

Chapter 1. Introduction

1.1 Historical Perspective and Materials Science

1.1.1 Historical Perspective

Materials are so important in the development of human civilization that the historians have identified early periods of civilization by the name of most significantly used material, e.g.: Stone Age, Bronze Age. This is just an observation made to showcase the importance of materials and their impact on human civilization. It is obvious that materials have affected and controlling a broad range of human activities through thousands of decades.

From the historical point of view, it can be said that human civilization started with *Stone Age* where people used only natural materials, like stone, clay, skin, and wood for the purposes like to make weapons, instruments, shelter, etc. Thus the sites of deposits for better quality stones became early colonies of human civilization. However, the increasing need for better quality tools brought forth exploration that led to *Bronze Age*, followed by *Iron Age*. When people found copper and how to make it harder by alloying, the *Bronze Age* started about 3000 BC. The use of iron and steel, a stronger material that gave advantage in wars started at about 1200 BC. Iron was abundant and thus availability is not limited to the affluent. This commonness of the material affected every person in many aspects, gaining the name *democratic material*. The next big step in human civilization was the discovery of a cheap process to make steel around 1850 AD, which enabled the railroads and the building of the modern infrastructure of the industrial world. One of the most significant features of the *democratic material* is that number of users just exploded. Thus there has been a need for human and material resources for centuries, which still going strong. It's being said and agreed that we are presently in *Space Age* marked by many technological developments towards development materials resulting in

stronger and light materials like composites, electronic materials like semiconductors, materials for space voyage like high temperature ceramics, biomaterials, etc.

In summary, materials constitute foundation of technology. The history of human civilization evolved from the Stone Age to the Bronze Age, the Iron Age, the Steel Age, and to the Space Age (contemporaneous with the Electronic Age). Each age is marked by the advent of certain materials. The Iron Age brought tools and utensils. The Steel Age brought railroads, instruments, and the Industrial Revolution. The Space Age brought the materials for stronger and light structures (e.g., composite materials). The Electronic Age brought semiconductors, and thus many varieties of electronic gadgets.

1.1.2 Materials Science

As engineering materials constitute foundation of technology, it's not only necessary but a must to understand how materials behave like they do and why they differ in properties. This is only possible with the atomistic understanding allowed by quantum mechanics that first explained atoms and then solids starting in the 1930s. The combination of physics, chemistry, and the focus on the relationship between the properties of a material and its microstructure is the domain of Materials Science. The development of this science allowed designing materials and provided a knowledge base for the engineering applications (Materials Engineering).

Important components of the subject Materials Science are structure, properties, processing, and performance. A schematic interrelation between these four components is shown in figure 1.1.

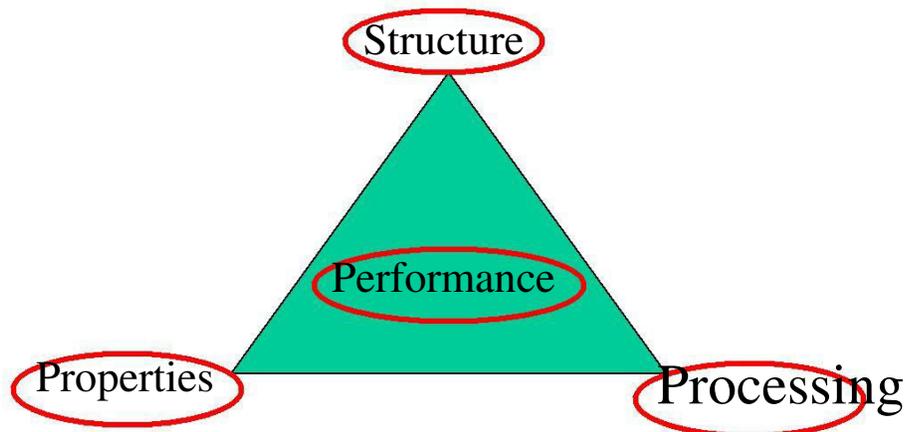


Figure 1.1: *Interrelation between four components of Materials Science.*

1.2 Why Study Materials Science and Engineering? and Classification of Materials?

1.2.1 Why Study Materials Science and Engineering?

All engineers need to know about materials. Even the most "immaterial", like software or system engineering depend on the development of new materials, which in turn alter the economics, like software-hardware trade-offs. Increasing applications of system engineering are in materials manufacturing (industrial engineering) and complex environmental systems.

Innovation in engineering often means the clever use of a new material for a specific application. For example: plastic containers in place of age-old metallic containers. It is well learnt lesson that engineering disasters are frequently caused by the misuse of materials. So it is vital that the professional engineer should know how to select materials which best fit the demands of the design - economic and aesthetic demands, as well as demands of strength and durability. Beforehand the designer must understand the properties of materials, and their limitations. Thus it is very important that every engineer must study and understand the concepts of Materials Science and Engineering. This enables the engineer

- To select a material for a given use based on considerations of cost and performance.
- To understand the limits of materials and the change of their properties with use.
- To be able to create a new material that will have some desirable properties.
- To be able to use the material for different application.

1.2.2 Classification of Materials

Like many other things, materials are classified in groups, so that our brain can handle the complexity. One can classify them based on many criteria, for example crystal structure (arrangement of atoms and bonds between them), or properties, or use. Metals, Ceramics, Polymers, Composites, Semiconductors, and Biomaterials constitute the main classes of present engineering materials.

Metals: These materials are characterized by high thermal and electrical conductivity; strong yet deformable under applied mechanical loads; opaque to light (shiny if polished). These characteristics are due to valence electrons that are detached from atoms, and spread in an *electron sea* that *glues* the ions together, i.e. atoms are bound together by metallic bonds and weaker van der Waalls forces. Pure metals are not good enough for many applications, especially structural applications. Thus metals are used in alloy form i.e. a metal mixed with another metal to improve the desired qualities. E.g.: aluminum, steel, brass, gold.

Ceramics: These are inorganic compounds, and usually made either of oxides, carbides, nitrides, or silicates of metals. Ceramics are typically partly crystalline and partly amorphous. Atoms (ions often) in ceramic materials behave mostly like either positive or negative ions, and are bound by very strong Coulomb forces between them. These materials are characterized by very high strength under compression, low ductility; usually insulators to heat and electricity. Examples: glass, porcelain, many minerals.

Polymers: Polymers in the form of thermo-plastics (nylon, polyethylene, polyvinyl chloride, rubber, etc.) consist of molecules that have covalent bonding within each molecule and van der Waals forces between them. Polymers in the form of thermo-sets (e.g., epoxy, phenolics, etc.) consist of a network of covalent bonds. They are based on H, C and other non-metallic elements. Polymers are amorphous, except for a minority of thermoplastics. Due to the kind of bonding, polymers are typically electrical and thermal insulators. However, conducting polymers can be obtained by doping, and conducting polymer-matrix composites can be obtained by the use of conducting fillers. They decompose at moderate temperatures (100 – 400 C), and are lightweight. Other properties vary greatly.

Composite materials: Composite materials are multiphase materials obtained by artificial combination of different materials to attain properties that the individual components cannot attain. An example is a lightweight brake disc obtained by embedding SiC particles in Al -alloy matrix. Another example is reinforced cement concrete, a structural composite obtained by combining cement (the matrix, i.e., the binder, obtained by a reaction known as hydration, between cement and water), sand (fine aggregate), gravel (coarse aggregate), and, thick steel fibers. However, there are some natural composites available in nature, for example – wood. In general, composites are classified according to their matrix materials. The main classes of composites are metal-matrix, polymer-matrix, and ceramic-matrix.

Semiconductors: Semiconductors are covalent in nature. Their atomic structure is characterized by the highest occupied energy band (the valence band, where the valence electrons reside energetically) full such that the energy gap between the top of the valence band and the bottom of the empty energy band (the conduction band) is small enough for some fraction of the valence electrons to be excited from the valence band to the conduction band by thermal, optical, or other forms of energy. Their electrical properties depend extremely strongly on minute proportions of contaminants. They are usually doped in order to enhance electrical conductivity. They are used in the form of single crystals without dislocations because grain boundaries and dislocations would degrade electrical behavior. They are opaque to visible light but transparent to the infrared. Examples: silicon (Si), germanium (Ge), and gallium arsenide (GaAs, a compound semiconductor).

Biomaterials: These are any type material that can be used for replacement of damaged or diseased human body parts. Primary requirement of these materials is that they must be biocompatible with body tissues, and must not produce toxic substances. Other important material factors are: ability to support forces; low friction, wear, density, and cost; reproducibility. Typical applications involve heart valves, hip joints, dental implants, intraocular lenses. Examples: Stainless steel, Co-28Cr -6Mo, Ti-6Al-4V, ultra high molecular weight poly-ethelene, high purity dense Al-oxide, etc.

1.3 Advanced Materials, Future Materials, and Modern Materials needs

1.3.1 Advanced Materials

These are materials used in *High-Tech* devices those operate based on relatively intricate and sophisticated principles (e.g. computers, air/space-crafts, electronic gadgets, etc.). These materials are either traditional materials with enhanced properties or newly developed materials with high-performance capabilities. Hence these are relatively expensive. Typical applications: integrated circuits, lasers, LCDs, fiber optics, thermal protection for space shuttle, etc. Examples: Metallic foams, inter-metallic compounds, multi-component alloys, magnetic alloys, special ceramics and high temperature materials, etc.

1.3.2 Future Materials

Group of new and state-of-the-art materials now being developed, and expected to have significant influence on present-day technologies, especially in the fields of medicine, manufacturing and defense. Smart/Intelligent material system consists some type of sensor (*detects an input*) and an actuator (*performs responsive and adaptive function*). Actuators may be called upon to change shape, position, natural frequency, mechanical characteristics in response to changes in temperature, electric/magnetic fields, moisture, pH, etc.

Four types of materials used as actuators: Shape memory alloys, Piezo-electric ceramics, Magnetostrictive materials, Electro-/Magneto-rheological fluids. Materials / Devices used as sensors: Optical fibers, Piezo-electric materials, Micro-electro-mechanical systems (MEMS), etc.

Typical applications: By incorporating sensors, actuators and chip processors into system, researchers are able to stimulate biological human-like behavior; Fibers for bridges, buildings, and wood utility poles; They also help in fast moving and accurate robot parts, high speed helicopter rotor blades; Actuators that control chatter in precision machine tools; Small microelectronic circuits in machines ranging from computers to photolithography prints; Health monitoring detecting the success or failure of a product.

1.3.3 Modern Materials needs

Though there has been tremendous progress over the decades in the field of materials science and engineering, innovation of new technologies, and need for better performances of existing technologies demands much more from the materials field. More over it is evident that new materials/technologies are needed to be environmental friendly. Some typical needs, thus, of modern materials needs are listed in the following:

- Engine efficiency increases at high temperatures: requires high temperature structural materials

- Use of nuclear energy requires solving problem with residues, or advances in nuclear waste processing.
- Hypersonic flight requires materials that are light, strong and resist high temperatures.
- Optical communications require optical fibers that absorb light negligibly.
- Civil construction – materials for unbreakable windows.
- Structures: materials that are strong like metals and resist corrosion like plastics.

Atomic Structure, Interatomic Bonding and Structure of Crystalline Solids

2.1 Atomic Structure and Atomic Bonding in Solids

2.1.1 Atomic Structure

Atoms are composed of electrons, protons, and neutrons. Electrons and protons are negative and positive charged particles respectively. The magnitude of each charged particle in an atom is 1.6×10^{-19} Coulombs.

The mass of the electron is negligible with respect to those of the proton and the neutron, which form the *nucleus* of the atom. The unit of mass is an atomic mass unit (*amu*) = 1.66×10^{-27} kg, and equals 1/12 the mass of a carbon atom. The Carbon nucleus has $Z=6$, and $A=6$, where Z is the number of protons, and A the number of neutrons. Neutrons and protons have very similar masses, roughly equal to 1 *amu* each. A neutral atom has the same number of electrons and protons, Z .

A *mol* is the amount of matter that has a mass in grams equal to the atomic mass in *amu* of the atoms. Thus, a mole of carbon has a mass of 12 *grams*. The number of atoms in a mole is called the Avogadro number, $N_{av} = 6.023 \times 10^{23}$. Note that $N_{av} = 1 \text{ gram}/1 \text{ amu}$.

Calculating n , the number of atoms per cm^3 of a material of density δ (g/cm^3):

$$n = N_{av} \frac{\delta}{M}$$

where M is the atomic mass in *amu* (*grams per mol*). Thus, for graphite (carbon) with a density $\delta = 1.8 \text{ g}/\text{cm}^3$, $M = 12$, we get $6 \times 10^{23} \text{ atoms/mol} \times 1.8 \text{ g}/\text{cm}^3 / 12 \text{ g/mol} = 9 \times 10^{22} \text{ C atoms}/\text{cm}^3$.

For a molecular solid like ice, one uses the molecular mass, $M_{(H_2O)} = 18$. With a density of 1 g/cm^3 , one obtains $n = 3.3 \times 10^{22} \text{ H}_2\text{O molecules/cm}^3$. Note that since the water molecule contains 3 atoms, this is equivalent to $9.9 \times 10^{22} \text{ atoms/cm}^3$.

Most solids have atomic densities around $6 \times 10^{22} \text{ atoms/cm}^3$. The cube root of that number gives the number of atoms per centimeter, about 39 million. The mean distance between atoms is the inverse of that, *or* 0.25 nm. This is an important number that gives the scale of atomic structures in solids.

2.1.2 Atomic bonding in solids

In order to understand the why materials behave like they do and why they differ in properties, it is necessary that one should look at atomic level. The study primarily concentrates on two issues: what made the atoms to cluster together, and how atoms are arranged. As mentioned in earlier chapter, atoms are bound to each other by number of bonds. These inter-atomic bonds are primarily of two kinds: Primary bonds and Secondary bonds. Ionic, Covalent and Metallic bonds are relatively very strong, and grouped as primary bonds, whereas van der Waals and hydrogen bonds are relatively weak, and termed as secondary bonds. Metals and Ceramics are entirely held together by primary bonds - the ionic and covalent bonds in ceramics, and the metallic and covalent bonds in metals. Although much weaker than primary bonds, secondary bonds are still very important. They provide the links between polymer molecules in polyethylene (and other polymers) which make them solids. Without them, water would boil at -80°C , and life as we know it on earth would not exist.

Ionic Bonding: This bond exists between two atoms when one of the atoms is negative (has an extra electron) and another is positive (has lost an electron). Then there is a strong, direct Coulomb attraction. Basically ionic bonds are non-directional in nature. An example is NaCl. In the molecule, there are more electrons around Cl, forming Cl^- and fewer electrons around Na, forming Na^+ . Ionic bonds are the strongest bonds. In real solids, ionic bonding is usually exists along with covalent bonding.

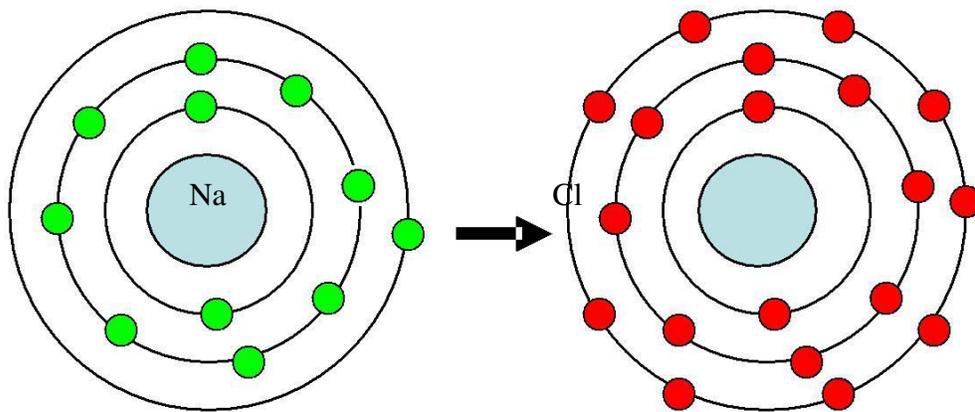


Fig.1 Schematic representation of ionic bonding. Here, Na is giving an electron to Cl to have stable structure

Covalent Bonding: In covalent bonding, electrons are shared between the atoms, to saturate the valency. The simplest example is the H_2 molecule, where the electrons spend more time in between the nuclei of two atoms than outside, thus producing bonding. Covalent bonds are stereo-specific i.e. each bond is between a specific pair of atoms, which share a pair of electrons (of opposite magnetic spins). Typically, covalent bonds are very strong, and directional in nature. The hardness of diamond is a result of the fact that each carbon atom is covalently bonded with four neighboring atoms, and each neighbor is bonded with an equal number of atoms to form a rigid three-dimensional structure.

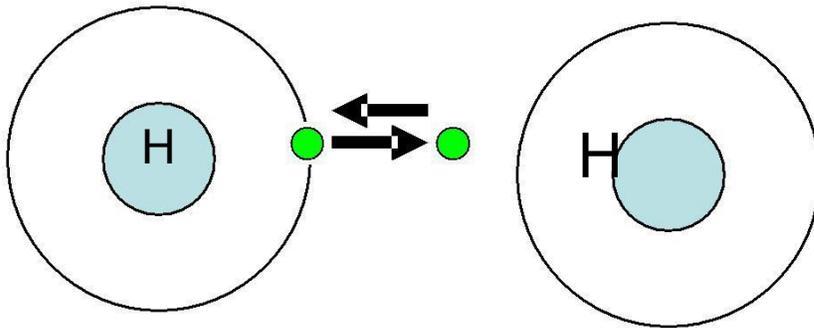


Figure 2. Schematic representation of covalent bond in Hydrogen molecule (sharing of electrons)

Metallic Bonding: Metals are characterized by high thermal and electrical conductivities. Thus, neither covalent nor ionic bondings are realized because both types of bonding localize the valence electrons and preclude conduction. However, strong bonding does occur in metals. The valence electrons of metals also are delocalized. Thus metallic bonding can be viewed as metal containing a periodic structure of positive ions surrounded by a sea of delocalized electrons. The attraction between the two provides the bond, which is non-directional.

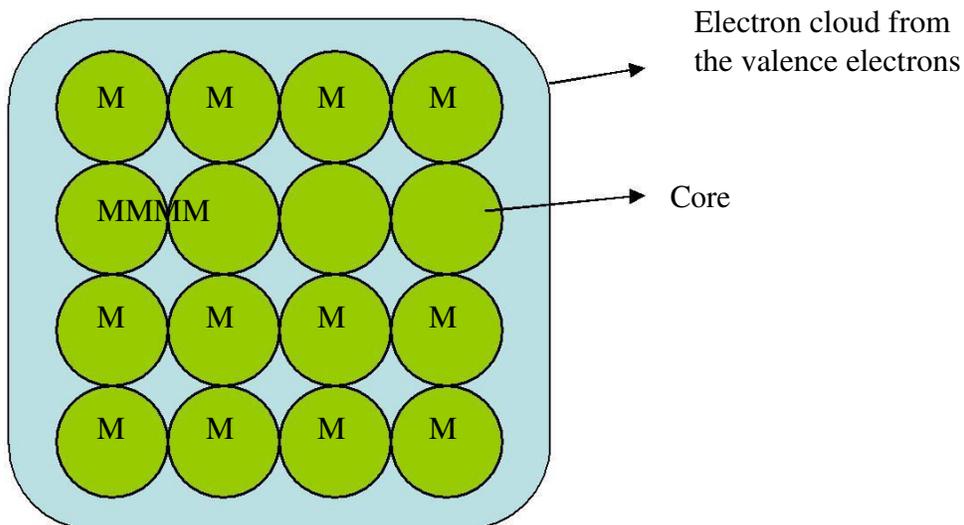


Figure 3. Metallic bonding

Fluctuating Induced Dipole Bonds: Since the electrons may be on one side of the atom or the other, a dipole is formed: the + nucleus at the center, and the electron outside. Since the electron moves, the dipole fluctuates. This fluctuation in atom A produces a fluctuating electric field that is felt by the electrons of an adjacent atom, B. Atom B then polarizes so that its outer electrons are on the side of the atom closest to the + side (or opposite to the – side) of the dipole in A.

Polar Molecule-Induced Dipole Bonds: Another type of secondary bond exists with asymmetric molecules, also called polar molecules because of positively and negatively charged regions. A permanent dipole moment arises from net positive and negative charges that are respectively associated with the hydrogen and chlorine ends of the HCl molecule, leading to bonding. The magnitude of this bond will be greater than for fluctuating induced dipoles.

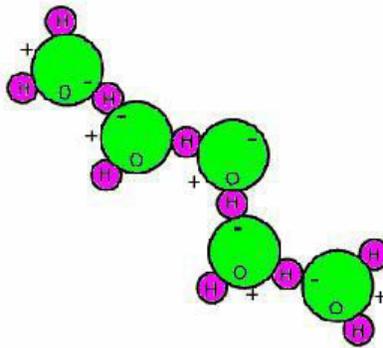


Figure 4. Dipole bond in water

These two kinds of bonds are also called van der Waals bonds. Third type of secondary bond is the hydrogen bond. It is categorized separately because it produces the strongest forces of attraction in this category.

Permanent Dipole Bonds / Hydrogen bonding: It occurs between molecules as covalently bonded hydrogen atoms – for example C-H, O-H, F-H – share single electron with other atom essentially resulting in positively charged proton that is not shielded any electrons. This highly positively charged end of the molecule is capable of strong attractive force with the negative end of an adjacent molecule. The properties of water are influenced significantly by the hydrogen bonds/bridges. The bridges are of sufficient strength, and as a consequence water has the highest melting point of any molecule of its size. Likewise, its heat of vaporization is very high.

2.2 Crystal Structures, Crystalline and Non-Crystalline materials

2.2.1 Crystal structures

All metals, a major fraction of ceramics, and certain polymers acquire crystalline form when solidify, i.e. in solid state atoms self-organize to form *crystals*. Crystals possess a long-range order of atomic arrangement through repeated periodicity at regular intervals in three dimensions of space. When the solid is not crystalline, it is called amorphous. Examples of crystalline solids are metals, diamond and other precious stones, ice, graphite. Examples of amorphous solids are glass, amorphous carbon (a-C), amorphous Si, most plastics.

There is very large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex structures for ceramics and some polymers. To discuss crystalline structures it is useful to consider atoms as being hard spheres, with well-defined radii. In this scheme, the shortest distance between two like atoms is one diameter. In this context, use of terms *lattice* and *unit cell* will be handy. *Lattice* is used to represent a three-dimensional periodic array of points coinciding with atom positions. *Unit cell* is smallest repeatable entity that can be used to completely represent a crystal structure. Thus it can be considered that a unit cell is the building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.

Important properties of the unit cells are

- The type of atoms and their radii R .
- Cell dimensions (Lattice spacing a , b and c) in terms of R and
- Angle between the axis α , β , γ
- a^* , b^* , c^* - lattice distances in reciprocal lattice , α^* , β^* , γ^* - angle in reciprocal lattice
- n , number of atoms per unit cell. For an atom that is shared with m adjacent unit cells, we only count a fraction of the atom, $1/m$.
- CN , the coordination number, which is the number of closest neighbors to which an atom is bonded.
- APF , the atomic packing factor, which is the fraction of the volume of the cell actually occupied by the hard spheres. $APF = \text{Sum of atomic volumes}/\text{Volume of cell}$.

Some very common crystal structures and relevant properties are listed in table 2.1.

Table 2.1: Common crystal structures and their properties.

Unit Cell	n	CN	a/R	APF
Simple Cubic	1	6	4/4	0.52

Body-Centered Cubic	2	8	$4/\sqrt{3}$	0.68
Face-Centered Cubic	4	12	$4/\sqrt{2}$	0.74
Hexagonal Close Packed	6	12		0.74

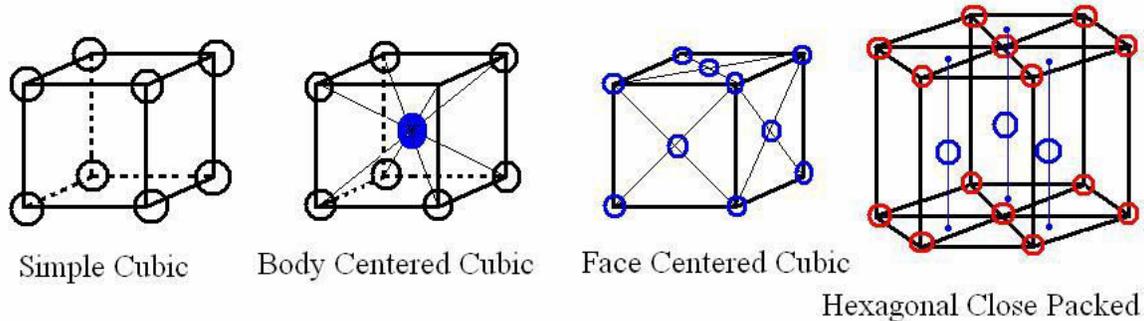


Figure 2.1: Common metallic crystal structures.

2.2.2 Crystalline and Non-crystalline materials

Single Crystals: Crystals can be *single crystals* where the whole solid is one crystal. Then it has a regular geometric structure with flat faces.

Polycrystalline Materials: A solid can be composed of many crystalline grains, not aligned with each other. It is called *polycrystalline*. The grains can be more or less aligned with respect to each other. Where they meet is called a *grain boundary*.

Non-Crystalline Solids: In amorphous solids, there is no long-range order. But amorphous does not mean random, since the distance between atoms cannot be smaller than the size of the hard spheres. Also, in many cases there is some form of short-range order. For instance, the tetragonal order of crystalline SiO_2 (quartz) is still apparent in amorphous SiO_2 (silica glass).

Point defects

Defects exist in any all solid materials. For ease of their characterization, defects are classified on the basis of their geometry, which is realistic as defects are disrupted region in a volume of a solid. Defects are:

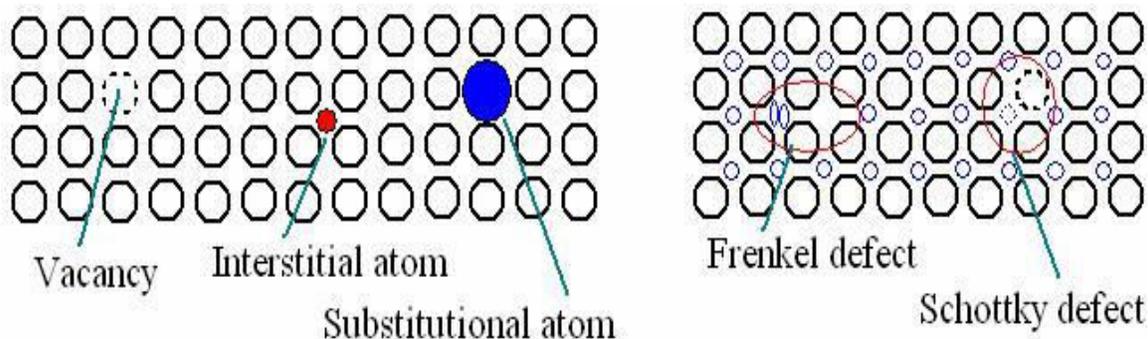
- Point defects (zero-dimensional)
- Line defects (single dimensional)
- Surface defects (two dimensional)
- Volume defects (three dimensional)

Point defects, as the name implies, are imperfect point-like regions in the crystal. Typical size of a point defect is about 1-2 atomic diameters. Different point defects are explained in the following paragraphs. *Figure-3.2* depicts various point defects.

A *vacancy* is a vacant lattice position from where the atom is missing. It is usually created when the solid is formed by cooling the liquid. There are other ways of making a vacancy, but they also occur naturally as a result of thermal excitation, and these are thermodynamically stable at temperatures greater than zero. At equilibrium, the fraction of lattice sites that are vacant at a given temperature (T) are:

$$\frac{n}{N} = e^{\frac{-Q}{kT}}$$

where n is the number of vacant sites in N lattice positions, k is gas or Boltzmann's constant, T is absolute temperature in kelvins, and Q is the energy required to move an atom from the interior of a crystal to its surface. It is clear from the equation that there is an exponential increase in number of vacancies with temperature. When the density of vacancies becomes relatively large, there is a possibility for them to cluster together and form voids.



Figur-3.2: Schematic depiction of various point defects

An *interstitial atom* or *interstitialcy* is an atom that occupies a place outside the normal lattice position. It may be the same type of atom as the rest surrounding it (self interstitial) or a foreign impurity atom. Interstitialcy is most probable if the atomic packing factor is low.

Another way an impurity atom can be fitted into a crystal lattice is by substitution. A *substitutional atom* is a foreign atom occupying original lattice position by displacing the parent atom.

In the case of vacancies and foreign atoms (both interstitial and substitutional), there is a change in the coordination of atoms around the defect. This means that the forces are not balanced in the same way as for other atoms in the solid, which results in lattice distortion around the defect.

In ionic crystals, existence of point defects is subjected to the condition of charge neutrality. There are two possibilities for point defects in ionic solids.

- when an ion displaced from a regular position to an interstitial position creating a vacancy, the pair of vacancy-interstitial is called *Frenkel defect*. Cations are usually smaller and thus displaced easily than anions. Closed packed structures have fewer interstitials and displaced ions than vacancies because additional energy is required to force the atoms into the interstitial positions.

- a pair of one cation and one anion can be missing from an ionic crystal, without violating the condition of charge neutrality when the valency of ions is equal. The pair of vacant sites, thus formed, is called *Schottky defect*. This type of point defect is dominant in alkali halides. These *ion-pair vacancies*, like single vacancies, facilitate atomic diffusion.

3.1.3 Line defects or Dislocations:

Line imperfections (one-dimensional defects) are also called Dislocations. They are abrupt changes in the regular ordering of atoms along a line (dislocation line) in the solid. They occur in high densities and strongly influence the mechanical properties of material. They are characterized by the Burgers vector (\mathbf{b}), whose direction and magnitude can be determined by constructing a loop around the disrupted region and noticing the extra inter-atomic spacing needed to close the loop. The Burgers vector in metals points in a close packed lattice direction. It is unique to a dislocation.

Dislocations occur when an extra incomplete plane is inserted. The dislocation line is at the end of the plane. Dislocations can be best understood by referring to two limiting cases - Edge dislocation *and* Screw dislocation.

Edge dislocation or *Taylor-Orowan dislocation* is characterized by a Burger's vector that is perpendicular to the dislocation line. It may be described as an edge of an extra plane of atoms within a crystal structure. Thus regions of compression and tension are associated with an edge dislocation. Because of extra incomplete plane of atoms, the atoms above the dislocation line are squeezed together and are in state of compression whereas atoms below are pulled apart and experience tensile stresses. Edge dislocation is considered *positive* when compressive stresses present above the dislocation line, and is represented by \perp . If the stress state is opposite i.e. compressive stresses exist below the dislocation line, it is considered as negative edge dislocation, and represented by \top . A schematic view of edge dislocations are shown in *figure 3.3*.

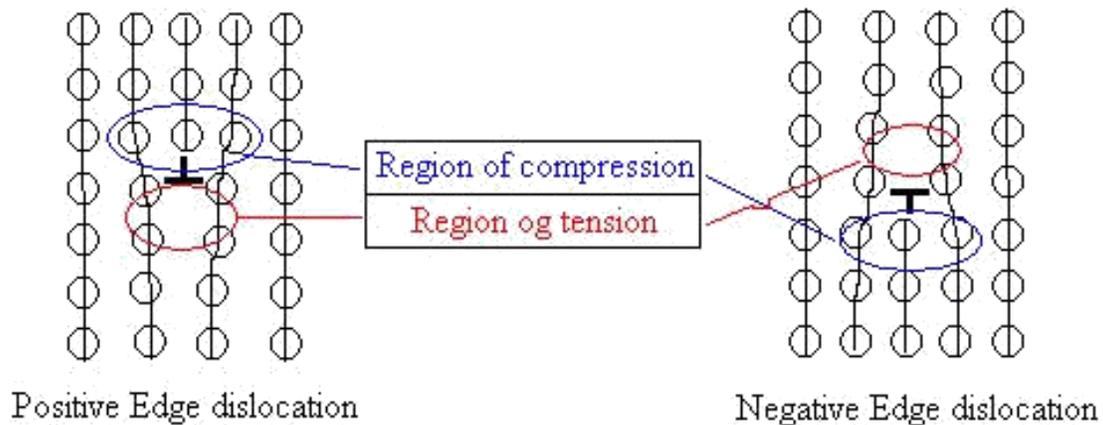


Figure-3.3: Edge dislocations.

A pure edge dislocation can glide or slip in a direction perpendicular to its length i.e. along its Burger's vector in the slip plane (made of \mathbf{b} and \mathbf{t} vectors), on which dislocation moves by slip while conserving number of atoms in the incomplete plane. It may move vertically by a process known as climb, if diffusion of atoms or vacancies can take place at appropriate rate. Atoms are added to the incomplete plane for negative climb i.e. the incomplete plane increases in extent downwards, and vice versa. Thus climb motion is considered as non-conservative, the movement by climb is controlled by diffusion process.

Screw dislocation or *Burgers dislocation* has its dislocation line parallel to the Burger's vector. A screw dislocation is like a spiral ramp with an imperfection line down its axis. Screw dislocations result when displacing planes relative to each other through shear. Shear stresses are associated with the atoms adjacent to the screw dislocation; therefore extra energy is involved as it is in the case of edge dislocations. Screw dislocation is considered positive if Burger's vector and \mathbf{t} -vector or parallel, and vice versa. (\mathbf{t} -vector – an unit vector representing the direction of the dislocation line). A positive screw dislocation is represented by “ \odot ” a dot surrounded by circular direction in clock-wise direction”, whereas the negative screw dislocation is represented by “ \ominus ” a dot surrounded by a circular direction in anti-clock-wise direction”. A schematic view of a negative screw dislocation is shown in *figure 3.4*.

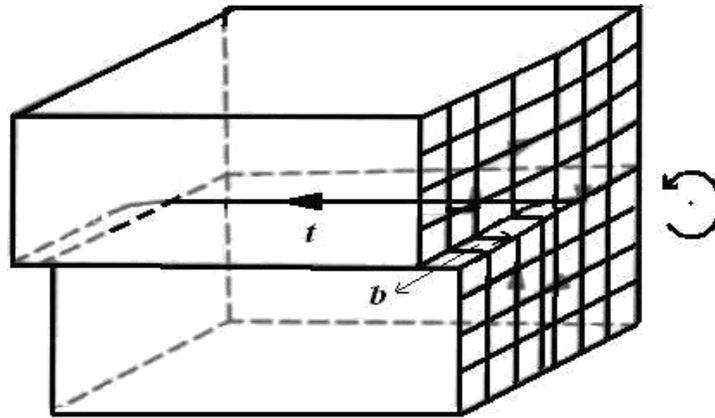


Figure-3.4: *Negative screw dislocation.*

A screw dislocation does not have a preferred slip plane, as an edge dislocation has, and thus the motion of a screw dislocation is less restricted than the motion of an Edge dislocation. As there is no preferred slip plane, screw dislocation can cross-slip on to another plane, and can continue its glide under favorable stress conditions. However, screw dislocation can not move by climb process, whereas edge dislocations can not cross-slip.

Dislocations more commonly originate during plastic deformation, during solidification, and as a consequence of thermal stresses that result from rapid cooling. Edge dislocation arises when there is a slight mismatch in the orientation of adjacent parts of the growing crystal. A screw dislocation allows easy crystal growth because additional atoms can be added to the 'step' of the screw. Thus the term screw is apt, because the step swings around the axis as growth proceeds. Unlike point defects, these are not thermodynamically stable. They can be removed by heating to high temperatures where they cancel each other or move out through the crystal to its surface. Virtually all crystalline materials contain some dislocations. The density of dislocations in a crystal is measured by counting the number of points at which they intersect a random cross-section of the crystal. These points, called etch-pits, can be seen under microscope. In an annealed crystal, the dislocation density is the range of 10^8 - 10^{10} m^{-2} .

Any dislocation in a crystal is a combination of edge and screw types, having varying degrees of edge and screw character. *Figure 3.5* depicts a schematic picture of a common dislocation.

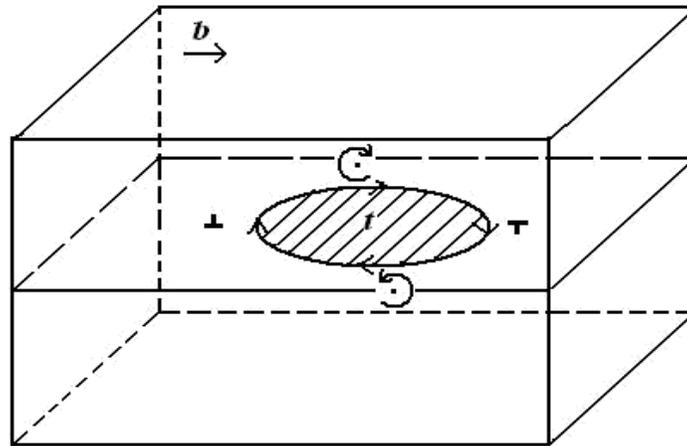


Figure-3.5: Typical dislocation in a crystal.

As shown in *figure 3.5*, the Burger's vector will have the same magnitude and direction over the whole length of dislocation irrespective of the character of the dislocation (edge, screw, or mixed) i.e. Burger's vector is invariant. Other geometrical characteristics of dislocations are:

- vectorial sum of Burger's vectors of dislocations meeting at a point, called node, must be zero.
- t-vectors of all the dislocations meeting at a node must either point towards it or away from it.
- a dislocation line can not end abruptly within the crystal. It can close on itself as a loop, or ends either at a node or at the surface.

Dislocations have distortional energy associated with them as is evident from the presence of tensile/compressive/shear stresses around a dislocation line. Strains can be expected to be in the elastic range, and thus stored elastic energy per unit length of the dislocation can be obtained from the following equation:

$$E \cong \frac{Gb^2}{2}$$

where G – shear modulus and b – Burger's vector.

Dislocations in the real crystal can be classified into two groups based on their geometry – full dislocations and partial dislocations. Partial dislocation's Burger's vector will be a fraction of a lattice translation, whereas Burger's vector is an integral multiple of a lattice translation for full dislocation. As mentioned above, elastic energy associated with a dislocation is proportional to square of its Burger's vector; dislocation will tend to have as small a Burger's vector as possible. This explains the reason for separation of dislocations that tend to stay away from each other!

2 Interfacial defects, Bulk or Volume defects and Atomic vibrations

3.2.1 Interfacial defects

Interfacial defects can be defined as boundaries that have two dimensional imperfections in crystalline solids, and have different crystal structures and/or crystallographic orientations on either side of them. They refer to the regions of distortions that lie about a surface having thickness of a few atomic diameters. For example: external surfaces, grain boundaries, twin boundaries, stacking faults, and phase boundaries. These imperfections are not thermodynamically stable, rather they are meta-stable imperfections. They arise from the clustering of line defects into a plane.

External surface: The environment of an atom at a surface differs from that of an atom in the bulk; especially the number of neighbors (coordination) at surface is less. Thus the unsaturated bonds of surface atoms give rise to a surface energy. This result in *relaxation* (the lattice spacing is decreased) or *reconstruction* (the crystal structure changes). To reduce the energy, materials tend to minimize, if possible, the total surface area.

Grain boundaries: Crystalline solids are, usually, made of number of grains separated by grain boundaries. Grain boundaries are several atoms distances wide, and there is mismatch of orientation of grains on either side of the boundary as shown in *figure-3.6*. When this misalignment is slight, on the order of few degrees ($< 10^\circ$), it is called *low angle grain boundary*. These boundaries can be described in terms of aligned dislocation arrays. If the low grain boundary is formed by edge dislocations, it is called *tilt boundary*, and *twist boundary* if formed of screw dislocations. Both tilt and twist boundaries are planar surface imperfections in contrast to high angle grain boundaries. For *high angle grain boundaries*, degree of disorientation is of large range ($> 15^\circ$). Grain boundaries are chemically more reactive because of grain boundary energy. In spite of disordered orientation of atoms at grain boundaries, polycrystalline solids are still very strong as cohesive forces present within and across the boundary.

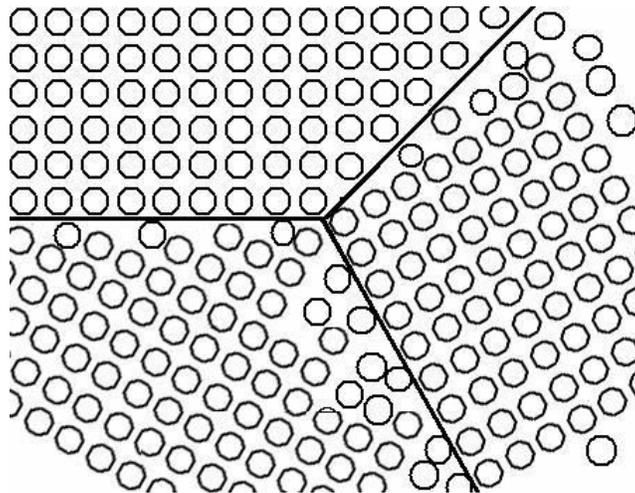


Figure-3.6: Schematic presentation of grain boundaries.

Twin boundaries: It is a special type of grain boundary across which there is specific mirror lattice symmetry. Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restored by the other (*figure-3.7*). The region between the pair of boundaries is called the twinned region. Twins which form during the process of recrystallization are called *annealing twins*, whereas *deformation twins* form during plastic deformation. Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure. Annealing twins are typically found in metals that have FCC crystal structure (and low stacking fault energy), while mechanical/deformation twins are observed in BCC and HCP metals. Annealing twins are usually broader and with straighter sides than mechanical twins. Twins do not extend beyond a grain boundary.

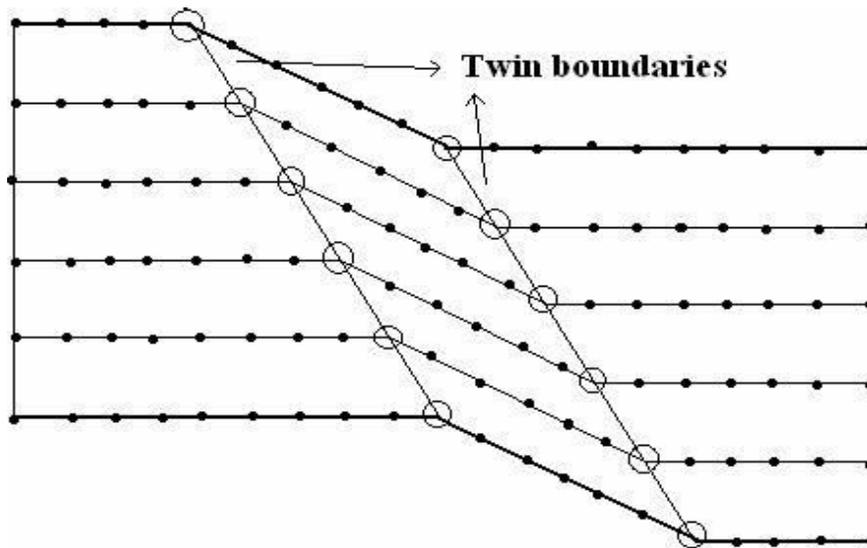


Figure-3.7: A pair of twin boundaries.

Stacking faults: They are faults in stacking sequence of atom planes. Stacking sequence in an FCC crystal is ABC ABC ABC ..., and the sequence for HCP crystals is AB AB AB.... When there is disturbance in the stacking sequence, formation of stacking faults takes place. Two kinds of stacking faults in FCC crystals are: (a) ABC AC ABC... where CA CA represent thin HCP region which is nothing but stacking fault in FCC, (b) ABC ACB CABC is called *extrinsic* or *twin stacking fault*. Three layers ACB constitute the twin. Thus stacking faults in FCC crystal can also be considered as submicroscopic twins. This is why no microscopic twins appear in FCC crystals as formation of stacking faults is energetically favorable. Stacking fault energy varies in range $0.01-0.1 \text{ J/m}^2$. Lower the stacking fault energy, wider the stacking fault, metal strain hardens rapidly and twin easily. Otherwise, metals of high stacking fault energy i.e. narrower stacking faults show a deformation structure of banded, linear arrays of dislocations.

Phase boundaries exist in multiphase materials across which there is sudden change in physical/chemical characteristics.

3.2.2 Bulk or Volume defects

Volume defects as name suggests are defects in 3-dimensions. These include pores, cracks, foreign inclusions and other phases. These defects are normally introduced during processing and fabrication steps. All these defects are capable of acting as stress raisers, and thus deleterious to parent metal's mechanical behavior. However, in some cases foreign particles are added purposefully to strengthen the parent material. The procedure is called dispersion hardening where foreign particles act as obstacles to movement of dislocations, which facilitates plastic deformation. The second-phase particles act in two distinct ways – particles are either may be cut by the dislocations or the particles resist cutting and dislocations are forced to bypass them. Strengthening due to ordered particles is responsible for the good high-temperature strength on many super- alloys. However, pores are detrimental because they reduce effective load bearing area and act as stress concentration sites.

3.2.3 Atomic vibrations

Atomic vibrations occur, even at zero temperature (a quantum mechanical effect) and increase in amplitude with temperature. In fact, the temperature of a solid is really just a measure of average vibrational activity of atoms and molecules. Vibrations displace *transiently* atoms from their regular lattice site, which destroys the perfect periodicity. In a sense, these atomic vibrations may be thought of as imperfections or defects. At room temperature, a typical vibrational frequency of atoms is of the order of 10^{13} vibrations per second, whereas the amplitude is a few thousandths of a nanometer. Many properties and processes in solids are manifestations of this vibrational atomic motion. For example: melting occurs once the atomic bonds are overcome by vigorous vibrations.