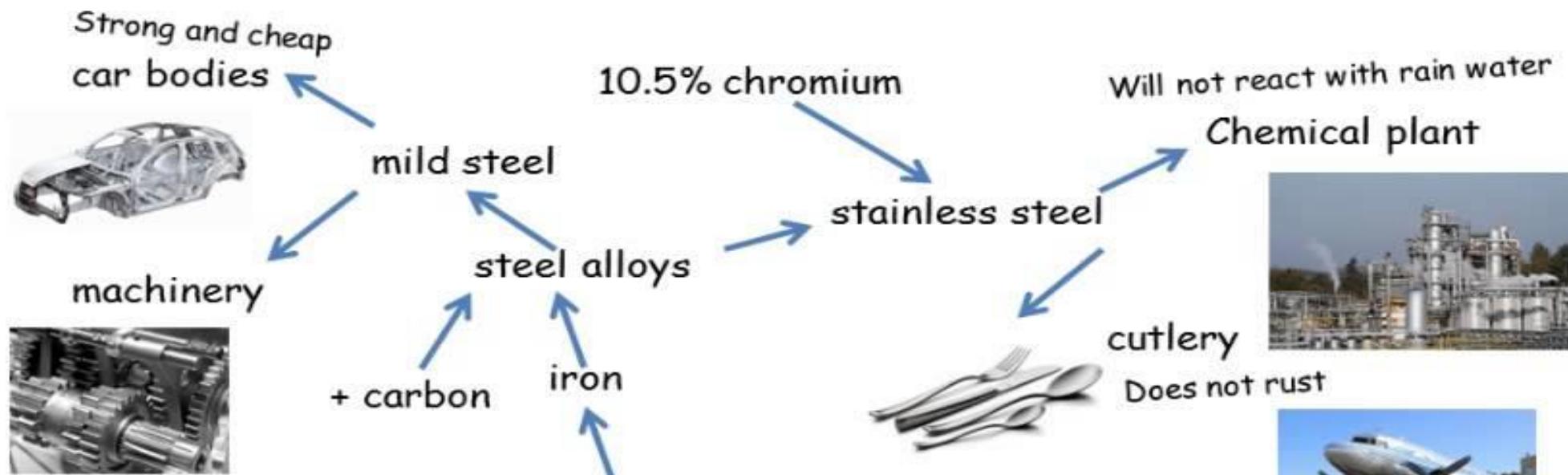
Does not have iron as Main constituent

Aluminum
Copper
Titanium
Tungsten

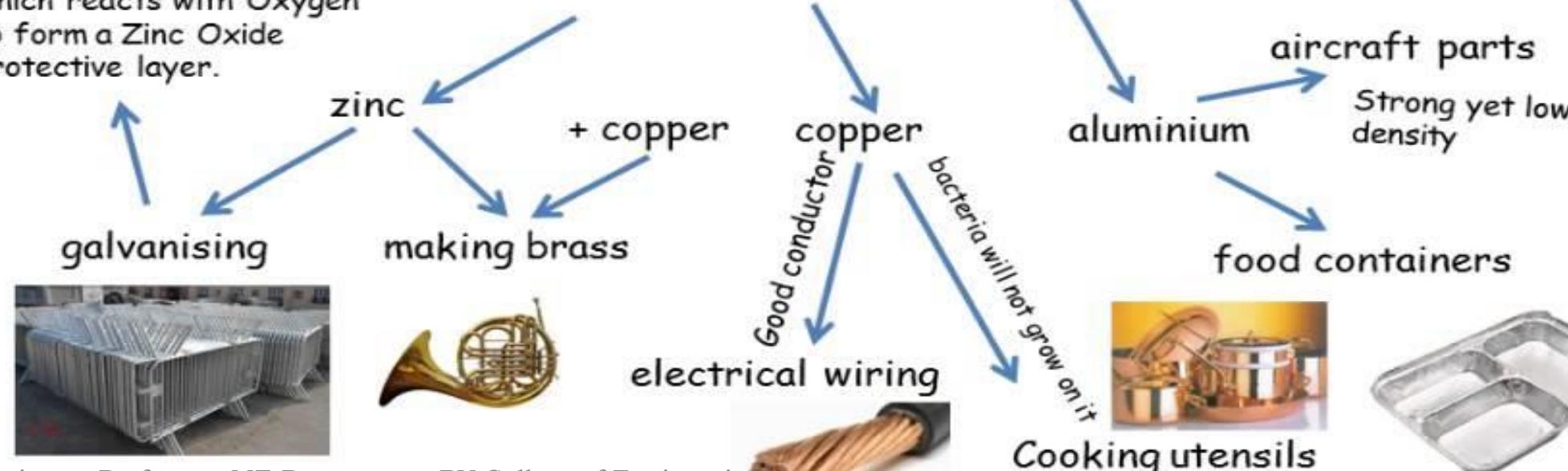


- Strong
- Malleable and ductile
- React with oxygen to form basic oxides
- Sonorous
- High melting and boiling points
- Good conductors of electricity
- Good conductors of heat
- Mainly solids at room temp. Exception mercury - liquid at room temp.
- Shiny when polished
- When they form ions, the ions are positive
- High density

- They are made into jewelry due to their hard and shiny appearance.
- They are used to make pans, since they are good conductors of heat.
- They are used in electrical cables, because they are malleable, ductile and good conductors of electricity.
- They are strong so used to build scaffolding and bridges.
- They make a ringing sound, sonorous, hence their use in bell making.



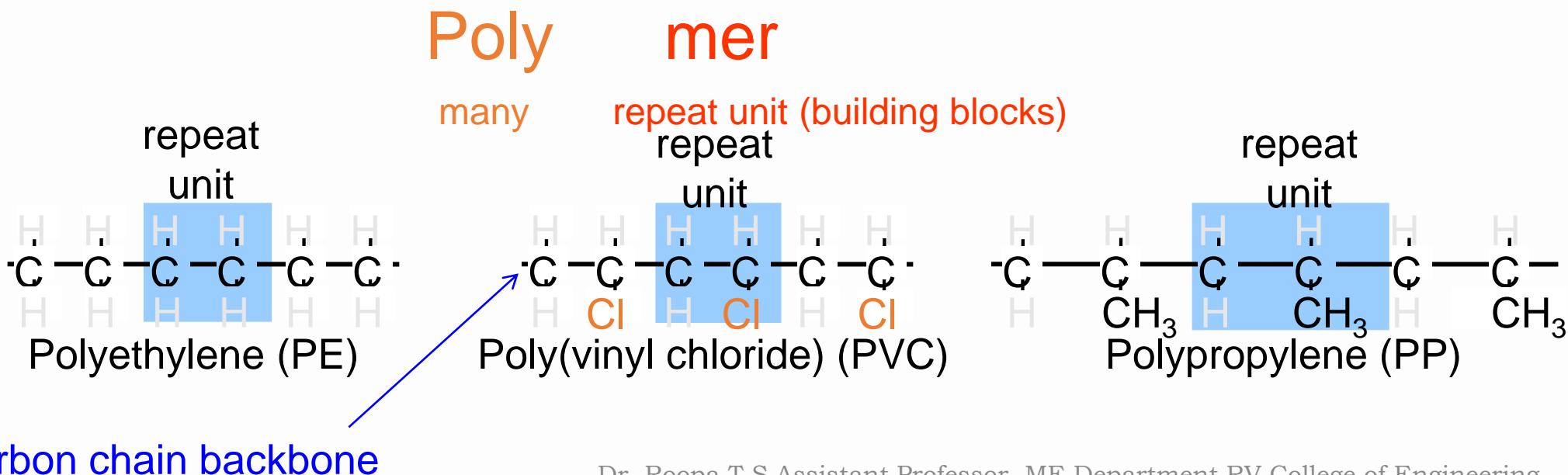
Coating Iron with Zinc which reacts with Oxygen to form a Zinc Oxide protective layer.



A compound of high molecular weight derived either by the addition of any smaller molecules, as polyethylene, or by the condensation of many smaller molecules with the elimination of water, alcohol, or the like, as nylon.

- **Natural polymers:** amber, wool, silk and natural rubber have been used for centuries.
- **Synthetic polymers:** includes synthetic rubber, phenol formaldehyde resin (or Bakelite) neoprene, nylon, polyvinyl chloride, polystyrene, polyethylene, silicone.

- A compound consisting of long-chain molecules, each molecule made up of repeating units connected together
- There may be thousands, even millions of units in a single polymer molecule
- The word polymer is derived from the Greek words **poly**, meaning **many**, and **meros** (reduced to mer), meaning **part**
- Most polymers are based on **carbon** and are therefore considered organic chemicals



- **Polymers can be separated into plastics and rubbers**
- As engineering materials, it is appropriate to divide them into the following three categories:
 1. Thermoplastic polymers
 2. Thermosetting polymers
 3. Elastomers

where (1) and (2) are plastics and (3) are rubbers

1. **Polymers have long chain structures.** The individual molecule of a polymer is very large, i.e., it may consist of thousands of similar small molecules, all bonded together covalently
2. **All polymers have one thing common, i.e., carbon,** which further bonds with hydrogen, nitrogen, halogens or other organic or inorganic substances
3. **Although, polymer's structure may be crystalline in simple materials but generally they are non-crystalline solids at room temperatures.** No doubt, polymers pass through a viscous stage during formation
4. **Polymers have light weight** and they can be easily fabricated and shaped.
5. **They are poor conductors of electricity** and their thermal conductivity is also low.
6. Moreover, **the polymers are resistant to chemical attack and decay**

Polymers

- ❖ Can be very resistant to chemicals.
- ❖ Can be both thermal and electrical insulators.
- ❖ Generally, polymers are very light in weight with significant degrees of strength.
- ❖ Can be processed in various ways.
- ❖ Are materials with a seemingly limitless range of characteristics and colors.
- ❖ Are usually made of petroleum, but not always.
- ❖ Can be used to make items that have no alternatives from other materials.

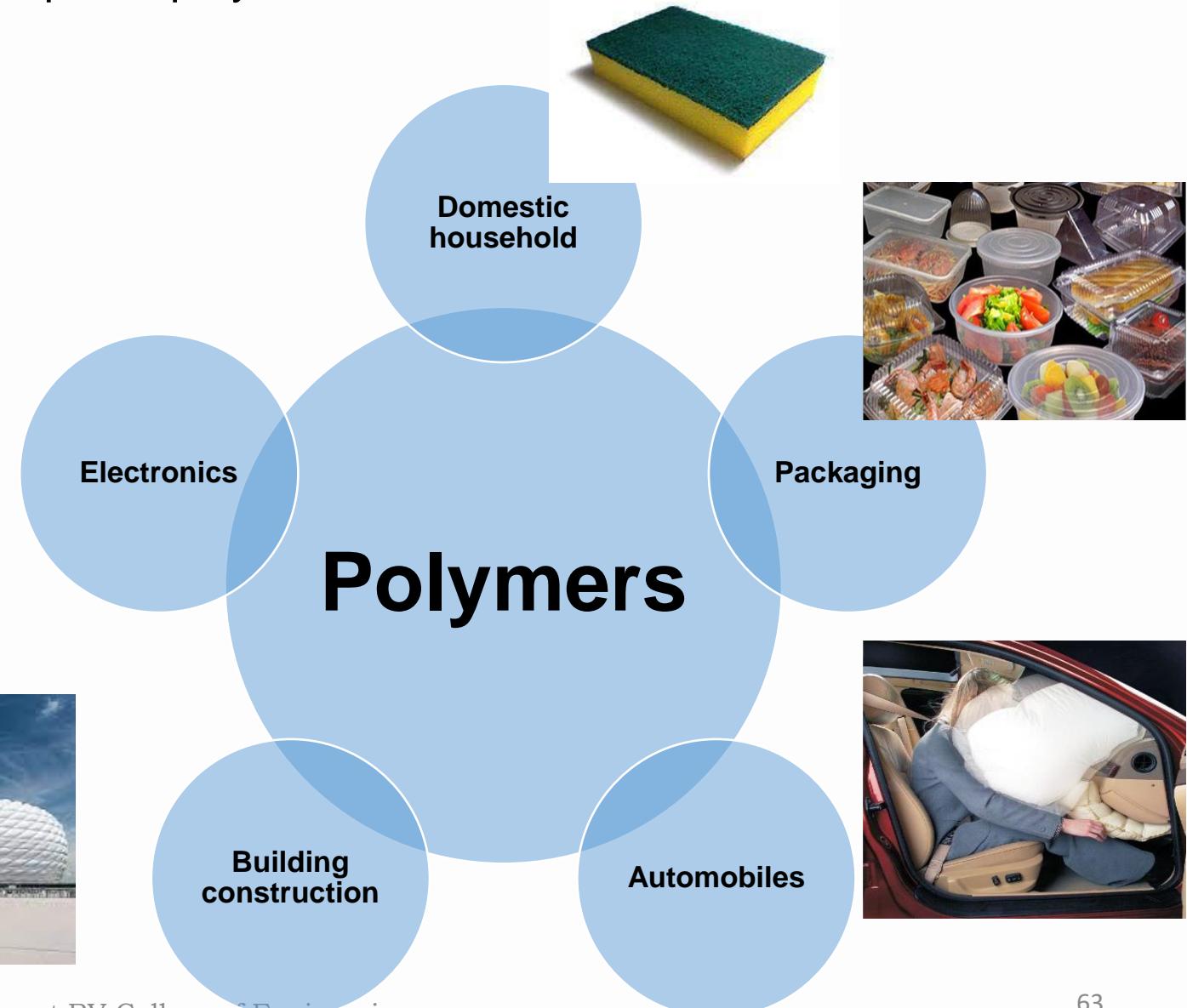
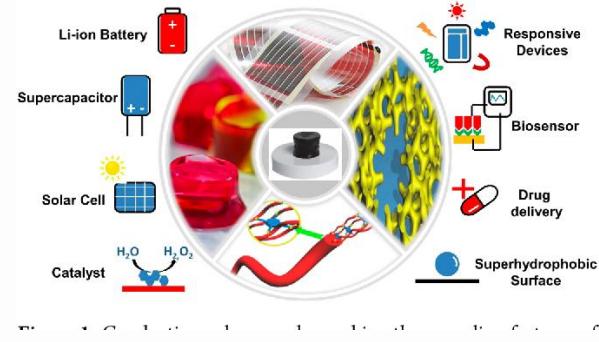
Sl No.	Thermosetting Plastics	Thermoplastics
1	Three dimensional network of primary covalent bonds with cross linking between chains	Linear polymers without cross linking and branching
2	Upon heating they retain their strength and prolonged heating causes roasting of polymers and ultimately depolymerisation	Upon heating the secondary bonds between individual chains break, the polymers become soft and on cooling hard and rigid because secondary bonds re-establish themselves
3	Harder, stronger and more brittle	strong and less brittle
5	It is difficult to fill an intricate mold with such plastics	They can fill the complicated mold quite easily
6	can not be recycled	can be recycled
7	Ex: polyesters, silicones, Bakelite etc.	PVC, Nylons, polyethylene
8	Applications: manufacture of telephones, electrical outlets, appliance handles etc.	Applications: Plastic walls, floor tiles, reflectors, plastic lenses etc.

- Polymers capable of large elastic deformation when subjected to relatively low stresses
- Some can be extended 500% or more and still return to their original shape
- **Two categories:**
 1. **Natural rubber** - derived from biological plants
 2. **Synthetic polymers** - produced by polymerization
- processes similar to those used for thermoplastic and thermosetting polymers

Characteristics of Elastomers

- **Elastomers consist of long-chain molecules that are cross-linked (like thermosetting polymers)**
- They owe their impressive elastic properties to two features:
 1. Molecules are tightly linked when unstretched
 2. Degree of cross-linking is substantially less than Thermosets

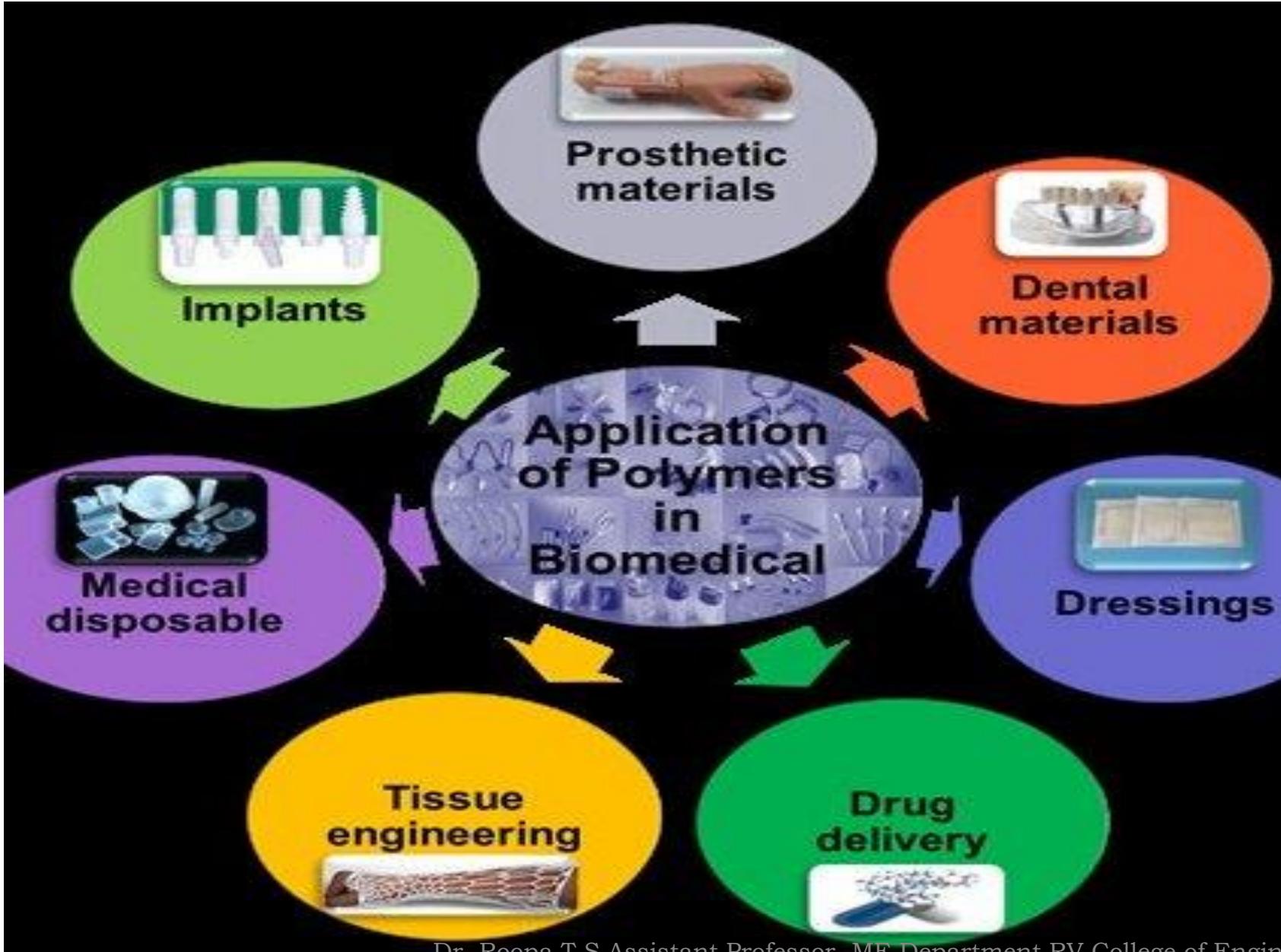
- ❖ While plastics are used as a common example of polymers, there are many other materials which are also polymers.
- ❖ Proteins, such as hair, nails, tortoise shell
- ❖ Cellulose in paper and trees
- ❖ DNA
- ❖ Rubber



Applications of Polymers

Go, change the world





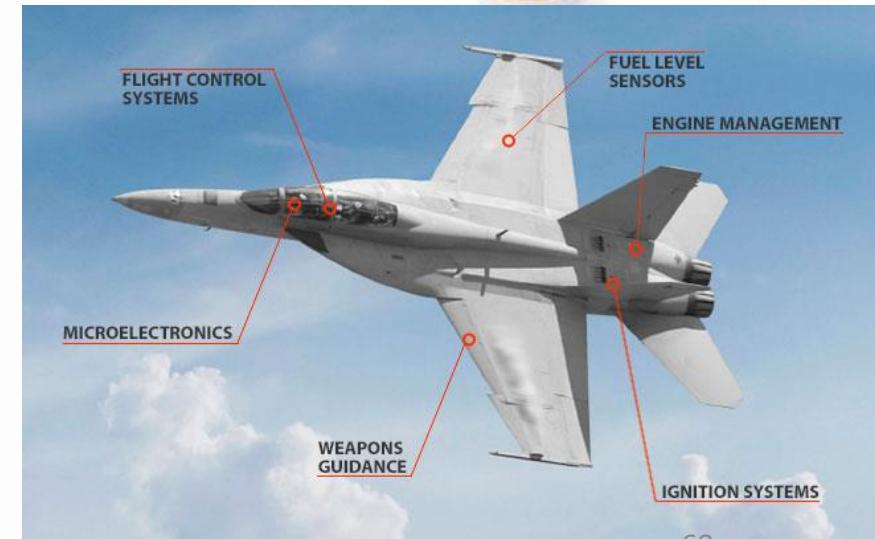
- Ceramic materials are inorganic, non-metallic materials made from compounds of a metal and a non metal. They are formed by the action of heat and subsequent cooling.
 - Are of 2 types : Crystalline & Non-crystalline-glass
- ▶ Some ceramics are semiconductors. Most of these are transition metal oxides that are II-VI semiconductors, such as zinc oxide.
- ▶ Under some conditions, such as extremely low temperature, some ceramics exhibit high temperature superconductivity.

- ❖ Hard, Brittle
- ❖ Wear-resistant
- ❖ Refractory
- ❖ Thermal and Electrical Insulators
- ❖ Nonmagnetic
- ❖ Oxidation Resistant
- ❖ Prone To Thermal Shock And
- ❖ Chemically Stable

Applications of Ceramics

Go, change the world

- **Aerospace:** space shuttle tiles, thermal barriers, high temperature glass windows, fuel cells
- **Consumer Uses:** glassware, windows, pottery, Corning™ ware, magnets, dinnerware, ceramic tiles, lenses, home electronics, microwave transducers
- **Automotive:** catalytic converters, ceramic filters, airbag sensors, ceramic rotors, valves, spark plugs,
- **Medical (Bio ceramics):** orthopedic joint replacement, prosthesis, dental restoration, bone implants
- **Military:** structural components for ground, air and naval vehicles, missiles, sensors
- **Computers:** insulators, resistors, superconductors, capacitors, ferroelectric components, microelectronic packaging
- **Other Industries:** bricks, cement, membranes and filters, lab equipment
- **Communications:** fiber optic/laser communications, TV and radio components, microphones



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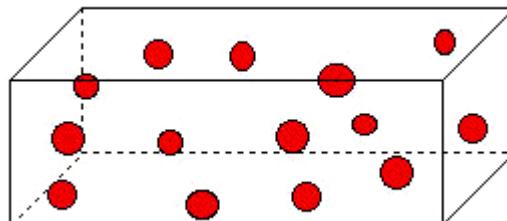
- **Composite materials** are **materials** made from two or more **constituent materials** with significantly different physical or chemical properties, that when combined, produce a **material** with characteristics different from the individual components

Typical engineered composite materials include:

- Composite building materials such as cements, concrete
- Reinforced plastics such as fiber-reinforced polymer
- Metal Composites

Particulate composite

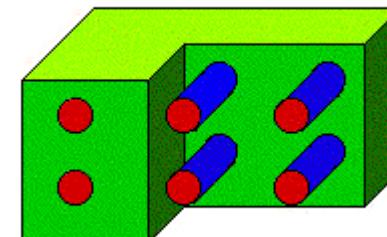
materials contain a large number of randomly oriented particles. Ex: ceramic particles dispersed in a metallic matrix.



Fiber-reinforced composites

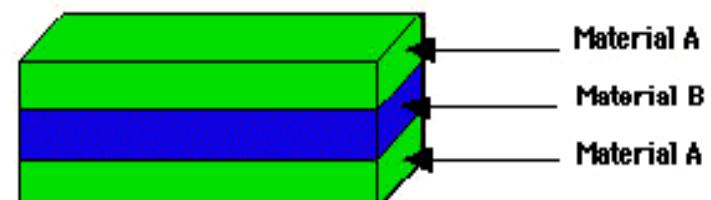
are composed of strong and stiff brittle fibers which are incorporated into a

matrix.

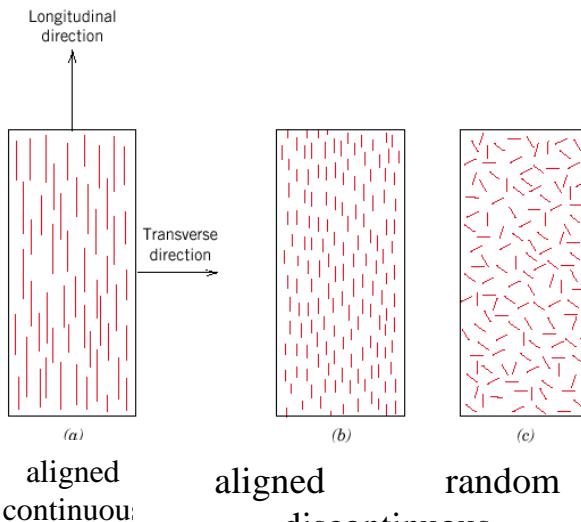
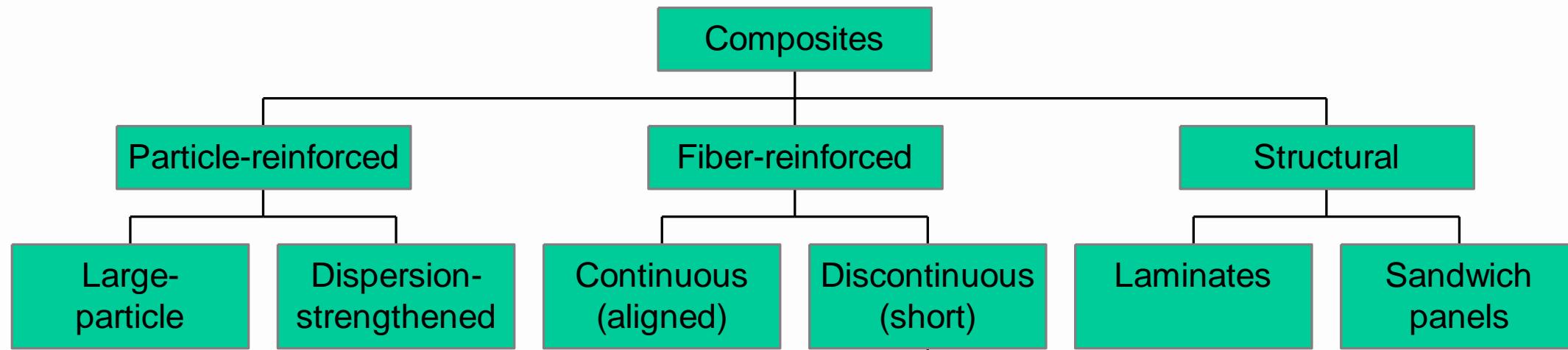


Laminar composites

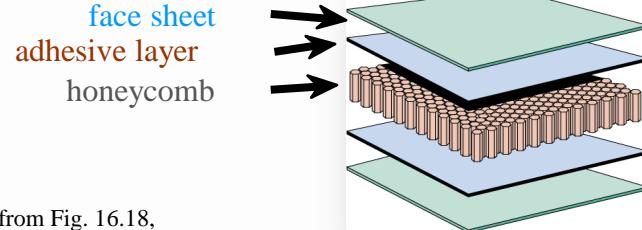
are Composed of layers of different materials, called laminates



Classification - Based on type of reinforcement



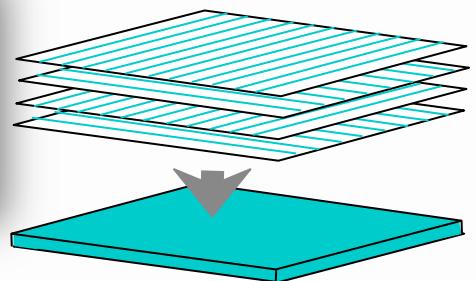
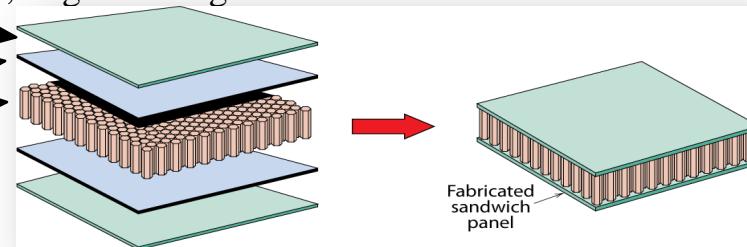
- **Sandwich panels**
 - low density, honeycomb core
 - benefit: light weight, large bending stiffness



Adapted from Fig. 16.18,
Callister 7e. (Fig. 16.18 is
from *Engineered Materials*
Handbook, Vol. 1, *Composites*, ASM International, Materials Park, OH, 1987.)

Laminate

- Stacked and bonded fiber-reinforced sheets
 - stacking sequence: e.g., $0^\circ/90^\circ$ or $0^\circ/45^\circ/90^\circ$
 - benefit: balanced, in-plane stiffness



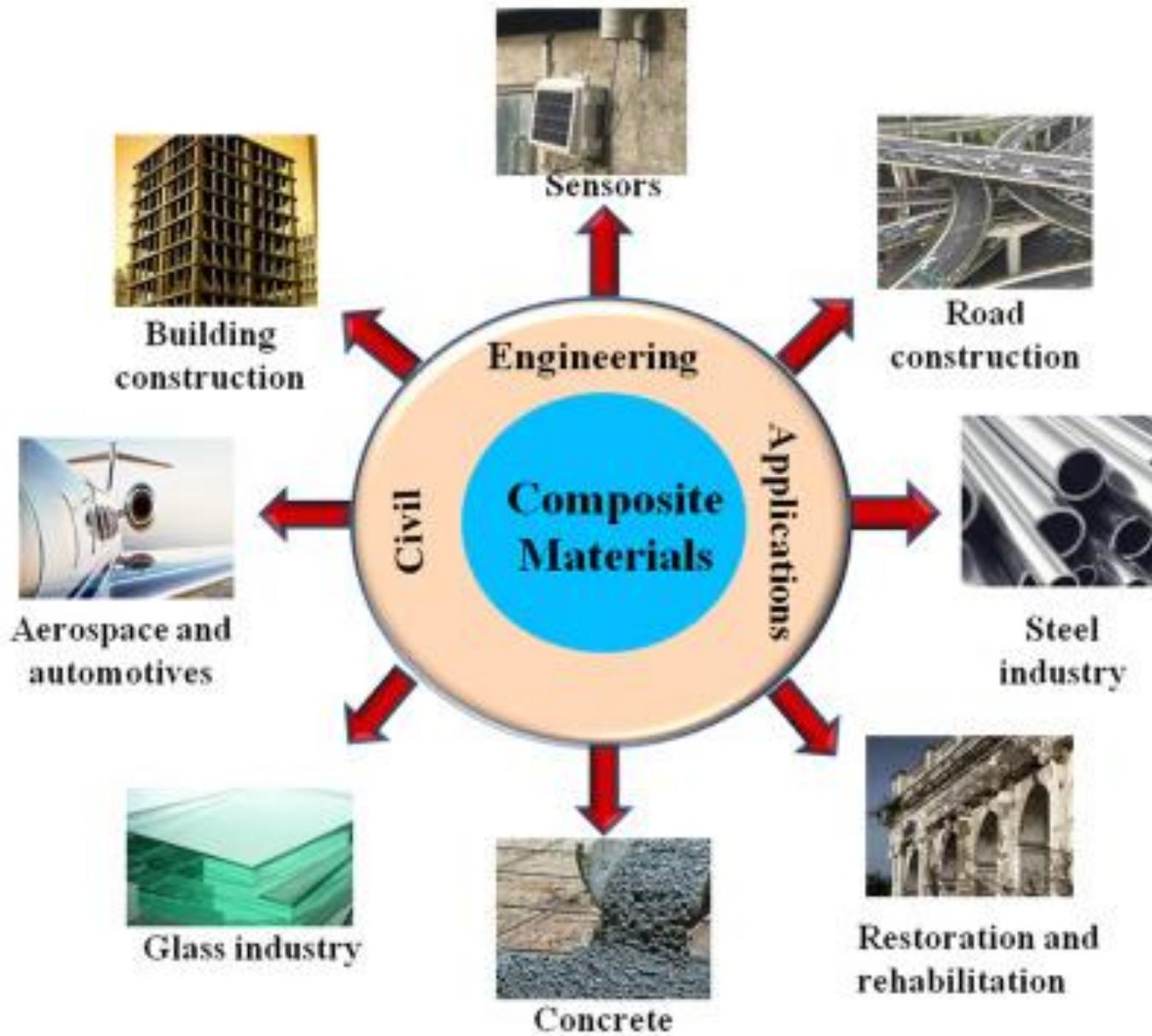
Adapted from Fig. 16.16, *Callister 7e*.

- **High Strength to Weight Ratio:** Fibre composites are extremely strong for their weight
- **Fire Resistance**
- **Chemical & Weathering Resistance:** Composite products have good weathering properties and resist the attack of a wide range of chemicals.
- **Translucency:** Polyester resins are widely used to manufacture translucent mouldings and sheets.
- **Manufacturing Economy:** due to their easy of production composite materials are economically easy to produce

- Light weight and strong - buildings, bridges and structures such as boat hulls,
- Carbon composite is a key material in today's launch vehicles and heat shields for the re-entry phase of spacecraft race car bodies,
- Used in storage tanks, imitation granite and cultured marble sinks and counter tops.
- Wood is a naturally occurring composite comprising cellulose fibers in a lignin and hemicellulose matrix.

- ❖ Applications:
 - ❖ Aerospace industry
 - ❖ Sporting Goods Industry
 - ❖ Automotive Industry
 - ❖ Home Appliance Industry

Applications of Composites



❖ Applications:

- ❖ Aerospace industry
- ❖ Sporting Goods Industry
- ❖ Automotive Industry
- ❖ Home Appliance Industry

(FRPs)

1. pipes, roofing's, storage containers, industrial floorings and automotive bodies
2. sports and recreational equipment's, pressure vessels and aircraft structural components.
3. military aircraft components, helicopter rotor blades and in some sporting goods.
4. Sic and Al₂O₃ fibre reinforced composites are used in tennis rackets, circuit boards and rocket cone noses.

(CMCs)

1. Concrete which contains steel rods in a matrix of cement , sand and crushed stones is extensively used in construction applications.
2. Sic particles reinforced in Titanium –di –boride matrix has good wear and corrosion resistance and hence can be used to produce heat exchangers.

(MMCs)

1. Boron fibre reinforced aluminium alloy matrix composites are used as structural members in space shuttles owing to its strength to weight ratio.
2. Al₂O₃ reinforced aluminium matrix finds applications in producing sporting equipment's and automobile engine parts.

