



# AN OVERVIEW ON MATERIAL SCIENCE

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## CHAPTER 1

### CLASSIFICATION AND SELECTION OF MATERIALS

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#### **ABSTRACT:**

A major component of materials science and engineering is the classification and selection of materials. It includes the process of selecting the best materials for particular applications as well as the systematic categorization of materials based on their qualities, composition, and structure. This abstract gives a general overview of the materials science classification and selection process and emphasizes the significance of taking a variety of aspects into account to guarantee the best possible material performance and functionality. One of the most important aspects of engineering and manufacturing processes is the classification and selection of materials. It entails classifying various materials according to their traits, traits, and appropriateness for particular uses. This abstract gives a general overview of material classification and selection while emphasizing the value of this procedure across a range of sectors and applications. In order to effectively classify materials, they must be grouped together according to attributes including composition, structure, mechanical qualities, thermal properties, electrical properties, and corrosion resistance. This classification aids in finding the best materials for particular engineering applications and offers a systematic framework for comprehending the behavior and performance of materials under various conditions.

The process of selecting materials is deciding which material is best for a certain application based on that material's characteristics, cost, availability, and other pertinent criteria. It necessitates in-depth knowledge of the application's requirements and limitations, as well as the performance traits of various materials. Mechanical strength, durability, thermal stability, electrical conductivity, chemical resistance, and environmental effect are all things that are taken into account throughout the choosing process.

#### **KEYWORDS:**

Alloys, Heat, Materials, Metals, Thermal.

#### **INTRODUCTION**

In today's research and technology-driven world, materials science and engineering are extremely important. To suit the needs of the plant and the individual, various types of materials are utilized in industry, housing, agriculture, transportation, etc. The quantum theory of solids has rapidly advanced, creating a wealth of prospects for improved comprehension and use of a variety of materials.

The astounding achievement in the field of space is largely attributable to the quick development of high-temperature and high-strength materials. A fairly complicated process goes into choosing a certain material for a given use [1]. However, if the specifics of:

- i. Operational Parameters,
- ii. Manufacturing methods,
- iii. Functional needs,
- iv. Cost factors are known, one can reduce the option.



## Engineering requirements

Properties like impact strength, tensile strength, and hardness are indicators of the acceptability for selection when choosing materials for engineering uses, but the design engineer must ensure that the radiography and other properties of the material are in accordance with the specifications. The component's production process, useful life, pricing, and other parameters are up for negotiation. To meet the various demands imposed on metallic materials, a particular surface treatment, such as hardening or normalizing, may be necessary. Additionally, the choice of materials for engineering purposes is influenced by the chemical qualities of such materials, such as structure, bonding energy, and resistance to environmental deterioration[2].Plastics and other polymeric materials have grown significantly in favor as engineering materials in recent years. Although they are less strong and temperature resistant than most metallic materials, these are still used in corrosive environments and in places where little wear is needed, such as small gear wheels, which were once made of hardened steel but are now made of nylon or Teflon. These materials work well, are silent, and don't need to be lubricated. Therefore, it is important to thoroughly understand the requirements of the process, operating limitations such as hazardous or non-hazardous conditions, continuous or non-continuous operation, availability of raw materials as well as spares, availability of alternate materials vis-à-vis life span of the instrument/equipment, cost, etc. before selecting a material or designing a component. diverse materials have diverse qualities to satisfy distinct technical requirements.

## Mechanical Properties

The following are the key mechanical characteristics influencing the choice of a material:

The material can resist the application of a tensile force thanks to its (i) tensile strength. The structural structure of the material provides internal resistance to sustain the tensile force.

(ii) Hardness: This refers to a material's resistance to wear, abrasion, and scratching. The same can be accomplished with the aid of heat treatment and alloying methods.

(iii) Ductility: A metal's ability to be stretched or pulled into wires without rupturing is known as this attribute. It is based on the size of the metal crystals' grains.

(iv) Impact Strength: This property measures how a material reacts to shock loading and is defined as the energy needed per unit cross-sectional area to fracture a specimen.

(v) Wear Resistance: The capacity of a material to withstand wear caused by friction under specific circumstances, i.e., to keep its physical dimensions when in sliding or rolling contact with another member.

(vi) Corrosion Resistance: Corrosion-resistant metals and alloys are those that can tolerate the corrosive action of a medium, meaning that corrosion processes occur in them at a relatively low rate.

(vii) Density: This is a crucial characteristic of a substance where mass and weight are crucial, such as in aero plane components[3], [4].

## b. Thermal Properties

The term "thermal properties" refers to a material's characteristics that depend on temperature. If one is familiar with thermal qualities, he or she can forecast how a machine component will behave under normal operating conditions. Several significant thermal properties of materials include specific heat, latent heat, thermal conductivity, thermal expansion, thermal stresses, thermal fatigue, etc.

When choosing a material for engineering purposes, such as when materials are being examined for high temperature service, these qualities are extremely important. Now, let's quickly go through a few of these characteristics:

(i) **Specific Heat (c):** The heat capacity of a homogeneous substance per unit mass.  $c = C/M$ , where  $C$  is the heat capacity and  $M$  is the body mass, for a homogeneous body. It can alternatively be described as the amount of heat needed to raise a substance's temperature by  $1^\circ\text{C}$  per unit mass. It is measured in  $\text{cal/g}^\circ\text{C}$ .

(ii) **Thermal Conductivity (K):** These measures how much heat is transferred over a unit area in a unit length of time when the temperature gradient across the heat-conducting material is equal to one unit. In actuality, a material's ability to conduct heat is referred to as its thermal conductivity. The rate at which heat will pass through a piece of a given size will increase with increasing thermal conductivity. Because copper and aluminium are effective heat conductors, they are frequently utilised whenever heat transfer is necessary. Due to its limited thermal conductivity, bakelite is frequently employed as a heat insulator.

The area ( $A$ ) and the thermal gradient ( $dt/dx$ ) have direct proportional relationships in terms of the heat flow through an area  $A$  that is perpendicular to the direction of flow.

(iii) **Thermal Expansion:** Solids of all types expand when heated and contract when cooled. You can experience linear, circular, or cubic thermal expansion. Thermally isotropic refers to a solid that expands uniformly in three mutually orthogonal directions. Linear expansion is the phrase used to describe how heating causes any linear dimension of a solid to increase, such as length, width, or height. The increase in length per unit length per degree increase in temperature is known as the coefficient of linear expansion. The term "cubical expansion" refers to a solid's increase in volume when heated. The lattice vibration, which is the cause of the thermal expansion of solids, gets stronger as the temperature rises [5], [6].

(iv) **Thermal Resistance (RT):** This is the resistance a conductor provides when heat flows between two places of the conductor because of a temperature difference.

(v) **Thermal Fatigue:** This is the mechanical result of continuous thermal strains brought on by continuous heating and cooling.

### (c) **Electrical Properties**

A material's conductivity, resistivity, and dielectric strength are a few crucial electrical characteristics. A substance is considered to be a good conductor of electricity if it presents little resistance to the flow of an electric current. A material's electrical resistance is determined by its dimensions and can be calculated using the formula  $\text{Resistance} = \text{Resistivity Length}$ .

#### **Area of a cross-section**

Typically, a material's resistivity is cited in the literature. Ohm-meter is the unit of resistivity.

Materials are categorized as conductors, semiconductors, and insulators based on their electrical resistivity. Metals are often effective conductors. Highly resistive materials include insulators. The most prevalent types of insulators are ceramic, which are used in household wiring, Bakelite handles for electric irons, and spark plugs for cars. Many metals and alloys attain the superconducting state, in which the dc resistivity is zero, when they are sufficiently chilled below their transition temperature,  $T_c$ .

### (d) **Magnetic Properties**

Magnetic materials are those in which a magnetic state can be induced. Magnetic materials can be categorized into one of five groups: Diamagnetic, paramagnetic, ferromagnetic,

antiferromagnetic, and ferrimagnetic materials are among them. The spontaneous magnetization of iron, cobalt, nickel, and several of their alloys and compounds. High frequencies could be employed with magnetic oxides like garnets and ferrites. These materials are used in a wide range of applications today, including magnetic recording tapes, inductors and transformers, memory components, microwave devices, bubble domain devices, recording hard cores, etc. because of their good magnetic characteristics and high electrical resistivity. In order to construct transformers and other electronic components, magnetic properties such as hysteresis, permeability, and coercive forces must be taken into account.

#### (e) **Chemical Characteristics**

Atomic weight, molecular weight, atomic number, valency, chemical composition, acidity, alkalinity, and other qualities are among these. These characteristics influence the choice of materials, especially in chemical plants.

#### (f) **Optical Characteristics**

Light transmission and reflection are influenced by a material's optical properties, such as refractive index, reflectivity, and absorption coefficient, among others.

#### (g) **Structure of Materials**

The internal configuration of the atoms and molecules has a major role in determining the qualities of engineering materials. We must remember that while choosing materials, being conscious of how different and similar different materials are is crucial. Pure metals are those that contain only one sort of atom. Since it is possible for the designer to realize an unlimited range of physical qualities in the product by modifying the metallic composition of the alloy, metals in practical commercial use are nearly exclusively alloys and not pure metals. Alloys are created using a variety of atom kinds. Alloys can be classed as multi-component alloys, ternary alloys, or binary alloys, each of which has three components. Multicomponent alloys are the norm in industry. Giving the percentage (either by weight or by atoms) of each element in an alloy helps to describe its composition.

The finished component, such as a shaft or a pulley, may not show the basic atomic arrangement or pattern, but the properties of the individual crystals within the metallic component controlled by the atomic arrangement are primarily to blame for their industrial application. The capacity of a piece of metal to tolerate external force to ascertain its strength. In order to counteract the size of the imposed load and maintain the constituent atoms in their ordered places, the structure of the metal or alloy reacts to the applied load internally. However, if the load is greater than the force holding the metal's atoms in place, the metallic bond breaks down and the atoms are pushed into new, displaced places. Slip is the word for the movement of atoms away from their initial locations in the metal. A metal's hardness can be determined by how easily its atoms slide about or move. We must keep in mind that a material's mechanical qualities directly depend on the relative movement of atoms or slide within the substance [7], [8].

### **3. Classification of Engineering Materials**

The chemical composition of the material, its mode of occurrence in nature, its refinement and manufacturing process, which it must go through before acquiring the necessary properties, its atomic and crystalline structure, as well as its industrial and technical use, are the factors that form the basis of different systems of classification of materials in material science and engineering.

The following six categories can be used to categories common engineering materials that are under the purview of material science and engineering:

(i) Ceramics (ii) Organic Polymers (iii) Composites (iv) Semi-conductors (v) Metals (ferrous and non-ferrous) and alloys (vi) Biomaterials (vii) Advanced Materials

Metals (i) According to their characteristics, all elements are roughly categorized into metals and non-metals. For the purpose of forming metallic bonds and conducting electricity, metals are elemental compounds that readily give up electrons. The following are some of the crucial fundamental characteristics of metals: (a) metals are typically excellent electrical and thermal conductors; (b) at room temperature, metals are typically solid; (c) to a certain extent, metals are malleable and ductile; (d) newly cut metal surfaces are lustrous; (e) struck metal produces a distinctive sound; and (f) the majority of metals form alloys. An alloy is created when two or more pure metals are melted together to create a new metal with distinct properties from the parent metals.

## DISCUSSION

Metallic materials have unique qualities including strength and flexibility. High luster, hardness, corrosion resistance, strong thermal and electrical conductivity, malleability, stiffness, magnetism, and other beneficial properties of metallic materials are only a few. Metals can either naturally be magnetic or non-magnetic. These characteristics of metallic materials are caused by (i) the atoms that make up those materials and (ii) how those atoms are arranged in the space lattice.

According to their applications in engineering, metallic materials are often categorized as follows:

(i) Pure Metals: Pure metal is typically quite hard to get by. They are often obtained by ore refinement. Pure metals are typically useless to engineers. To get pure metals (purity 99.99%), such as aluminum, copper, and others, one must use specialized, extremely expensive procedures.

(ii) Alloyed Metals: Alloys are created by mixing two or more metals, at least one of which must be a metal. An alloy's characteristics might differ greatly from those of its basic elements. For instance, low carbon steel, which has a carbon content of less than 0.15%, is incredibly strong, incredibly ductile, and highly resistant to corrosion. It also contains 18% chromium and 8% nickel. We must keep in mind that these characteristics are very different from how original carbon steel behaved.

(iii) Ferrous Metals: These ferrous metals mostly consist of iron. Non-ferrous metals are present in non-ferrous alloys in significant amounts. For engineering applications, ferrous alloys are crucial. These can be divided into the following categories depending on how much carbon and other alloying elements are present:

(a) Mild steels: These materials typically include 0.15% to 0.25% carbon. These can be well welded and are moderately robust. These materials are inexpensive to produce.

(b) Medium Carbon Steels: These are made with carbon that ranges from 0.3% to 0.6%. These materials have a high degree of strength but a relatively low degree of weld ability.

High carbon steels (c) include carbon in amounts ranging from 0.65% to 1.5%. Heat treatment makes these materials strong and tough, but their weld ability is poor.

Plain carbon steel is created with a carbon concentration of up to 1.5%, silica up to 0.5%, manganese up to 1.5%, and traces of other components.

(d) Cast irons: These materials typically include 2% to 4% carbon. These materials are employed as ferrous casting alloys because of their relatively low production costs.

Non-Ferrous Metals (iv): These materials are made up of metals other than iron. These might, however, have trace amounts of iron. Only seven non-ferrous metals—out of a number—are moderately affordable, available in sufficient quantities, and utilized as standard engineering metals. These are zinc, magnesium, copper, tin, aluminum, and tin. There are a total of fourteen different non-ferrous metals that are produced in comparatively small amounts yet are extremely important in contemporary industry. These include manganese, titanium, tantalum, chromium, mercury, cobalt, tungsten, vanadium, molybdenum, antimony, cadmium, zirconium, beryllium, and niobium[9], [10].

(v) Sintered Metals: These materials have radically different structures and properties from the metals from which they were cast. Sintered metals are created using a technology called powder metallurgy. The metals that will be sintered are first produced in powdered form, which is followed by a precise mixing procedure. They are appropriately combined, placed in the die of the desired shape, and then treated under specific pressure. Finally, one has the furnace sinter them. It is important to note that while the mixture created in this way is not an actual alloy, it does have some typical alloy characteristics.

(vi) Clad Metals: In order to take advantage of the qualities of both materials, a "sandwich" of two materials is formed. Cladding is the name given to this method. By rolling the two metals together when they are extremely hot, mild steel is mostly imbedded into stainless steel using this method. One surface cannot corrode with this procedure. Duralumin covered in thin sheets of pure aluminum is another example of how this method is used. Duralumin's inner layer provides high strength, while the outer layers of aluminum's surface resist corrosion. The cost of manufacturing this method is not too high.

### **Organic, inorganic and biological materials**

Carbon compounds and their derivatives make up organic materials. They are crystalline solids made of extensive molecular chains. Given that carbon compounds make up every component of biological systems, the study of organic compounds is crucial. There are also some biologically derived materials, like limestone, that lack an organic content.

### **Organic materials**

These substances are carbon compounds, in which carbon has chemical bonds with oxygen, hydrogen, and other non-metallic elements. These compounds have a complicated structural makeup. Plastics and synthetic rubber are two examples of common organic materials, sometimes known as organic polymers. Wood, a variety of waxes, and petroleum-derived compounds are more examples of organic materials. In polymerization reactions, simple molecules are chemically joined into long chain molecules or three-dimensional structures to create organic polymers. Solids called organic polymers are made of extensive molecular chains. These substances are strong and have a low specific gravity. The two main categories of organic polymers are: (a) thermoplastics, which soften when heated and then re-harden when cooled, including nylon, polythene, etc.

(b) Thermosetting plastics: These substances, such as urea-formaldehyde, phenol-formaldehyde, etc., cannot be re-softened after polymerization. These materials are brittle, robust, non-swelling, and cross-linked as a result of cross-linking. These substances are excellent for casting and molding into components. They are resistant to corrosion well.

The polymeric materials have been established due to their superior corrosion resistance, ease of fabrication into desired shapes and sizes, fine luster, light weight, strength, and stiffness, and these materials are quickly replacing many metallic components. Building cladding,

roofing, and glazing are all common applications for PVC (Polyvinyl Chloride) and polycarbonate polymers. Plastics are also utilized to lighten the weight of movable things like cars, rockets, and aero planes. When making tanks and pipelines, polyethylene and polypropylene are employed.

1. To stop water from seeping into canals and lagoons, thermo-plastic sheets are frequently utilized as liner.
2. Plastics are utilized as surface coverings on metallic structures to prevent corrosion. Adhesive primary ingredients often include plastics. Plastic materials are more prone to attack by insects and rodents than other materials because of their lesser toughness.
3. Plastics can burn because of the carbon they contain. 100°C or such is the maximum service temperature. Due to their decreased heat conductivity, these materials are employed as thermal insulators.
4. Plastic materials have a low stiffness modulus, which can be raised by adding fillers, like glass fibers.
5. Thermoplastic materials include natural rubber, which is an organic substance with biological origins. It is made from a fluid that the rubber trees provide. Rubber is frequently used in toys, metal component insulation, car tyres, and other rubber products.

### **Inorganic Materials**

These materials come from minerals and include metals, clays, sand, rocks, gravel, minerals, and ceramics.

These substances are not biological substances; rather, they are products of the organic growth and development of living things.

The components of the earth's crust are rocks. The following are the top three rock types:

- (i) **Igneous Rocks:** Also known as volcanic rocks or lava rocks, igneous rocks are created when semi-liquid or liquid material (magma) solidifies. Plutonic rocks are formed when this consolidation occurs deep beneath the earth. Granite is igneous plutonic, whereas basalt is igneous volcanic.
- (ii) **Sedimentary Rocks:** Shale and sandstone rocks are examples of sedimentary rocks, which are generated when the broken-down remnants of previous rocks are compressed under pressure. The rocky material that lies above provides the pressure needed for the development of sedimentary rocks.
- (iii) **Metamorphic Rocks:** These rocks, such as marble and slates, are essentially sedimentary rocks that are transformed into new rocks by extreme heat and pressure. These rocks have a structure that falls somewhere between igneous rocks and sedimentary rocks.

Construction of buildings, homes, bridges, monuments, arches, tombs, etc. frequently uses rock materials. The extremely hard slate is still utilized as a roofing material. Crushed stones of basalt, dolerite, and rhyolite are utilized as concrete aggregate and road construction materials.

Engineers are particularly interested in a different class of minerals called pozzolanics because they are silicious compounds, either naturally occurring or manmade, that hydrate to produce cement. Examples of pozzolanic materials include volcanic ash, fly ash, certain shales, and blast furnace slag. Pozzolans-portland cement, which sets more slowly than regular portland cement and has stronger resistance to sulphate solutions and sea water, is created when the cement contains 10- 20% pulverised blast furnace slag.

The naturally existing materials exist in nature in the form in which they are to be used, including rocks, stone, wood, copper, silver, and gold. However, there aren't many naturally occurring materials. Most materials are now produced to specific specifications. It goes without saying that the manufacturing method used to create materials with the desired qualities is related to the study of engineering materials. Natural metals like copper, silver, gold, and others are largely chemically inert, highly malleable and ductile, and remarkably corrosion-resistant in their free condition. These metals' alloys are more durable than the base metals. Metals that are more reactive include carbonates, sulphates, and sulfide ores.

### **Biological materials**

Biological materials include leather, limestone, bone, horn, wax, and wood, among others. There are various uses for wood, which is a fibrous composition of cellulose, lignin, and hydrocarbons. In addition to these elements, wood also contains trace amounts of gum, starch, resins, wax, and organic acids. Wood can be divided into soft wood and hard wood. Fresh wood has a high water content, therefore seasoning is necessary to remove that moisture. If the wood is not properly seasoned, defects including cracks, twists, and warps may appear.

After cleaning and tanning procedures, leather is made from animal skin. These days, it is employed in the production of belts, boxes, shoes, handbags, etc. The process of tanning is used to preserve leather. Two popular tanning methods are as follows:

Vegetable tanning (a) involves immersing the skin in tanning liquid for a number of days before drying it to the best possible leather conditions.

(b) Chrome tanning: This method revolves a drum filled with a chromium salt solution while the skin is pickled in an acidic solution. The leather is then cured and rolled.

A significant non-organic substance with biological origins is limestone. Limestone and calcium carbonate make up the majority of it. It is frequently used to make cement. Limestone in its purest form is utilized as flux in the iron and steel industries.

In the past, tools and weapons were made from animal bones. Today, bones are used to make glue, gelatin, and other products. The organic materials, phosphates, and calcium carbonates that make up bones are laminated together. Compared to tension, these are stronger in compression.

### **Semiconductors**

These are the materials whose electrical characteristics fall in between those of electrical insulators and conductors. Because impurity atom concentrations may be regulated across very small spatial regions, semiconductors' electrical properties are particularly sensitive to their presence. The electronic industry is built on semiconductors. The development of integrated circuitry, which completely transformed the electronics and computer industries, was made possible by semiconductors. They have an impact on every aspect of life, including communication, computing, biomedicine, power, aviation, defense, and entertainment. The semiconductor industry is evolving quickly, and this trend is anticipated to last for the ensuing ten years. During this decade, organic semiconductors are anticipated to play a significant role. Diamond will be crucial as a semiconductor. Circuits will be integrated in three dimensions using optoelectronic devices, and optical computing.

### **Biomaterials**

These are used in parts that are implanted into people's bodies to replace sick or injured body parts. Biomaterials must be compatible with bodily tissues and not produce hazardous

byproducts (i.e., they must not have negative biological effects). Metals, ceramics, polymers, composites, and semiconductors, to name a few, can all be employed as biomaterials.

### **Current trends and advances in materials**

The materials that are employed in great quantities for engineering purposes include cement, steel, and wood. Any nation's steel consumption is seen as a barometer of its overall economic health.

The need for diverse high steel alloys keeps growing for high temperature applications, such as steam and gas turbines. Iron-based alloys with chromium, nickel, molybdenum, and tungsten are more appropriate for the aforementioned purposes. Material scientists and engineers are working hard to develop newer materials that have combination resistance to high temperature and corrosion. Despite being challenging to form and process, several ceramic materials are in demand for use in high-temperature applications. Improved fatigue qualities can be added to aircraft components by using newly developed metallic materials and manufacturing methods like iso-static pressing and isothermal forging.

While creating finished surfaces and lowering the cost of metal cutting, powder metallurgy is also very capable of transferring better mechanical properties under various loading circumstances. Surprisingly, rapid cooling technology is being used to produce metal powders that can be used in temperature-resistant parts manufacturing processes like powder metallurgy and hot iso-static pressing. This technology achieves cooling rates in the neighborhood of one million degrees Celsius per second. To achieve anticorrosion qualities at high temperatures, metallurgists nowadays have created a variety of molybdenum and aluminum alloys as well as alloys of titanium and nickel. More than any other material, polymeric materials are expanding in bulk at a 9% annual rate. Plastics have taken the place of metals, wood, glass, and paper in a number of applications. The creation of synergistic plastic alloys, which have superior qualities than the separate components making up the alloy, is a recent development in plastic technology. The recent discovery of plastic conductors may soon have a larger influence.

Ceramics are mostly employed as materials that can carry light loads at high temperatures. Brittleness and difficulties in cutting and shaping are ceramics' main flaws. Cerments, which are predicted to be practical cutting materials, are produced when ceramic powder is combined with metal powder, such as molybdenum. Tool bits made of cermet's are anticipated to have a variety of uses in order to achieve fast cutting speeds and produce higher surface finishes. It is anticipated that molybdenum fibers will successfully reinforce the well-known ceramic alumina. The attempts to improve strength in such composite ceramics have not yet been effective due to the micro-cracking of molybdenum fibers. However, it has been discovered that these composites have better impact and thermal shock resistance.

The development of solar cells, electronic digital circuits, computers used in factory automation, and the usage of robots in various industrial applications have all increased the need for silicon chips and silicon-based materials. Semiconductors are the foundation of electronics today, and they have an impact on a wide range of devices and businesses, including those involved in communications, computers, biomedicine, power, aviation, defense, entertainment, etc.

### **Advanced materials**

Advanced materials are sometimes used to refer to materials used in high-technology (or high-tech) applications. High technology includes things like electronic devices (VCRs, CD players, etc.), computers, fibre optic systems, spaceships, aeroplanes, and military rocketry that operate or function utilising quite complex and sophisticated concepts. These advanced



materials are often either freshly created high performance materials or conventional materials whose qualities have been improved. Advanced materials can also be made of any sort of material (for example, metals, ceramics, or polymers), and they are typically quite expensive. The characteristics and uses of many advanced materials are covered in later chapters, including those used in lasers, integrated circuits (ICs), magnetic information storage, liquid crystal displays (LCDs), fibre optics, and the thermal projection system for the space shuttle orbiter.

### Smart Materials

Smart or intelligent materials are a class of cutting-edge materials that are now being created and that will significantly impact many of our technology. The term "smart" refers to the ability of these materials to sense changes in their surroundings and then react to these changes in predetermined ways—qualities also present in live beings. Additionally, highly complex systems made of both smart and conventional materials are being included in the idea of smart materials.

The goal of the field of smart materials is to merge the control circuit, the actuator, and the sensor—each of which detects an input signal—into a single, cohesive whole. In reaction to changes in temperature, electric fields, and/or magnetic fields, actuators may be required to alter shape, location, natural frequency, or mechanical qualities. Shape memory alloys, piezoelectric ceramics, magnetostrictive materials, and electrorheological/magnetorheological fluids are typically the four types of materials most frequently utilised for actuators. Shape memory alloys are metals that, when their temperature is adjusted after they have been deformed, return to their original shapes. Piezoelectric ceramics respond to an applied electric field (or voltage) by expanding and contracting; on the other hand, these materials also produce an electric field when their dimensions are changed. With the exception of their receptivity to magnetic fields, the behaviour of magnetostrictive materials is similar to that of piezoelectric ceramic materials. Additionally, liquids that exhibit substantial variations in viscosity in response to the application of electric and magnetic fields, respectively, are known as magnetorheological and electrorheological fluids.

The integrated circuit (IC) device that combines a sensor, actuator, and control circuit simulates a biological system. Smart sensors, microsystem technology, or micro-electromechanical systems (MEMS) are the terms used to describe them. Optical fibers, piezoelectric materials (including certain polymers), and MEMS are among the materials and gadgets used as sensors. For instance, one kind of intelligent technology is applied to helicopters to lessen the noise that the revolving rotor blades make in the cockpit. Blade strains and deformations are monitored by piezoelectric sensors that are installed into the blades; feedback data from these sensors are supplied into an adaptive device that is computer controlled and produces noise-cancelling antidote.

MEMS devices are compact, lightweight, inexpensive, and dependable thanks to large-batch fabrication techniques. They typically consist of actuators to change and regulate the environment in the desired way, integrated electronics to analyse the data acquired, and sensors that gather environmental data such as pressure, temperature, acceleration, etc. There are many different types of materials used in MEMS technology.

Due to its superior mechanical qualities and established micro-fabrication methods, including lithography, etching, and bonding, silicon also serves as the structural backbone of these systems. Along with silicon, several materials with piezoelectric, piezoresistive, ferroelectric, and other characteristics are frequently utilised for sensing and actuation tasks. During this decade, the field of MEMS is anticipated to revolutionise industrial processes, aviation, and pollution management, affecting every part of our life.

## Nanostructured materials and Nanotechnology

Materials with nanostructures feature structural components with sizes between 1 and 100 nm, such as clusters, crystallites, or molecules. Generally speaking, these compact collections of atoms are referred to as nanoparticles, nanocrystals, quantum dots, and quantum boxes. Since it was discovered that nanostructured materials and nanotubes may be used in high-tech engineering applications a decade ago, significant research has been conducted in these fields. As one moves from a "infinitely extended" solid to a material particle made of a countable number of atoms, one observes striking changes in the fundamental electrical, optical, and magnetic properties. Nano-sized silicon powders, silicon-nitride (SiN), and silicon-carbide (SiC) thin films are among the numerous forms of nanostructured materials that have been taken into consideration for use in opto-electronic devices and quantum-optic devices. Because their strength and hardness increase when the grain size decreases, certain of them are also used as advanced ceramics with controlled micro structures. Fullerenes and nanotubes, two examples of carbon-based nanomaterials and nanostructures, are becoming more and more common in nanoscale research and technology. Nanotechnology is currently being hailed as the upcoming enabling technology that will completely reimagine the future of a number of technologies, goods, and markets. In a separate chapter, a brief overview of nanostructured materials is given, with a focus on carbon-based nanomaterials and nanostructures.

### Quantum Dots

Three-dimensional bulk systems have been reduced to two-dimensional, one-dimensional, and finally zero-dimensional systems as a result of quick advancements in the production of semiconductor structures. Future applications like semiconductor lasers and microelectronics exploit these decreased dimensional systems. The final step in reducing the dimensionality of semiconductor devices is represented by quantum dots. These are nanometer-sized, three-dimensional semiconductor structures that confine electrons and holes. QDs are utilized as the gain material in lasers because they operate at the level of a single electron, which is unquestionably the highest possible level for an electronic device. Quantum dot lasers, QD memory technology, QD photo-detectors, and even quantum cryptography all make use of QDs. A quantum dot's emission wavelength depends on its size. In order to create light of various colors, one can make dots of various sizes.

## CONCLUSION

Materials science and engineering depend heavily on the classification and selection of materials since it establishes whether a material is suitable for a given application. The main ideas and factors involved in this process have been examined in this essay. Grouping materials based on their characteristics, makeup, and structure is the process of classification. This enables a methodical comprehension of the many kinds of materials and their behavior under varied circumstances. Metals, ceramics, polymers, composites, and semiconductors are examples of common classes. Materials can be further categorized within each group according to certain traits like electrical conductivity, thermal qualities, mechanical strength, or chemical resistance.

The process of selecting materials entails deciding which material is best for a certain purpose. During this process, a number of elements need to be taken into account. Mechanical characteristics like toughness, strength, and stiffness are among them, as are thermal characteristics, electrical conductivity, corrosion resistance, and cost. Aesthetics, environmental impact, availability, and manufacturability are possible additional factors. Materials databases, handbooks, and computer-aided tools are frequently utilized to speed up the selection process. These sources offer knowledge about the characteristics, capabilities, and potential uses of various materials, assisting in making well-informed choices.

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## CHAPTER 2

### ATOMIC STRUCTURE AND ELECTRONIC CONFIGURATION

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#### ABSTRACT:

Chemistry and physics both depend on fundamental ideas like atomic structure and electrical arrangement. The arrangement and organization of the nucleus, protons, neutrons, and electrons as well as other subatomic particles within an atom is referred to as atomic structure. The distribution of electrons around the nucleus at various energy levels and orbitals is referred to as their electronic configuration. In this abstract, the importance of understanding atomic structure and electrical configuration in relation to understanding the characteristics and behavior of atoms and elements is highlighted. Chemistry relies heavily on an understanding of atomic structure and electrical configuration to explain the behavior and properties of elements and compounds. In this abstract, the importance of atomic structure and electrical configuration in describing the structure and behavior of atoms and molecules is highlighted. The content and arrangement of subatomic particles within an atom are referred to as its atomic structure. The nucleus, which houses protons and neutrons, sits at the core of an atom. Neutrons are electrically neutral, whereas protons have a positive charge. Negatively charged electrons that reside in particular energy levels or shells around the nucleus. An atom's atomic number and element identity are both determined by the number of protons present in it. The arrangement of electrons within the various energy levels or shells is known as the electronic configuration of an atom. Prior to populating higher energy levels, electrons occupy the lowest accessible energy levels. The Aufbau principle, Pauli exclusion principle, and Hund's rule are only a few of the guidelines that the electron configuration adheres to. These laws control how orbitals are filled, which affects how stable and reactive atoms are.

#### KEYWORDS:

Atoms, Atomic Number, Electron, Energy, Mass, Model, Nucleus.

#### INTRODUCTION

Atoms, the smallest indivisible particles, are the building blocks of all materials, whether they be in solid, liquid, or gaseous form. In contrast to atoms of various elements, which differ in weight, size, and other characteristics, atoms of the same element are similar to one another in every respect, including weight, size, and other attributes. The atoms are of the order of  $10^{-10}$  m in size. An element is a substance made up of only one sort of atom. A few examples of elements include nitrogen, carbon, hydrogen, aluminum, copper, gold, and iron. Molecules are groups of atoms that typically coexist in a stable state, such as H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, etc. Many molecules in nature are made up of atoms from many elements, such as water (H<sub>2</sub>O), etc. molecules with one atom (sometimes referred to as monoatomic), two atoms (often referred to as diatomic), three atoms (also referred to as triatomic), or more atoms (also referred to as polyatomic).

Scientists including Sir J.J. Thomson, Ernest Rutherford, Niels Bohr, and many more discovered that although an atom is unbreakable, it is made up of smaller particles named electrons, protons, and neutrons at the turn of the 20th century. Neutrons are neutral, whereas protons and electrons are electrical in nature. The mass of an atom is concentrated at its nucleus, or center, as demonstrated by Rutherford and colleagues. The electron, proton, and

neutron are the three main subatomic particles that make up an atom, which essentially has an electrical structure.

The atom is thought to be composed of a hefty nucleus made up of protons and neutrons that is encircled by highly organized configurations of electrons that orbit the nucleus at a significantly greater distance from it. The atomic nucleus is  $10^{-14}$  m in size and has a density of  $2 \times 10^{17}$  kg/m<sup>3</sup>, according to research. White dwarf stars have densities that are very close to that of pure nuclear stuff. The mass of an atom is mostly determined by the protons and neutrons inside the nucleus because the mass of the electron is extremely small in comparison to that of protons and neutrons [1], [2].

### The electron

The first experimental proof that electrical charge was not indefinitely divided but rather existed in discrete units was supplied by M. Faraday in his experiments on the laws of electrolysis in 1833. When J.J. Thomson was researching the flow of electricity through low-pressure gases in 1897, he noticed that light rays appeared to leave the cathode's surface and move away from it through the discharge tube in straight lines. Since they emanate from the cathode of the discharge tube, these rays are known as cathode rays. W. Crookes investigated the characteristics of these cathode rays and demonstrated that they (i) move straight forward and produce shadows (ii) carry a negative charge and have enough momentum (iii) have a high kinetic energy and can cause some chemical processes and trigger fluorescence on specific materials. J.J. Thomson believed that the cathode rays are made up of a stream of particles with a mass of  $m$  and a charge of  $e$  ( $= 1.602 \times 10^{-19}$  C) that originate at the cathode of the discharge tube to best explain these characteristics of the cathode rays. They are referred to as electrons. When Thomson calculated the specific charge ( $e/m$ ), which is the ratio of the electronic charge to the mass of the electron, he discovered that it was  $1.76 \times 10^{11}$  C/kg. It has now been discovered that electrons are a universal component of all matter. These facts lend credence to this:

(i) The electrons determined to be the same and having the same effects in all applications, such as radio and television (electromagnetic waves), X-ray applications, producing fluorescence effects, producing photoelectric effects, etc., can be obtained from many sources around the world.

(ii) It has been discovered that the cathode ray electrons emitting in various cathode ray discharge tube modes display the same characteristics.

(iii) Electrons from any source have the same effective radius,  $r_e$  ( $= 4.6 \times 10^{-6}$  nanometer), rest mass,  $m_0$  ( $= 9.109 \times 10^{-31}$  kg), and charge,  $e$  ( $= -1.602 \times 10^{-19}$  C), respectively.

The electrons move in a variety of orbits and shells around the nucleus. It has an electric charge that is opposite to that of a proton ( $1.602 \times 10^{-19}$  C), as was before mentioned. De Broglie wavelength,  $= h/mv$ , experimental determination yield  $= 1.66 \times 10^{-10}$  m  $= 0.166$  nm for electron, which exhibits properties of both a tiny particle and an energy wave [3], [4].

Different orbitals are occupied by the electrons that surround the atom's nucleus. An exact description of an electron's momentum and position is impossible, according to the Heisenberg uncertainty principle. The relationship between the uncertainty in the momentum  $p$  and the uncertainty in the location  $x$ , where  $h$  ( $= 6.626 \times 10^{-34}$  J-s) is Planck's constant, states that the product of the two uncertainties cannot be smaller than a specific value. The uncertainty principle has the effect of making it impossible to imagine an electron orbital as a discrete path around the nucleus. The orbital will have to be viewed as the nucleus's surrounding electron probability density cloud. A discrete level of energy—an integral multiple of quanta of fundamental energy units—represents each discrete orbit or quantum state in Bohr's model of the atom in which an electron can only go around the nucleus. Most

of the technical qualities of materials, such as bonding with other atoms, electrical and optical capabilities, chemical reactivity, etc., are determined by the electrons in the outermost shell or orbit.

## DISCUSSION

### Protons

The proton is the name for the hydrogen atoms nucleus. The unit positive charge of a proton is the same as that of an electron ( $1.602 \times 10^{-19}$  C). A proton has a mass of  $1.672 \times 10^{-27}$  kg. The nucleon, also known as a proton or neutron, is thought to be a single particle with two distinct charge states. The charge  $Z$  of the specified nucleus, often known as the charge number, refers to how many protons are present in the nucleus.

### Neutrons

These are 1.008 times heavier than protons and electrically neutral particles. Each neutron has a mass of  $1.675 \times 10^{-27}$  kg. One proton and one electron make up each neutron, hence neutron = proton + electron. The mass number of the nucleus is defined as  $A = N + Z$ , the sum of all the nucleons in the nucleus. There are other particles besides the three stated above, such as positrons or positive electrons, neutrinos and antineutrinos, mesons, deuterons, alpha particles, etc. Mesons are particles with intermediate mass between the electron and the proton. Mesons come in two varieties: (pie) mesons and (mu) mesons, with the former being a little heavier. Mesons of both sorts can have either a positive or negative charge. There are also neutrinos and antineutrinos, which are tiny particles with no charge. It has been hypothesized that these particles exist in order to explain energy shifts that occur when electrons and positrons emit radioactively, respectively. Antineutrino is said to occupy the same location with regard to the positron as neutrino and share the same energy as it [5], [6].

### Atomic Number

$Z$  stands for this essential atomic characteristic. The number of protons in the nucleus, or the amount of positive charge on the nucleus, is quantitatively equal to the element's atomic number. We must keep in mind that every atom of a given element has the same atomic number, which indicates the element's place in the periodic table of elements. Since a typical atom is electrically neutral, it has an equal number of protons and electrons. For instance, the number of protons in an iron atom is 26 ( $Z = 26$ ), hence the number of balancing electrons is also 26. 26 clearly indicates where the element iron is located in the periodic table.

### Atomic Weight and Mass number

The average relative weight of an element's atoms in relation to the assumed weight of one oxygen atom, which is 16, is known as its atomic weight. This means that the atomic weight of an element is the ratio between the weight of one element's atom and 1/16th of the weight of an oxygen atom. Not to be confused with the mass number, this. The total amount of protons and neutrons makes up the mass number. The common abbreviation for the mass number is  $A$ .  $A$  is equal to the sum of the protons and neutrons. For instance, the nucleus of an atom of chlorine contains 17 protons and 18 neutrons. Clearly, 35 mass number of chlorine.

### Isotopes

Isotopes are all atoms with various atomic weights that are part of the same element; the atomic number of isotopes in a given element does not change. Isotopes obviously have the same number of protons and electrons. As a result, the isotopes are atoms with the same atomic number and same element but differing weights. Because there are various numbers of neutrons in the nuclei, different isotopes of the same element have different masses. For

instance, there are three isotopic types of hydrogen. Hydrogen has an atomic number of 1. There are three types of hydrogen: (i) Common hydrogen, with an atomic mass of 1.

(ii) Deuterium ( ${}_1\text{D}^2$ ), which has an atomic mass of 2.

(iii) Tritium ( ${}_1\text{T}^3$ ), which has an atomic mass of 3.

The two isotopes of chlorine are  ${}_{17}\text{Cl}^{35}$  and  ${}_{17}\text{Cl}^{37}$ .

### Isobars

Isobars are atoms that have the same mass but come from various chemical elements. Naturally, the quantity of protons and electrons in the atoms of isobars varies. Each nucleus' total number of protons and neutrons is also the same. Calcium and argon are an illustration of the first pair of isobars. The atom of argon (atomic number 18) contains 18p, 18e, and 22 n. The atoms of calcium, which carries the number 20, contain 20p, 20e, and 20 n [7], [8].

### Isotones

These are the nuclides with varied Z and A but the same amount of neutrons (N). The isotones  ${}^{13}_6\text{C}$  and  ${}^{14}_7\text{N}$  are two examples. Naturally, not all isotones with a particular value of N correspond to the same chemical element. The examination of the characteristics of isotopes, isotones, and isobars enables us to reveal a number of atomic nucleus characteristics. Such approach enables us to forecast what will happen to a nucleus' stability when an additional n or p is introduced to the nucleus.

### Avogadro's Number

The term "Avogadro's number" (abbreviated N) refers to how many atoms there are in one gram of a substance. It has a mass of  $6.023 \times 10^{23}$  mol. It has always existed.

### Atomic Nucleus

In order to investigate the atomic structure, Rutherford used radioactive particles in 1911. He measured the angles at which a beam of particles scattered after being directed through a thin layer of gold foil. Rutherford was able to deduce that the nucleus, which had a positive charge, contained the majority of the mass of the gold atom. It is discovered that the radius of the gold nucleus is less than  $2.8 \times 10^{-14}$  m, or considerably less than 1/10,000 of the radius of the entire atom. The nucleus radius for the examined metals is around 10–14 metres. The nuclear radius, also known as the "nuclear force radius," is the distance from the nucleus's centre where an outside, uncharged nucleon first senses its influence. Recent research using more precise methods has revealed that an atomic nucleus' radius falls between the ranges of 10-14 m and 10-15 m. It is important to keep in mind that a nucleus lacks definite boundaries. The nuclear radius obviously has arbitrary significance. Nuclear matter has an average density of  $1.5 \times 10^{18}$  kg/m<sup>3</sup>. This offers us a sense of the degree of compactness of the nucleons in a nucleus and is approximately 10<sup>15</sup> times larger than the density of matter in bulk. Since the majority of the mass is contained in the nucleus, it also demonstrates that matter in its pure form is essentially empty. We must also keep in mind that it is not always correct to assume that the nucleus is spherical is not always true.

### Atomic Models

We have read about the existence of some elementary particles that are more fundamental than chemical elements in the sections above. For instance, electrons are a fundamental component of all matter and are shared by all the elements. After getting quantitative measurements on electrons and positive rays, numerous atomic models of atomic structure have been established over the years in order to have a clear picture of the extra-nuclear electronic structure, primarily with the aid of positive rays and mass spectroscopy. The main

atomic models put out by Sir J.J. Thomson, Rutherford, Niels Bohr, Sommerfeld, and the contemporary atomic model will now be discussed.

### **J.J Thomson's Atomic Model**

The plum-pudding model of atomic structure was proposed by J.J. Thomson in 1911. The following statements are made in accordance with this model:

- (i) The electron is a component of all matter;
- (ii) The electron has a rest mass of  $9.1085 \times 10^{-31}$  kg;
- (iii) The electron has a negative charge of  $1.602 \times 10^{-19}$  C. Atoms are uniform spheres in which electrons are distributed along with positive charges, much like plums in a pudding. The atom has no electrical charge.
- (iv) The electrons emit light by vibrating in relation to their equilibrium position.

Thomson calculated the total number of electrons in an atom using a variety of spectroscopy techniques.

A significant accomplishment, Thomson's demonstration of the presence of electrons in atoms served as a necessary foundation for the theories of atomic structure that followed. Thomson proved that the charge to mass (e/m) ratio of the electron always yields the same value by employing various filament wire types. This demonstrates unequivocally that the electron is a component of all matter. The periodicity of elements, the occurrence of spectral lines in ions, and the kinetic theory of gases might all be explained by Thomson's model. Thomson's model was unable to account for (i) Rutherford's experiment's scattering of  $\alpha$ -particles on thin gold foil. (ii) The atoms' emission of spectral series. Rutherford's alpha particle scattering investigations forced the abandonment of Thomson's model of the atom [9], [10].

### **Rutherford Nuclear Atomic Model**

In 1911, Rutherford and associates carried out differential scattering tests and put forth a new atomic model. Rutherford focused particles on a thin piece of gold foil that was  $4 \times 10^{-6}$  meters thick. He noticed that while certain particles were dispersed throughout the area, others were seen to pass through the film. The particles that were passing through the thin gold sheet also dispersed widely and produced luminescence on a fluorescent zinc sulphide screen. About 1 in 10,000 particles had a deflection of more than  $90^\circ$ , which is a very small number of big angle deflections. A  $\alpha$ -particle rarely deflected through 180 degrees, or reversed back along its original path.

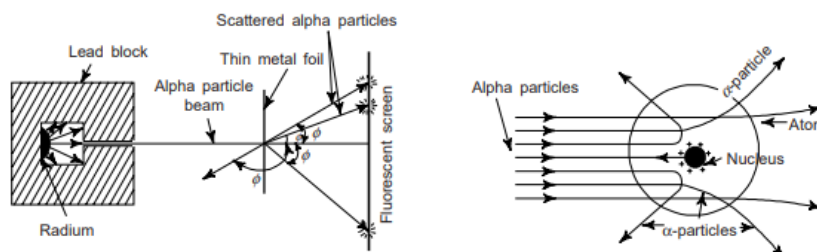
The Thomson's atomic model's uniform distribution of positive charge in a sphere with atomic-scale dimensions was proven to be false by Rutherford particle scattering studies. Only if it is accepted that the positive charge in a sphere or atom is concentrated in the centre and the negatively charged particles surround it loosely, leaving enough space for  $\alpha$ -particles to pass through, can Rutherford's findings be explained. Atoms must therefore have a significant amount of unoccupied space. The idea that an electron is too light of a particle to create any discernible deflection of the particle can be used to explain the large angle scattering that has been seen. Only if an atom's whole positive charge and mass are concentrated in a compact core, which Rutherford referred to as the atom's nucleus, with extremely small dimensions, might it be feasible for an atom to have an equal or even greater mass than itself. The observations of Rutherford can be summed up as follows:

- (i) The nucleus of an atom, which has very small dimensions, is where all of the positive charge and mass of the atom are concentrated.



(ii) An atom's diameter is approximately  $10^{-10}$  m, whereas the nucleus' diameter is between  $10^{-15}$  and  $10^{-14}$  m. Of course, the atom's nucleus takes up a space that is one million times smaller than the entire atom. As a result, the atom has a lot of empty space.

(iii) An atom is made up of a positive nucleus with electrons whirling around various orbits very quickly (Fig. 1). Atoms are electrically neutral because the overall negative charge of electrons equals the positive charge of the nucleus.



**Fig. 1 shows alpha scattering experiment and deflection of alpha particles in vicinity of nucleus(newagepublishers.com).**

According to Rutherford's hypothesis, the centrifugal force that the electrons experienced as a result of moving in orbits around the nucleus balanced the force of attraction between them and the nucleus. The following is how this model describes  $\alpha$ -particle scattering. The  $\alpha$ -particles are hefty and positively charged. It is possible to ignore the interactions between electrons electrical force of repulsion is needed. The particle that enters the atom at a significant distance from the nucleus encounters essentially no electrostatic repulsion and almost passes without deflection and  $\alpha$ -particles.  $\alpha$ -particles move at a high speed, therefore to deflect them at enormous angles, a significant.

This demonstrates how the atom contains a lot of unused space. The massive positive core (nucleus), on the other hand, exerts a very strong repulsive force on  $\alpha$ -particles that are travelling close to it, causing them to scatter along a wide angle in a single encounter. When a particle is directed towards the nucleus, the repulsive force causes it to slow down, eventually come to a stop, and then be repulsed away along its own route. Therefore, the main interaction is between the positively charged core nucleus at the heart of the atom with integral number  $Z$  and charge  $+Ze$ , and the doubly charged particle ( $+2e$ ). A particle approaching the nucleus directly with a mass of  $m$  and a velocity of  $v$  has kinetic energy equal to

$$\text{K.E. of alpha-particle, } E_k = \frac{1}{2} mv^2$$

### Drawbacks of Rutherford Atomic Model

The atom model proposed by Rutherford has a significant defect. Its shortcomings include the following:

(i) In this atomic model, the electrons orbit the nucleus in a Coulomb field just like planets do. We are aware that a particle travelling along a curved path is speeding up, and that a charged particle speeding up emits electromagnetic radiation while continuously losing energy. According to Newton's rule of motion and Maxwell's electromagnetic field equations, the atom would radiate all of its energy in a period of time of the order of  $10^{-10}$  seconds, and the electron would eventually fall into the nucleus. The atom would be destroyed as a result of this. Accordingly, it is impossible for an atom to contain separately charged positively and negatively, which defies both the laws of classical mechanics and empirical data.

(ii) The electromagnetic theory of radiations states that an electron in motion must continuously release radiations with increasing frequency. Contrary to what has been

observed, elements only emit spectral lines at specific fixed frequencies and not at all frequencies.

(iii) The distribution of electrons in different orbits around the nucleus is not governed by any rules.

The renowned Danish scientist Niels Bohr presented some new ideas in 1913 that were based on the quantum concept that Max Planck had put forth a few years previously in an effort to overcome the aforementioned Rutherford atomic model limitations.

### **Bohr's Atomic Model**

Bohr regarded the hydrogen atom as the most basic of all atoms. He agreed with the atom's Rutherford model. According to the Rutherford model, the hydrogen atom's orbit around its single proton-containing nucleus contains just one electron. Bohr believed that the electron had an orbit that was round. It should be noted that some ionized atoms can be described using the same straightforward model of the hydrogen atom. There are two electrons present in the helium atom. The helium ion  $\text{He}^+$ , which has only one electron circling in the orbit around the nucleus and carries two electronic units of positive electricity, is left behind as a result of the removal of one electron from it. The hydrogen atom is similar to the  $\text{He}^+$  ion as a result. Other instances outside  $\text{He}^+$  include  $\text{Li}^{++}$  ( $Z = 3$ ),  $\text{Be}^{+++}$  ( $Z = 4$ ),  $\text{B}^{+++}$  ( $Z = 5$ ), etc. The electrons are thought to be in a fixed, definite planetary system (in circular orbits) in Bohr's concept of the atom. Energy levels are the name given to these stationary states. Since each orbit has a specific amount of potential energy attached. Bohr believed that any atom's electron might exist in more than one energy level in this concept of the atom.

### **Bohr's Postulates**

A single electron can rotate around the nucleus of a hydrogen atom in one of several distinct orbits known as stationary orbits. Only orbits for which the angular momenta of the planetary electron are integral multiples of  $h/2\pi$  or, where  $h$  is the Planck constant, are allowed for the electrons. As a result, relation (9) provides the electron's angular momentum. Bohr's initial premise is this. Despite what the electromagnetic theory of light predicts, an electron in a stationary orbit does not emit electromagnetic radiation. Only when an electron transitions from a higher to a lower energy state does radiation take place. According to Planck's rule, the energy  $h\nu$  of the emitted radiation will be  $h\nu = E_2 - E_1$  (10), where  $\nu$  is the frequency of the emitted radiation and  $\omega = 2\pi\nu$  is the angular frequency, if the transition is from a higher energy orbit  $E_2$  to a lower energy orbit  $E_1$ . A photon is a unit of energy that is released from an atom as a result of an energy difference, abbreviated to  $h\nu$ . This demonstrates how atoms are where light waves originate. Unsurprisingly, an electron does not emit light when it is in one of its fixed orbits; instead, it emits light only when it changes orbits. Bohr's second postulate is this.

It is important to note that the aforementioned Bohr postulates directly conflict with both Maxwell's electromagnetic theory and the rules of classical mechanics. All orbits for the electron spinning around the nucleus are allowed under Kepler's equations in classical mechanics, just as they are for planets revolving in orbits around the sun. As a result, Bohr's first hypothesis involving fixed orbits defies the precepts of classical mechanics. A rotating electron must emit electromagnetic radiation since it is moving with centripetal acceleration, again in accordance with the electromagnetic theory of light. The electromagnetic theory of light obviously conflicts with Bohr's second postulate, which states that when the electron rotates in a stationary orbit, no radiation is emitted or absorbed.

The Bohr postulates were introduced as ad hoc hypotheses, it is important to remember that. Bohr acknowledged that the laws regulating the mobility of electrons are those of classical mechanics. He set several limitations on the permitted orbits within the quantum condition. No mechanics were proposed by Bohr to explain the velocity of the electron. Bohr went on to

assume that the centrifugal force ( $=mv^2/r$ ) needed for rotation is provided by an inward electrostatic force of attraction between the positively charged nucleus and the negatively charged electrons in the case of a hydrogen atom. This is done to keep the electron in its orbit around the small, heavy center of the atom known as the nucleus and prevent it from spiraling towards or away from it to escape. According to Bohr, the electron was a negatively charged particle that travelled in a circle at a distance of  $r$  from the nucleus.

### **The Hydrogen Spectrum**

It was recognised towards the end of the 19th century that light with a discrete collection of light pictures known as spectral lines results from light with a continuous frequency distribution. These lines can be examined based on their frequency distribution or hue. Additionally, it was found that the wavelengths of a spectrum's lines group together into distinct groups known as series. Multiple series may be displayed by an element. An empirical formula that is similar for all the series of a particular element can be used to represent each series. J.J. Balmer made the first such discovery in 1885 while studying the visual spectrum of hydrogen, the simplest element and likely the simplest structure. Balmer series of hydrogen is the current name for this series.

### **Normal and Excited States of Atom**

A hydrogen atom is considered to be in the normal or ground state when its lone electron is in the ground state, or the innermost orbit, with  $n = 1$ . Now, if we allow an electrical discharge to pass through a container containing hydrogen gas, cathode rays (electrons) moving at a high speed frequently collide with electrons, forcing some of the electrons into one of the outer allowed orbits, i.e.,  $n = 2, 3, 4, 5, 6, \dots$ . The atom is said to be ionised when the electron has been totally expelled, or when  $n = \infty$ . The ionisation potential ( $V_i$ ) is the name given to the equivalent potential. The unit of measurement for ionisation energy or potential is the electron volt (eV;  $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$ ). The highest ionisation energies are found in inert or noble gases because these elements have stable electronic configurations. A shell or subshell is totally filled with electrons. We can see that alkali atoms, such as lithium and sodium, have low ionization potential because they have one electron in their outermost and innermost subshells, which is outside of the stable configuration and can therefore be removed from the atom with ease. Ionization energy is also related to the concept of electron affinity. This is the energy that is released when an electron is added to a neutral atom. The energy needed to transfer an electron from atom 1 to atom 2 is equal to the difference between their respective atoms' ionization energy  $I_1$  and electronic affinity  $E_2$ . Halogen atoms have the highest electron affinities, as can be seen.

However, the atom is said to be excited when the electron is compelled into an outer orbit (let's suppose  $n = 2, 3, 4, 5, \dots$ ). The electron is in its lowest energy level at the bottom in the unexcited normal state, also known as the ground state, with  $n = 1$ . The electron is said to be in a stable state when it moves constantly in this orbit without giving off or absorbing energy. An excited electron absorbs energy (let's suppose  $n = 2, 3, 4, 5, \dots$  orbits). An energetic emission occurs when an electron transitions from the excited state to one of the lower levels.

### **Limitations of Bohr's Theory of Hydrogen Atom**

The Bohr model of the hydrogen atom is somewhat successful, and the quantization of atomic energy idea is true, but the model is lacking in the following areas:

(i) The notion that only circular orbits are permitted, despite the fact that elliptical orbits are likewise feasible.

These presumptions are obviously arbitrary and unreasonable.

- (ii) Complex atoms, or systems having two or more planetary electrons, cannot be modelled using this atom's generic structure.
- (iii) The model provides no details regarding the distribution or arrangement of electrons within the atom.
- (iv).The model is incapable of handling unbound systems
- (v) The model is based on the planetary model, which merely introduces the principal quantum number,  $n$ .
- (vi) The model does not explain why some spectral lines are more intense than others, and it does not offer a way to determine how quickly one energy level changes to another.
- (vii) Model is unable to account for electrons' wave-like characteristics.
- (viii) The model is unable to account for the fine hydrogen structural lines.
- (ix) The model is unable to explain how interactions between individual atoms lead to an exaggerated amount of matter.
- (x) Model doesn't explain chemical bonding in any way.

### **Sommerfeld Wilson's Model of Atom**

The electron in Bohr's atomic model is thought to be circular. However, if the force  $F \propto 1/r^2$ , the centre of the force is at one of the foci of the ellipse and the orbit of the particle is affected by an attractive force directed towards a fixed point (central force) and the particle's energy  $E$  is negative. Only in certain circumstances is the orbit circular. In addition to demonstrating how to loosen the Bohr atomic model's constraint to circular orbits, Sommerfeld and Wilson made a relativistic modification to it in 1916. Sommerfeld and de Broglie have considered a number of adjustments to account for the fine structure as well as the observable spectra of complex atoms with two or more planetary electrons. According to Newtonian mechanics, elliptical orbits are also possible, and Sommerfeld expanded Bohr's theory to include them. For this he preserved the quantum number  $n$ , which is now defined in terms of the total momentum, and introduced a second quantum number  $l$ , which is equivalent to the angular momentum number  $l$  introduced earlier. Sommerfeld undoubtedly introduced two new quantum numbers.

### **Periodic Table**

109 elements have been found by scientists. In 1869, Mandeleev developed a method for tabulating all the known elements based on the periodicity of their chemical characteristics. Mandeleev's periodic table is what it is called.

### **Mandeleev Periodic Table**

Mandeleev found that the elements with comparable qualities appear at regular intervals if the elements are organised in the order of increasing atomic weights. Based on this finding, Mandeleev developed a law that states that an element's properties are a periodic function of its atomic weight. In order to ensure that elements with comparable properties are placed next to one another in the same vertical columns or groups, Mandeleevorganised all of the known elements at the time in horizontal rows in ascending order of their atomic weights. Seven horizontal rows, or periods, and eight vertical columns, or groups, made up Mandeleev's periodic table. He left some gaps in his periodic table to ensure that elements with comparable properties fell into the same vertical column or group. These holes were probably left to accommodate elements that weren't yet understood.

Although the Mandeleev periodic table of elements was very important for studying elements, it was unable to explain where isotopes were located. Isotopes didn't have their own spot in the periodic table. Additionally, it was discovered that occasionally, elements with greater atomic masses emerge before those with lower atomic masses. Later researchers came to the conclusion that atomic weight cannot be used as the basis for classifying elements as a result of these disadvantages.

## CONCLUSION

Understanding how atoms and elements behave and exhibit certain qualities depends on the study of atomic structure and electrical configuration. This essay examined the major ideas surrounding these subjects and emphasized how crucial they are to physics and chemistry. The organization of subatomic particles within an atom is shown by its atomic structure. Protons and neutrons make form the nucleus, which is in the center, while electrons are found in various energy levels called shells all around it. The total number of protons and neutrons determines the atomic mass, whereas the number of protons determines the atomic number, defining the identity of the element. The distribution of electrons at various energy levels and orbitals is referred to as their electronic configuration. There are a few rules that govern how electrons are arranged, including the Aufbau principle, Pauli exclusion principle, and Hund's rule. These laws control the atoms' stability and reactivity as well as how their orbitals are filled.

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## CHAPTER 3

### APPLICATIONS OF CRYSTAL GEOMETRY, STRUCTURE AND DEFECTS

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#### ABSTRACT

Fundamental concepts in materials science and solid-state physics are flaws, crystal geometry, and crystal structure. A three-dimensional arrangement of atoms or molecules, a crystal, has clearly defined geometric structures and recurring patterns. While crystal defects are imperfections or departures from the ideal crystal structure, crystal structure refers to the configuration of atoms or molecules within a crystal lattice. The summary of crystal geometry, structure, and flaws in this abstract emphasizes the importance of these factors in comprehending the characteristics, behavior, and applications of crystalline materials. Fundamental characteristics of solid-state materials such as crystal geometry, structure, and defects are critical in defining their physical and chemical properties. In order to comprehend the behavior and properties of crystalline materials, this abstract gives a general overview of crystal geometry, structure, and flaws. The arrangement and organization of atoms or ions in a crystal lattice is referred to as crystal geometry. Crystals are three-dimensional collections of unit cells that repeat and are distinguished by certain geometric properties including lattice constants, angles, and symmetry. The overall shape, symmetry, and characteristics of the crystal are determined by its geometry, which is influenced by interactions between atoms or ions. The arrangement of atoms, ions, or molecules within a crystal lattice's unit cell is referred to as the crystal structure. The orientations of the individual particles, their separation from one another, and the bonding patterns that hold the crystal together are all described in great detail. Utilizing methods like X-ray crystallography, which makes it possible to identify the locations of atoms inside a crystal lattice, crystal structures are frequently described.

#### KEYWORDS

Atoms, Crystal, Lattice, Planes, Space, Structures, Symmetry.

#### INTRODUCTION

Introduction length can be as per the nature of the topic. Hence it can be prepared as per the discretion of the author. In nature, there are primarily two types of solids: crystalline and non-crystalline (amorphous), which have quite different properties. The majority of crystalline solids are composed of millions of minuscule grains, or single crystals, which make up their microstructure and are referred to as polycrystalline. This grain is positioned randomly in relation to one another. But a single grain is a single crystal, no matter how big it is. Metal single crystals of volumes several cubic centimeters are reasonably simple to manufacture in a lab. Regular polyhedrons, single crystals are polyhedral whose shape is determined by their chemical makeup. Crystalline bodies keep their structure and remain solid up to a specific temperature, or melting point, where they transition from a solid to a liquid state. At the specific solidifying temperature or point, the reversal process of solidification occurs during cooling. Both times, the temperature stays the same until the material has completely melted or solidified, accordingly [1], [2].

Amorphous substances lack crystalline structure when condensed; examples include common glass, sulphur, selenium, glycerine, and the majority of high polymers. When heated, amorphous bodies progressively become softer across a large temperature range, become

viscous, and only finally transform into a liquid state. The process moves in the reverse direction during cooling. An amorphous body's instability may cause a partial or total shift to the crystalline state during repeated heating, protracted holding at 20–25°C, or, in some situations, deformation. The turbidity effect that appears in inorganic glasses upon heating or in optical glasses after prolonged usage are examples of such shifts from an amorphous to crystalline state. Other examples include the partial crystallisation of molten amber upon heating and the further crystallisation and strengthening of nylon threads under strain.

Ions, atoms, or molecules in crystalline solids are arranged in an organised manner. The electrical structure of atoms and the type of interactions they have within the crystal, the spatial arrangement of their ions, atoms, or molecules, and the composition, size, and form of the crystal all affect the properties of crystals [3], [4]. A crystalline substance can either be a single crystal or an aggregate of several crystals, known as polycrystalline, that are divided by sharp borders known as grain boundaries. Because the crystals in polycrystalline materials have distinct orientations with regard to one another and grain boundaries prevent dislocations from moving, polycrystalline materials are stronger than conventional ones. These crystals are called isotropic because they display the same properties in all planes and directions, in contrast to anisotropic single crystals.

## Crystals

These solids are composed of flat faces that are ordered oriented in relation to one another, converge at their edges and vertices, and have regular periodic arrangements in their component parties. A crystal is symmetrical with respect to specific elements, such as points, lines, or planes, thus if it were to rotate around these elements, it would be impossible to tell the difference between its new position and its original position. This symmetry is a crucial trait depending on the crystal's internal structure. One can categorise crystals and describe their behavior using symmetry. All solids can remain in their crystalline state at temperatures lower than those required for crystallization.

## Single Crystal

The majority of substances are polycrystalline, however some substances, such as sugar, sodium chloride (common salt), diamond, etc., are single crystals. Single crystals are created artificially from a material's vapor or liquid state and depict it in its perfect state. We may examine the behaviors and flaws of the material using these crystals under optimal circumstances.

## Whiskers

These are extremely thin filaments, solitary crystals that resemble hair, measuring around 13 mm in length and possibly 10–4 cm in diameter. These are generated as free crystal dislocations and have no structural flaws. Because of this, whiskers are much more durable than polycrystals made of the same material. By incorporating fibres of one material into a matrix of another, these are utilised as reinforcements in materials to boost strength. These fibre- or whisker-reinforced composites' characteristics can frequently be customised for a particular application. The whiskers' increased diameter boosts their ductility while reducing their strength. The main drawback of the technology is the high cost of the whiskers and the pricey fabrication. The most flawless crystalline solids now on the market are called whiskers. The most well-known composite material is arguably fibre glass, which is made of glass-reinforcing fibres embedded in a matrix of polyester or an epoxy polymer. Fibre glass can withstand significant stresses at both low and relatively high temperatures [5], [6].

Specialised procedures can be used to create single crystals of SiC, Al<sub>2</sub>O<sub>3</sub>, S-Glass, graphite, boron, iron, silver, copper, and tin. A wide range of materials, including mercury, graphite, sodium and potassium chlorides, copper, iron, and aluminum oxide, have all had their



whiskers produced from extremely saturated media. These whiskers can grow up to a few inches long and have a diameter of a few micrometres. Some demonstrate outstanding strength in both tension and bend testing.

The electrical, magnetic, or surface properties of whiskers are frequently extraordinary in addition to their strength. This behavior suggests that the crystal structure of whiskers is almost flawless, especially in terms of line flaws. In reality, it seems that some whiskers have line flaws while others don't. However, no clear relationship between whisker structure and characteristics has been found.

### **Lattice Points and Space Lattice**

The term "crystal structure" refers to the arrangement of atoms in a crystal. There is a regular arrangement of atoms in a flawless crystal. In a model of a crystal, the ions, atoms, or molecules that make up its structure can be visualised as spheres that are in regular contact with one another and organised in various directions. In a straightforward representation of crystal structure, points in place of spheres represent the centres of ions, atoms, or molecules. Ions, atoms, and molecules are typically arranged in periodic ways that vary in different directions. It is quite convenient to visualise the locations of these atoms, ions, or molecules in space. Lattice points are such points in space. A crystal lattice or space lattice is created when all of the lattice points are combined. A lattice is referred to as a Bravais lattice if all of the atoms, molecules, or ions at the lattice points are identical.

### **DISCUSSION**

A three-dimensional coordinate system that has the coordinate axis correspond with any three of the crystal's edges that overlap at one point and do not lie in a single plane is used to describe the space lattice of crystals. The three-dimensional space-lattice is obviously a finite array of points in three dimensions where each point has the same environment as every other point in the array. When comparing the symmetry of real crystals, the space lattice is a very helpful reference. The basis for describing a crystal structure can be found in a space lattice. It is important to understand the difference between a lattice and a crystal structure. A crystal structure is created by joining an assembly of atoms that are similar in composition, arrangement, and orientation to each lattice point. R.J. Haüy developed the space-lattice theory to explain the unique geometric characteristics of crystal polyhedrons. An elementary unit with all the qualities of a crystal was said to exist, or alternatively, a crystal was created by juxtaposing such simple units[7], [8].

When three vectors (OA, OB, and OC) are used to define the mathematical points that make up a parallel-piped OABC's vertices, translations parallel to and equal to these vectors can be used to create a space lattice. The unit cell is referred to as the parallel-piped. We regularly come with complicated lattices in metals, which are made up of numerous primitive translation lattices that are displaced from one another. The majority of metallic crystals have atoms that are tightly packed and extremely symmetrical. The three most prevalent varieties of space lattices are hexagonal closed packed (HCP) lattices, body-centered cubic (BCC) lattices, and face-centered cubic (FCC) lattices.

### **Basis**

A collection of hypothetical points that are arranged in space in such a way that each point has the same surrounds is known as a space lattice. It is important to highlight that atoms, not points, are always used to describe the crystal structure. In order to create a crystal structure, one atom or group of atoms must be regularly positioned on each lattice point. The basis is a single atom or group of atoms that serves as the structural or building block for the entire crystal structure. It is obvious that a lattice and a basis together create the crystal structure. Because there are so many distinct types of basis accessible, it is obvious that one

can create a vast number of crystal structures using just fourteen space lattices. One obtains a monoatomic crystal structure when the basis is just one atom. One material with monoatomic face-centered cubic structures is copper. In biological materials, complex bases are found as examples.

### Unit Cell

As we've seen, the atomic arrangement of crystalline solids shows that even the smallest groups of atoms repeat themselves. Therefore, it is generally advantageous to divide the structure into repetitive little repeat units called unit cells when describing crystal formations; this means that some fundamental grouping of particles is repeated in every crystal. Undoubtedly, a unit cell is the space lattice's smallest unit. Fig. 1 shows lattice parameter of unit cell.

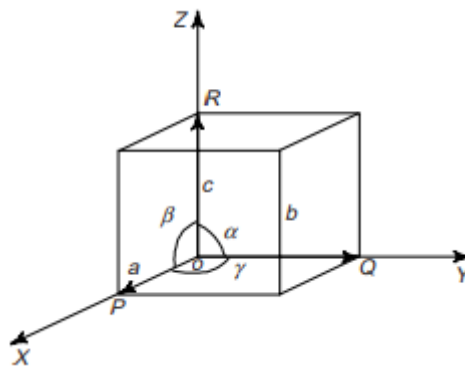


Fig. 1 shows lattice parameter of unit cell(newagepublishers.com).

### Primitive cell

This is a geometric design that, when repeated indefinitely in three dimensions, will completely cover the available space and correspond to one lattice point, i.e., the unit cell that only has one lattice point at the corners. Although the unit cell and the primitive cell may occasionally be the same, the former generally varies from the latter in that it is not limited to being the equivalent of one lattice point. Non-primitive cells are unit cells that have more than one lattice point. Although some primitive cells may be unit cells, not all primitive cells must be unit cells.

### Crystal glasses

In the crystalline state, atoms, molecules, or ions are arranged in a predictable, repeated, and symmetrical pattern; nevertheless, the crystal will only have an externally symmetrical structure if no restraint is applied during crystal growth. Crystals have symmetry in that any given direction within the crystal corresponds to one or more directions that, in terms of the attributes under consideration, are exactly the same. Symmetry operations, which cause the crystal to coincide with itself in various places, are used to study the symmetry of crystals. The most basic symmetry-related operations (rotation, reflection, and translation-parallel displacement) are related to these elements. The axis and planes of symmetry are the most basic symmetry components. If a crystal's shape includes one or more symmetrical components, it is considered to be symmetrical. A symmetry class is a collection of symmetry operations that often combines rotations, reflections, and rotations with reflection. An example of symmetry is:

(i) The Symmetry Plane: If a plane divides the shape of the crystal into two identical halves or two mirror images of one another, the shape is said to be symmetrical about that plane. We must keep in mind that the faces are only perfectly equal in size in an ideal crystal.

(ii) The Symmetry Axis: A shape is said to be on an axis if it can be rotated about it to occupy the same relative location in space more than once during a full rotation.

These axes might have 2, 3, 4, or 6 folds. When rotating by 360 degrees around its axis of symmetry, the crystal can occupy more than one congruent position.

(iii) The Centre of Symmetry: Within a crystal, there is a location where faces that are crystallographically comparable are arranged in parallel and equivalent positions, such as the center of a cube. We should be aware that a tetrahedron lacks such a center. The shape of a cube is highly symmetrical, and it has numerous planes and axes of symmetry.

The primary axes of a cube are quadruple, meaning that the crystal travels through four identical places during each full rotation about the axis. Six two-fold and three fold axes make up the body diagonal axes. The hexagonal prism's vertical axis is made up of six axes. An operation that leaves the crystal and its surroundings unchanged is known as a symmetry operation. Point group symmetry operations and space group symmetry operations are two different types of symmetry operations that are done around a point, line, or both. We must keep in mind that crystals display both symmetries alone and in appropriate combinations. Crystals display the following types of point group symmetry: (i) the center of symmetry, also known as the inversion center; (ii) reflection symmetry; and (iii) rotation symmetry[9], [10].

### Crystals Systems

The lattice is referred to be a Bravais lattice if all of the atoms at the lattice sites are the same. In two dimensions, there are four systems and five potential Bravais lattices. The oblique, rectangular, square, and hexagonal crystal systems are the four types of two-dimensional space. There are two Bravais lattices in the rectangular crystal system: rectangular primitive and rectangular centered. There are only fourteen distinct ways to organise points in three-dimensional space so that each arrangement satisfies or confirms the definition of a space lattice, based solely on symmetry considerations. Bravais lattices are these 14 space lattices with 32 point groups and 230 space groups. The mix of symmetry elements they display can be identified if they are seen as solids. Each space lattice has a unit cell that may be used to define it. This unit cell can be replicated in space an endless number of times to produce the full space lattice. The 14 various types of unit cells are organized into seven distinct classes of crystal lattices, hence seven distinct co-ordinate systems of reference axes are needed to explain basic crystal structures.

The features of 14 three-dimensional Bravais lattices are described, together with the axial connection for the class of crystal lattices seven systems to which each belongs.

1. Simple Cubic
2. Body centered cubic
3. Face-centered cubic
4. Tetragonal
5. Body-centered tetragonal
6. Orthorhombic
7. Base-centered orthorhombic
8. Body-centered orthorhombic
9. Face-centered orthorhombic
10. Monoclinic
11. Base-centered monoclinic
12. Triclinic
13. Trigonal
14. Hexagonal

## Crystal structures for Metallic Elements

In order for most common metals to crystallize, body-centered cubic structures (BCC) and face-centered cubic structures (FCC) are the most prevalent types of space lattice or unit cells. Structures with hexagonal closed packing (HCP)

(i) **Body-centered Cubic Structure (BCC):** In a BCC system, the unit cell has one atom at each corner that is shared by the eight adjacent cubes as well as the one in the body's center. Each unit cell naturally shares 8 atoms, one on each of its corners and an additional atom in the body's core.

(ii) **Face-centered Cubic Structure (FCC):** The atoms in this kind of lattice structure, sometimes referred to as a cubic packed structure, are situated in the middle of each face and at each of the cube's eight corners. The BCC structure is less frequent in metals than this sort of structure. Additionally, it crystallizes in ceramics. Common examples of metals with this kind of structure are Cu, Al, Ag, Au, Fe, Ca, Co, and Iron (910°C to 1400°C).

(iii) **Hexagonal Closed Packed (HCP) Structures:** In HCP structures, the unit cell has three additional atoms inside of it in addition to one atom at each of the hexagonal faces' centres and one atom at each of the hexagonal prism's corners. Due to the differences between the environments of the inside atoms and the corner atoms, the HCP structure does not constitute a space lattice.

## Atomic Radius

This is explained as being equal to half of an element's closest neighbors in its crystal structure. Atomic radius is stated in terms of the cube edge element and is indicated by the symbol  $r$ . By assuming that atoms are spheres in contact within a crystal, it is possible to calculate the atomic radius.

- (i) **Simple cubic structure-** Aspects of the lattice are touched by atoms in the SC structure.
- (ii) **Body centered structure-** the atoms are in contact with one another along the cube's diagonal. The diagonal in this situation is obviously  $4r$ .
- (iii) **Face centered structure-** Along the diagonal of every cube face, atoms in this structure touch. The diagonal is  $4r$  in length.

## Directions, Lattices and Miller Indices

There are directions and lattice planes in a crystal that have a lot of atoms in them. With the use of crystal directions, a variety of crystal properties, notably mechanical ones, are connected to the crystal structure. By examining the atomic locations within a unit cell, it is possible to acquire a comprehensive description of the crystal structure. Finding directions and lattice planes is crucial for crystal analysis

- (i) **Crystal Directions:** We take any lattice point on the line as the origin and define the vector connecting this to any other lattice point on the line as follows to specify the direction of a straight-line connecting lattice points in a crystal lattice.
- (ii) **Crystallographic planes:** The crystal lattice can be thought of as an amalgamation of a number of parallel, evenly spaced planes that run through the lattice points and are referred to as lattice planes, or atomic planes. The lattice planes for a given lattice can be selected in a variety of ways. The hardening reaction, plastic deformation, and other characteristics as well as the behavior of metal are significantly influenced by these crystal planes and crystal orientations.

**Miller Indices of Crystal Planes:** Key Features Several crucial characteristics of Miller indices of crystal planes include:

- (a) The Miller indices are identical for all parallel, equidistant planes. Miller indices undoubtedly specify a collection of parallel planes.
- (b) The Miller index is 0 because a plane that is perpendicular to one of the coordinate axes has an intercept of infinity.
- (c) Two planes are considered to be parallel to one another if their Miller indices have the same ratio, such as 844 and 422 or 211. In other words, all parallel planes with the same orientation and equal spacing have the same index number [hkl].
- (d) The only index ratio that matters is that miller indices of planes are represented by (hkl), meaning that the plane divides the axes into equal segments at the points h, k, and l. [xyz] square brackets are used to represent the directions in space.
- (f) The typical inside brackets are used singly, not in combination. Clearly, (111) should be read as 1+1 rather than "100-11."
- (g) Miller indices may also be negative, and when they are, a bar is placed over the digit, as in (0, 10).

### Crystal Growth

The following sequence of processes typically results in crystal growth: (i) diffusion of the crystallising substance's molecules through the crystal's environment (or solution) to its surface; (ii) diffusion of these molecules over the crystal's surface to specific sites; (iii) incorporation of molecules into the crystal at these sites; and (iv) diffusion of the crystallization process' heat away from the crystal surface. Any of these four steps has the potential to restrict the crystal growth rate. Nucleation is the first development of the centers from which crystal growth begins. The rate of crystal development can be increased by independently raising the temperature or the super-saturation of the crystallizing component. But in many physical circumstances, lowering the temperature raises the super-saturation. In these conditions, the rate of crystal development initially rises with falling temperature, reaches a maximum, and then falls. The growth is frequently significantly slowed down by presence of certain contaminants. The crystals in the medium develop apart from one another for a while after nucleation. However, if numerous crystals with various inclinations are forming, they may eventually collide, and inter-crystalline (grain) borders will be created. In these polycrystalline aggregates, the larger grains develop at the expense of the smaller ones through a process known as grain growth that occurs at relatively high temperatures.

### Anisotropy

If a body's physical characteristics are independent of the direction in which they are measured, the term "isotropic" is used to describe it. An isotropic body only has one refractive index, one dielectric constant, etc. Most liquids, but not all, and aggregates formed of tiny crystals distributed randomly in space are isotropic in every way. Single crystals may or may not be isotropic with regard to a particular property depending on their symmetry; for instance, single crystals with a cubic structure are isotropic with regard to electrical resistivity but not with regard to elastic deformability.

As a result of an ordered arrangement of atoms (ions, molecules), crystals have varying properties depending on their crystallographic direction. The condition is known as anisotropy. Atomic interactions control the characteristics of crystals. Because the distances between atoms in crystals vary along different crystallographic directions, different characteristics result. Almost all of a crystal's qualities are anisotropic. However, the

phenomena is more obvious in crystals with asymmetrical structures. Certain single crystals may exhibit higher resistivity along a certain crystallographic direction than along directions perpendicular to it when tested with the electric field. As a result, these crystals are anisotropic in terms of resistivity.

### Methods of Determining Crystals Structure

Crystal structure can be determined using the following techniques: (i) X-ray diffraction (a) The Bragg spectrometer technique (a) Laue's approach Powder technique (c) Diffraction of electrons and neutrons are two further examples.

#### Laue's Method

This is a key technique for researching X-ray diffraction and figuring out crystal structure. In this technique, a single crystal is positioned in the X-ray beam's path, and the glancing angle is maintained. The crystal is given permission to receive a wide variety of wavelengths of white radiation. Each crystal plane set chooses the proper wavelength value in accordance with Bragg's law. Each set of planes will undoubtedly result in a place that satisfies Bragg's law. A  $90^\circ$  polychromatic X-ray beam is directed towards the crystal's plane. As the rays travel through the crystal, they collide with Bragg's planes, which have varying  $d$  interplanar spacings. These several sets of planes create various angles depending on the X-ray beam's direction. It is clear that some combinations of  $n$  and  $d$  satisfy the Bragg's condition, increasing the intensity of diffracted X-rays. Fig. 1 shows Laue's Method.

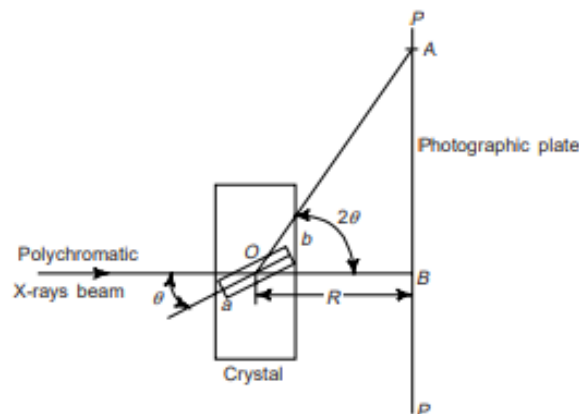


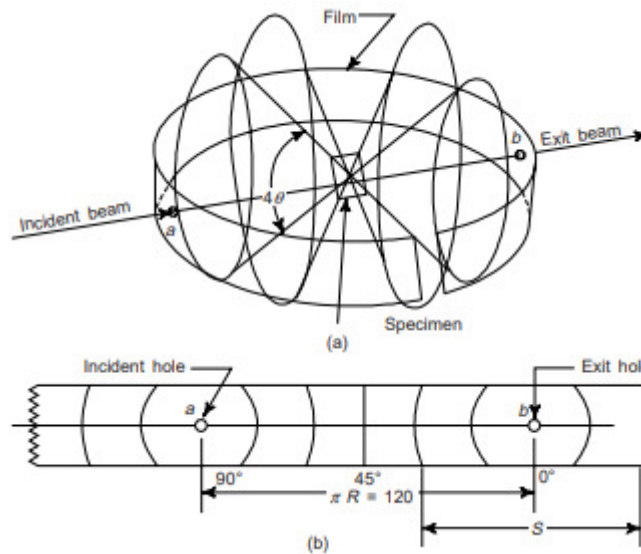
Fig.1 shows Laue's Method.(newagepublishers.com)

A black patch at B is created on photographic plate PP when primary rays are permitted to pass through the crystal. The fundamental X-rays contain a variety of wavelengths, which causes them to generate less conspicuous spots surrounding this focal spot. Let A be any location (other than the centre spot) on PP,  $ab$  be the position of one of the potential Bragg's planes, the associated angle, and B the corresponding angle's value. Finding  $AB = R \tan 2\theta$  (17) from AOB. One can determine the equivalent plane by using AB and R. For a single crystal of a considerable size, Laue's approach is particularly helpful.

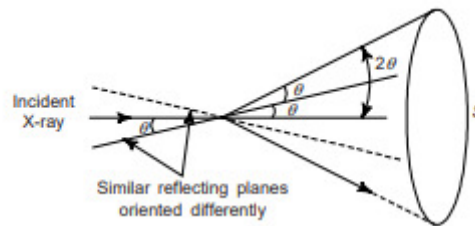
#### Powder Method

When there aren't any huge single crystals accessible, this procedure is very helpful. It is possible to determine a crystalline solid's structure using a method. The material that was used is a thin powder made up of several small crystallites that have random orientations. It is made by crushing the widely accessible polycrystalline material, which avoids the time-consuming task of generating the individual crystals. The powder is squeezed and bonded into a thin spindle, plastered on a thin wire, or inserted in a capillary tube. A strip of circular photographic film is fixed around the centre of this powder specimen. Fig. 2 shows powder

method (a) photographic film position (b) flattened photographic film after developing and indexing of different lines. Fig. 3 A cone produced by reflection of X-rays from identical planes having different orientations.



**Fig. 2 shows powder method (a) photographic film position (b) flattened photographic film after developing and indexing of different lines(newagepublishers.com).**



**Fig. 3 A cone produced by reflection of X-rays from identical planes having different orientations(newagepublishers.com).**

## Electron and Neutron Diffraction

We must monochromatize the thermal neutrons from nuclear reactors because of their wide energy distribution. The crystal is exposed to these neutrons, and one of the reflected beams is chosen. This is permitted to land on the test sample that is being looked at. Through a counter, the scattered beam's intensity is determined. Though there are numerous similarities between the X-ray and neutron diffraction studies, it is important to emphasise that there are also many discrepancies. Neutrons are dispersed by nuclei, whereas electrons scatter X-rays. Since X-rays are unable to produce exact results when studying low atomic weight elements, neutron diffraction can be used to analyse a variety of these elements. We are aware that a neutron has a magnetic moment and that this magnetic ordering results in extra scattering. Since X-ray or electron diffraction investigations cannot show this structure, neutron diffraction studies have become crucial in determining magnetic structure. Additionally, neutrons can be used to examine lattice vibrations.

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### Crystals Growth Method

Large, high-quality single crystals of semiconductors and related electronic materials were in high demand with the development of semiconductor-based technologies. In order to increase the degree of flexibility in the material properties, significant semiconductor crystal components' compositions were changed over relatively short distances as semiconductor devices became more complex. It is frequently necessary to use single-crystal structures that are thin, multilayered, and even include compositional variations that are both normal and lateral to the direction of growth.

### CONCLUSION

In solid-state physics and materials research, the investigation of crystal geometry, structure, and defects is fundamental. This essay has examined the key ideas surrounding these subjects and has emphasized their significance for comprehending the characteristics, behavior, and uses of crystalline materials. The geometric configuration of atoms or molecules in a crystal lattice is referred to as crystal geometry. Crystals have particular symmetries and shapes, such as cubes, spheres, or prisms, depending on how the individual particles are arranged. The interpretation and prediction of numerous material properties, including as optical, electrical, and mechanical behavior, are made possible by our understanding of crystal geometry. The arrangement of atoms or molecules within a crystal lattice is referred to as crystal structure. It entails locating and describing unit cells, which are the recurring structural elements that make up the crystal. Understanding the crystal structure reveals information on the spatial arrangement of atoms inside the lattice, the density of the crystal, and the bonds that hold together individual atoms or molecules.

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## CHAPTER 4

# EXPLORING THE OF DEFECTS OR IMPERFECTIONS IN CRYSTALS

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### ABSTRACT

The ideal, organized structure of crystalline materials is deviated from by defects or faults in crystals. These flaws have a substantial impact on the characteristics and behavior of materials and can develop during crystal formation, processing, or as a result of outside causes. This abstract gives a general overview of the several forms of crystal defects, such as point, line, and planar defects, and emphasizes how they affect the properties and uses of materials. A variation from the ideal atomic arrangement within the crystal lattice constitutes a defect or imperfection in a crystal. These flaws can be found at many scales, from atomic-level flaws to extended flaws, and they can significantly affect a material's mechanical, electrical, optical, and physical properties. The types, formation processes, and consequences on material behavior of flaws or faults in crystals are highlighted in this abstract. Three primary forms of flaws can be found in crystals: point flaws, line flaws (dislocations), and planar flaws (interfaces and grain boundaries). Point defects are localized departures from the ideal atomic arrangement caused by additional or missing atoms in the crystal lattice. Interstitials, vacancies, substitutional impurities, and self-interstitials are a few examples of point defects. Numerous characteristics, including electrical conductivity, diffusion, and optical activity, can be impacted by these flaws. Line defects, also known as dislocations, are one-dimensional flaws that develop when atoms are arranged incorrectly along a particular path in the crystal lattice. Dislocations can affect the mechanical strength, plastic deformation, and creep behavior of a material. They are vital in defining how the material reacts to outside stressors and can cause crystal structural flaws to form during production or processing.

### KEYWORDS

Atoms, Crystal, Dislocation, Flaws, Lattice.

### INTRODUCTION

Atoms were organized in regular patterns in perfect crystals. Real crystals' structure, however, differs from ideal crystals. Real crystals are never completely flawless; as a result, the arrangement of atoms within a crystal's volume is never absolutely regular. Natural crystals always have flaws, frequently a lot of flaws, because of the chaotic conditions in which they developed. These crystals may be valued as gems if they have color-altering flaws, like in ruby (which results from chromium replacing a small portion of the aluminum in aluminum oxide, or  $Al_2O_3$ ). Even though there is significant control over their type, concentration, and distribution, laboratory-prepared crystal will always have flaws.

Defect relevance varies depending on the material, defect kind, and qualities taken into account. A modest defect concentration will have very little impact on several properties because they are inversely correlated with defect concentration, such as density and elastic constants. Other characteristics, such as an insulating crystal's color or a semiconductor crystal's conductivity, may be significantly more sensitive to the presence of a tiny number of flaws. Even though faults are often associated with unwanted features, they are also responsible for many of the crucial characteristics of materials. A large portion of material science is around studying and engineering defects to give solids the appropriate

characteristics. The usage of silicon in electronic devices is reliant upon minute quantities of chemical impurities such as phosphorus and arsenic which give it desired qualities. A defect free, i.e. ideal silicon crystal would be of little value in current electronics. While many properties of greatest technical importance, such as mechanical strength, ductility, crystal growth, magnetic hysteresis, dielectric strength, and semiconductor condition, which are referred to as structure sensitive, are greatly affected by the relatively minor changes, some properties of materials, such as stiffness, density, and electrical conductivity, which are referred to as structure-insensitive, are not affected by the presence of defects in crystals. On the basis of their geometry, crystalline flaws can be categorized as follows:

There are four types of imperfections: point, line, surface, and grain boundary flaws, as well as volume flaws. A point defect's size is comparable to an interatomic space's. When it comes to linear faults, their length is significantly larger than their breadth. While surface imperfections' breadth and length may be several orders larger than their depth, they have a modest depth. Volume flaws (pores and cracks) could be at least a few tens of in size in all measurements[1], [2].

### **Point Imperfections**

The lattice flaws at isolated lattice sites, known as point defects, are caused by improper atom packing during crystallization. Point defects are also a result of atoms vibrating at high temperatures. Point flaws only have a local impact, such as a vacant lattice location. In crystals, point defects are always present, and their presence causes the free energy to drop. (i) Vacancies: A void is the most basic point fault. Such defects may result from either improper packing during initial crystallization or from thermal vibrations of the atoms at higher temperatures. This refers to an empty (unoccupied) site in a crystal lattice, i.e., a missing atom or vacant atomic site. In the latter scenario, there is always a greater chance that individual atoms will leave their positions of lowest energy when the thermal energy brought on by vibration is increased.

An equilibrium concentration of vacancies and interstitial atoms exists for each temperature; an interstitial atom is an atom that has been moved from a site into an interstitial position. For instance, copper can have between 10 and 13 vacancies per 10<sup>4</sup> atoms when the temperature is between 20 and 25 °C, and it can have as many as 0.01% of vacancies when the temperature is close to the melting point. The mentioned thermal energy is on the order of 1 eV per vacancy for the majority of crystals. As temperature rises, atoms' thermal vibrations get louder. The vacancies can be solitary or they can combine into a di-vacancy or a tri-vacancy if there are two or more of them. The lattice planes are distorted because the atoms next to a vacancy have a tendency to be closer together. A specific percentage of vacancies are present in a crystal at thermal equilibrium, increasing the structure's unpredictability. Vacancies are more concentrated and are able to shift locations more frequently at higher temperatures. The most significant type of point defects are vacancies, which speed up all atomic displacement processes like diffusion and powder sintering.

## **DISCUSSION**

### **Interstitial Imperfections**

If the atomic packing factor is low in a closed packed structure of atoms in a crystal, an additional atom may lodge within the crystal structure. This type of location, or voids, is referred to as interstitial. Only when an extra atom is significantly smaller than its parent atoms can it reach the interstitial space or void between the regularly spaced atoms, failing which it will result in atomic distortion. The resulting flaw is referred to as an interstitial defect. The greatest size of an atom that can fit in the interstitial void or space in closely packed structures, such as FCC and HCP, has a radius that is around 22.5% of the radii of the

parent atoms. Additionally, interstitialcies might be single, double, or triple interstitial. We must keep in mind that interstitialcy and vacancy are opposite phenomena[3].

**Frenkel Defect:** The defect formed when a missing atom, which is in charge of creating a vacancy, occupies an interstitial site (in charge of creating an interstitial defect), is referred to as a Frenkel defect. Vacancy and interstitial flaws are, of course, both components of the Frenkel defect. Due to the energy needed to move an ion into a new place, these faults are less frequent. Because positive ions are smaller in size and can easily lodge in the interstitial regions, this sort of flaw is more prevalent in ionic crystals.

**The Schottky Defect:** These flaws resemble vacancies. Every time a pair of positive and negative ions is missing from a crystal, this defect results. This kind of flaw preserves charge neutrality. In contrast to vacancies and Schottky defects, closed-packed structures featureless interstitialities and Frenkel defects because it takes more energy to move the atoms into their new places.

**Substitutional Defect:** When a foreign atom replaces the lattice's parent atom and takes its place, a defect known as substitution defect results. In this kind of defect, the parent atom's replacement atom may be the same size, slightly smaller, or slightly larger than the parent atom.

**Phonon:** Thermal vibrations occur as the temperature rises. As a result, the symmetry is flawed and the shape of the atoms deviates. The magnetic and electric properties are significantly impacted by this imperfection[4]. The crystal lattice is distorted by various point defects, which also have an effect on the material's physical characteristics. Point flaws in commercially pure metals increase the electric resistance while having little to no impact on the mechanical qualities. The ductility and other characteristics of irradiated metals are only significantly diminished at high defect concentrations.

Point flaws can develop through a variety of processes in addition to temperature variations. Quenching (rapid cooling) from a higher temperature is one way to increase the amount of point defects at a specific temperature. The crystal lattice can also be severely deformed, such as by hammering or rolling, to produce extra flaws. We must keep in mind that even though many faults are added, the lattice still mostly preserves its crystalline character. Excessive point defects can also be produced by external bombardment with atoms or high-energy particles, such as neutrons from a nuclear reactor or the cyclotron's beam. A point defect is produced when the first particle collides with the lattice atoms and moves them. The quantity of point defects produced in this way does not depend on temperature, but solely on the crystal's composition and the blasting particles[5], [6].

### **Line Defects or Dislocations**

Dislocations are irregularities in lines. Dislocation is a linear disturbance, or one-dimensional flaws in the atomic arrangement's geometry, that can very readily happen in the slip plane through a crystal. Edge and screw dislocation linear flaws are the most significant types. Both of these categories are created during the deformation process. These two flaws, which are the most obvious flaws, cause the useful feature of ductility in metals, ceramics, and crystalline polymers.

(i) **Edge Dislocation-** An additional partial plane of atoms is added to the crystal to create this particular sort of dislocation. A dislocation's edge is basically a 'additional' half-plane in the crystal lattice, as seen in its cross-section. Elastic distortion occurs in the lattice surrounding the dislocation. Zones of compression and tension in the crystal lattice are what cause the deformation in the crystal close to the dislocation. In contrast to below this line, where it is in tension, the lattice is compressed above the line of dislocation. It is important to remember that the dislocation line has a higher energy level than the remainder of the crystal.

The Burgers vector is referred to as the distortion criteria. If a closed contour is made around a zone in an ideal crystal by moving from one site to another as illustrated and the process is subsequently repeated around a zone in a real crystal that has a dislocation, the zone's existence can be ascertained. The contour described in the genuine crystal turns out to be unclosed. The Burgers vector is the one needed to close the contour. An edge dislocation's Burgers vector is parallel to the dislocation line and equal to interatomic space.

(ii) Screw Dislocation- The creation of a screw dislocation is depicted. In this, the atoms are moved in two different planes that are orthogonal to one another. Atoms are arranged in screw dislocations in a way that resembles a screw or a helical surface.

### **Climb motion is not present in a screw dislocation**

The following consequences of screw dislocation are crucial.

(i) It's likely that more force is needed to create and move a screw dislocation than to start an edge dislocation.

(ii) Plastic deformation is feasible at low stress levels without disrupting the continuity of the lattice.

(iii) Screw dislocation results in spiral distortion of the planes and distorts the crystal lattice for a significant distance from the line's center. We must keep in mind that both forms of dislocations, i.e., combinations of edge and screw dislocations, are strongly related to crystallization and deformation[7], [8].

The dislocation density is the sum of the lengths of all the dislocation lines in a given volume. In semiconductor crystals, it might be equal to  $10^4$ – $10^5$  cm<sup>2</sup> and in annealed metals,  $10^6$ – $10^8$  cm<sup>2</sup>. The dislocation density may increase to  $10^{11}$ – $10^{12}$  cm<sup>-2</sup> after cold plastic deformation. Any attempts to increase the dislocation density above  $10^{12}$  cm<sup>-2</sup> quickly result in the metal breaking and failing. Dislocations first occur during crystallization; at this point, their density may be quite high, and they have a significant impact on the characteristics of materials. Dislocations take part in phase changes and recrystallization along with other defects. They can also act as the nuclei for the precipitation of a secondary phase from solid solution. The rate of diffusion through a crystal lattice with defects is several orders of magnitude slower than that along dislocation lines. Since this lessens lattice distortions, dislocations are used as sites for the accumulation of impurity atoms, particularly interstitial impurities. The Cottrell atmospheres, which prevent dislocation movement and fortify the metal, can arise when impurity atoms cluster around dislocations.

Dislocations have a particularly noticeable impact on crystal strength. Metals' experimentally determined yield strengths are only one thousandth of their theoretical values, with mobile dislocations being mostly responsible for the loss. A metal's strength can be increased several times beyond its strength in the annealed condition by significantly increasing the dislocation density and lowering the dislocation mobility. Metals with no flaws, especially long, thin "whiskers" formed by crystallization from the gaseous phase, have strengths that are close to their theoretical values.

Dislocations have specific geometrical properties, such as (i) the requirement that the vectorial sum of the Burgers vectors of dislocations converging at the node must be zero, which is comparable to Kirchhoff's law for electrical currents converging at a junction, and (ii) the impossibility of a dislocation line abruptly terminating inside a crystal. Either a node or the surface serves as its conclusion. A dislocation line can also loop back on itself to shut. The compressive and tensile strains around an edge dislocation or the shear strains around a screw dislocation show that dislocations have distortional energy associated with them. One can assume that these strains are elastic strain as a first approximation.

## Surface and Grain Boundary Defects

Structure-related surface and grain boundary defects are two-dimensional and result from changes in the arrangement of atomic planes on or across a boundary. One of the planes' orientations or the order in which they are stacked may have changed. High-angle and low-angle borders, stacking faults, and twin boundaries are the most significant surface flaws. External and interior surface defects are the two main categories. A material's external surface is inherently flawed since the atomic bonds stop there. While atoms inside the crystal have neighbors on both sides of them, surface atoms only have neighbors on one side. The energy of surface atoms is higher than that of inside atoms because they are not completely surrounded by other atoms. The energy of the surface atom for the majority of metals is on the order of  $1 \text{ J/m}^2$  [9], [10]. Defects such as grain boundaries, tilt boundaries, twin boundaries, and stacking faults are examples of internal surface imperfections.

### Grain Boundaries

Single crystal or polycrystalline materials are both acceptable for engineering purposes. There is a tone of tiny grains in a polycrystalline alloy. Grain boundary imperfections are those surface flaws that, during the nucleation or crystallization of a polycrystalline aggregation, divide crystals or grains with various orientations. The existence of neighboring grains frequently has an impact on a grain's form. A border between any two grains is effectively a transition layer with a thickness of 1–5 nm because the lattices of adjacent grains are orientated randomly and differently. This layer could contain an unorganized atomic structure, clusters that are dislocated, and a significant number of contaminants.

A transition zone that is not aligned with either grain exists between two adjacent grains at grain borders where the atomic packing is poor. We therefore observe that boundary atoms in such situations cannot have a complete complement of surrounding atoms. The neighboring grain's orientation mismatch results in a less effective packing of atoms at the boundary. As a result, the atoms at the boundary are more energetic than those found inside the grains. The nucleation of polymorphic phase shifts is also influenced by the boundary atoms' greater energy. An interphase border, also known as an interface, is the boundary between two crystals with differing crystallographic layouts or compositions. Atomic diffusion is favored by the boundary's reduced atomic packing. High angle grain borders are defined as those where there is a greater than  $10^\circ$ – $15^\circ$  variation in orientation between two neighboring grains. Sub grains or blocks make up each grain in turn. A section of a crystal with a comparatively uniform structure is called a sub-grain. Walls of dislocations serve as sub-grain borders, dividing a grain into several sub-grains or blocks. Because the mis-orientation angle between adjacent sub-grains is small (less than  $5^\circ$ ), their boundaries are referred to as having a "low angle." Low angle borders might act as areas where contaminants build up.

### Tilt Boundaries

The orientation difference between two nearby crystals is less than  $10^\circ$ , making this a low-angle border surface flaw. Due to this, the boundary disruption is not as severe as it is in the high angle boundary. This kind of boundary is made up of edge dislocations stacked one on top of the other and is linked to relatively low energy. Low-angle boundaries can generally be described by adequate arrays of dislocation. Angle or tilt =  $b/D$ , where  $b$  is Burgers vector's magnitude and  $B$  is the typical vertical spacing between dislocations.

### Twin Boundaries

This is yet another flaw in a planar surface. The atomic configuration on one side of a twin boundary mirrors the configuration on the other. Twinning can happen when materials are deformed or while crystals are growing. Twin boundaries appear in pairs, restoring the orientation shift that was caused by one boundary. The twinned region is the area that lies

between the two boundaries. Twin borders are clearly discernible under an optical microscope. Mechanical twins are twins that occur during the process of recrystallization, or mechanical working, whereas annealing twins are twins that form as a result of annealing after plastic deformation.

### **Stacking Faults**

This is a region of an atomic plane that is limited between dislocations and where there is a disruption in the usual alternation of atomic layers. This particular fault type results from the stacking of two out-of-order atomic planes while the lattice on either side of the fault is flawless. For instance, close-packed atomic layers in FCC lattice alloys typically alternate in the pattern ABC ABC AB. Upon overcoming a stacking fault. For instance, their alternation may become ABC BCA BC. The stacking fault in the situation under consideration acts as, in a sense, a thin plate of an HCP lattice in the structure of an FCC lattice since the BCBC alternation is typical of an HCP lattice. Here, an ideal FCC crystal's stacking sequence is given as ABC ABC, while a stacking error may cause the sequence to alter to ABC ACAB.

### **Volume Imperfections**

When there is only a slight electrostatic difference in the stacking sequences of closely packed planes in metals, volume defects, such as cracks, may develop. Additionally, when atom clusters are missing, a significant emptiness or void results, which is also a volume imperfection. Volume imperfections are also known as foreign particle inclusions, big voids, or non-crystalline regions with size of the order of 0.20 nm.

### **Liquid Crystals**

These liquids have some degree of order in their molecular structure. Liquid crystals sit in between normal liquids with disordered molecules and crystals due to the ordered arrangement of their molecules. Although fluid like other liquids, liquid crystals have crystal characteristics that are anisotropic. There are several types of liquid crystals that are known today; among them, some organic substances with molecules of an elongated form are significant. Due to some peculiarities in molecular interaction, these elongated molecules are ordered in a specific order upon melting. In the temperature range between the melting point and the point at which the liquid crystal transforms into an isotropic liquid, the intermediate state of a liquid crystal with ordered structure is kept. Thermal oscillations grow and the organized molecular structure totally vanishes at this transition, turning the substance transparent. This is why the brightening point—the maximum temperature at which a liquid crystal can exist—is so named.

### **Anisotropy**

If a body's physical characteristics are independent of the direction in which they are measured, the term "isotropic" is used to describe it. An isotropic body only has one refractive index, one dielectric constant, etc. Most liquids, but not all, and aggregates formed of tiny crystals distributed randomly in space are isotropic in every way. Single crystals may or may not be isotropic with regard to a particular property depending on their symmetry; for instance, single crystals with a cubic structure are isotropic with regard to electrical resistivity but not with regard to elastic deformability. As a result of an ordered arrangement of atoms (ions, molecules), crystals have varying properties depending on their crystallographic direction. The condition is known as anisotropy. Atomic interactions control the characteristics of crystals. Because the distances between atoms in crystals vary along different crystallographic directions, different characteristics result. Almost all of a crystal's qualities are anisotropic. However, the phenomena is more obvious in crystals with asymmetrical structures. Certain single crystals may exhibit higher resistivity along a certain

crystallographic direction than along directions perpendicular to it when tested with the electric field. As a result, these crystals are anisotropic in terms of resistivity.

### **Theory of Dislocations**

In the study of dislocations, the phrases (i) Burger vector, (ii) Dislocation climb, (iii) Cross slip, (iv) Jogs in dislocation, and (v) Perfect and Partial dislocations are constantly employed.

### **Dislocation Climb**

Grain boundaries, interface planes, or dislocations intersecting the slip plane are just a few examples of the different obstructions that prevent dislocation movements. Some barriers can be overcome via dislocations under high stress. For instance, these are the dislocations that cross the slip plane.

Contrarily, dislocations cannot overcome other barriers, including grain boundaries, and these later build up in front of them. A stress field is produced by a buildup (pile-up) of dislocations that repels any incoming dislocation. The repulsion is stronger and the metal is more difficult to deform the more dislocations there are in a cluster. A crack initiates in a place when the dislocation density in a cluster reaches a specific value.

When heated to temperatures more than  $0.3 T_m$ , a different mechanism of dislocation movement is activated. Dislocation climb is what it is called. It fundamentally involves the diffusional displacement of a dislocation into adjacent lattice planes by attachment of a dislocation into adjacent lattice planes by attachment of vacancies. A surplus half-plane's edge is successively attached with vacancies, which corresponds to the edge being moved one atomic row upward. Vacancies 'attack' the displacement at different locations and take the form of steps on it. The dislocation shifts over tens of lattice planes along a significant portion of its length when vacancies are filled. The secondary phase particles' retarding influence is lessened by the dislocation climb. Under the influence of the load, the climbed dislocations are then slipped. Vacancies become quite mobile at temperatures over  $0.3 T_m$ , and the necessary amount of vacancies can be created through plastic deformation. One of the crucial phenomena that occurs during the annealing process is the dislocation climb.

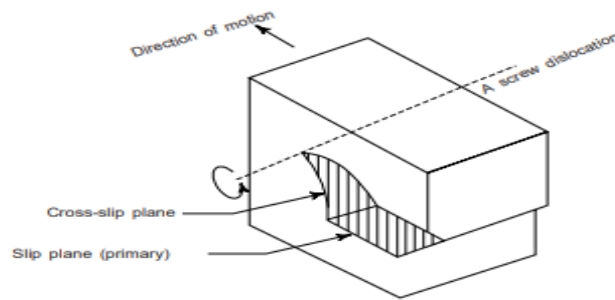
### **Cross-slip**

A screw dislocation can alter its slip orientation more easily than an edge dislocation can. The probable slip planes of a screw dislocation need not be parallel as is needed for edge dislocation because the Burger vector in a screw dislocation is parallel to the line of dislocation.

The screw dislocations can avoid barriers by a mechanism known as cross-slip, whereas the dislocation only modifies slip planes. A screw dislocation can cross-slip from one easy slip-plane to another when the planes of easy slip coincide.

On all easy slip-planes, the resolved shear stress is not equal, meaning that it is lower on the plane of cross-slip than it is on the slip-plane that contains the obstacle. Cross-slip consequently happens at larger strains than regular slide. We must keep in mind that crystals with several slip systems are those where cross-slip happens most frequently. In the FCC and BCC structures, respectively, there are four and six simple slip planes, and these planes intersect. They obviously meet the cross-slip requirement. The cross-slip or occurrence of greater stress values affects the work-hardening properties of different materials used in engineering. Fig. 1 presents a cross slip illustration.

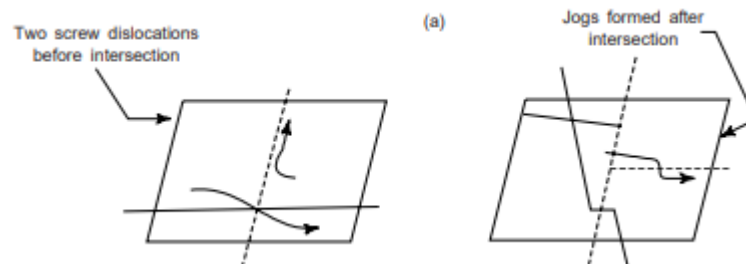




**Fig. 1 shows Cross-slip.(newagepublishers.com)**

### Jogs in Dislocation

A jog in a dislocation can be controlled as a brief length of dislocation that does not lie in the same plane as the main plane but has the same Burger vector. The vector dislocation that jumps from one plane to another is referred to as a jog. This is because dislocation may travel from one slip plane to another slip plane rather than being restricted to a single plane. A crystal may develop jogs when two edge or screw dislocations are used. Fig.2 provides an illustration of jogs in dislocation.

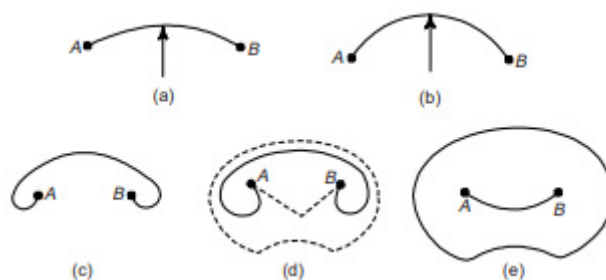


**Fig. 2 shows Jogs in crystal dislocation(newagepublishers.com)**

### Frank Read Source

Numerous crystal surfaces exhibit strong slip, which is found to cause the movement of hundreds of dislocations. There must, of course, be some efficient designers or some mechanisms that cause these multiple dislocations to occur on a specific slip plane. Frank-Read sources are what these are known as. Numerous new dislocations can be created from a single Frank-Read dislocation source. Practical studies show that under relatively high pressures, plastic deformation occurs often in most metals due to the coordinated movement of thousands to millions of dislocations within individual crystals. In actual crystals, plastic deformation is caused by dislocations moving in succession.

So-called dislocation mills or the amplification of dislocations are explained by the Frank-Read mechanism. Think about a dislocation line, represented by AB in a crystal. The dislocation line or Frank-Read source, as we can see, consists of the two nodes A and B. A shear stress parallel to the figure's plane will act on the dislocation line AB in the first scenario when the Burger vector is perpendicular to the line AB. Shear tension caused the dislocation line to bend outward, producing slip. Typically, a slip plane has tens of dislocations. The dislocation line AB assumes a specific radius of curvature for a given stress. The dislocation line becomes unstable and continues to grow when the load is raised. Fig. 3 shows sequence of formation of read source.



**Fig. 3 shows sequence of formation of read source.(newagepublishers.com)**

## CONCLUSION

The properties, behavior, and uses of crystalline materials are strongly influenced by defects or faults in the crystals. This essay has examined various crystal flaws and emphasized their importance in materials research. Point defects, which include vacancies, interstitials, and impurities, are small, localized departures from the ideal crystal lattice. These flaws can change a material's electrical, optical, and mechanical characteristics. For instance, adding free charge carriers to a semiconductor through doping can alter conductivity. Interstitials and voids can influence diffusion rates and material stability, while impurities can change the characteristics of optical absorption or emission. Line defects, also known as dislocations, are linear flaws that occur when there are additional or missing atomic planes in the crystal lattice. Dislocations have a big impact on the strength, ductility, and deformation mechanisms of materials, which changes how they behave mechanically. They may serve as obstacles to dislocation motion, which may alter the material's flexibility and fracture resistance.

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## CHAPTER 5

### FEATURES OF AN OVERVIEW OF THE BONDS IN SOLIDS

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#### ABSTRACT

Atoms or molecules are held together to create solid materials by bonds, which are the forces that bind them. These bonds are essential in defining the strength, conductivity, and stability of solids as well as their other physical and chemical characteristics. This abstract gives a general review of the various kinds of bonds found in solids, such as ionic, covalent, metallic, and van der Waals bonds, and emphasizes how important these bonds are for comprehending the behavior and uses of solid materials. Materials science is based on an understanding of the nature and behavior of chemical bonding in solids, which is essential for describing the properties and behavior of various kinds of materials. This abstract gives a general review of the characteristics of solid-state bonding, emphasizing the several kinds of bonds that exist, how they form, and how important they are in determining a material's structural, mechanical, electrical, and thermal properties. Solids form stable arrangements and structures as a result of interactions between atoms or ions, which result in the formation of chemical bonds. Three primary kinds of chemical bonding can be seen in solids:

#### KEYWORDS

Atoms, Bonds, Covalent, Energy, Electrons, Metallic.

#### INTRODUCTION

There are many different forms of solids found in nature. A lot of solids are collections of atoms. The nature, potency, and directionality of chemical binding forces, cohesive forces, or chemical bonds affect the arrangement of atoms in any solid material. These holding forces are referred to as atomic interaction forces. In comparison to the gaseous and liquid forms, atoms, molecules, and ions are more densely packed and bound together by powerful mutual forces of attraction and repulsion in solids. On the basis of this, one may characterize the atomic arrangement in elements and compounds.

The electrical structure of interacting atoms controls the kind of link that develops between them in crystals. A crystal's state of maximal thermodynamic stability is reached when its atoms are a specific distance apart from one another. These separations are influenced by the crystallographic interaction forces. Electrostatic forces are primarily the source of the attractive interactions between atoms. The interatomic distance  $r$  and some powers of its magnitude are related. The periodic table is intimately related to the various bonding types since they are dependent on the electronic structure of the atoms in question. The type of bonding present in a material has a significant impact on its electrical, chemical, and physical properties. When the space between the atoms is reduced to the point where they are very close to one another, repulsive forces are created. These forces intensify more quickly than attraction forces do. The repulsive forces are also influenced by the attraction between positively charged nuclei. A power of  $r$  also determines how strong the overall repulsive force is. When these attracting and repulsive forces are in balance, which occurs when two atoms or molecules are at an equilibrium distance  $r_0$ [1], [2].

#### Types of Bonds

Seitz divided solids into five categories in 1940 based on the atoms' bonds, and this division has since been widely adopted. During a chemical reaction, atoms of various sorts move

closer to one another and unite, and these bonds are typically referred to as chemical bonds. Common bonds are primarily divided into two groups according to their strength, the direction of the bonding forces, the cohesive forces (chemical bonds), and the characteristics of any solid material which are:

(i) **Primary Bonds:** These are interatomic bonds held together by electrostatic force. These bonds experience the development of relatively substantial atomic forces, which increase their stability and strength. Their bond energy ranges from 1 to 1.5 eV. These bonds are often referred to as alluring bonds. Typically, the interatomic distance is  $1-2r$ . The three basic bonds listed below are present in various materials. (i) Ionic or electrostatic bonds (ii) Covalent, atomic or homo-polar bonds (iii) Metallic bond

(ii) **Secondary Bonds:** An intermolecular secondary bond is less stable and stronger than a main bond. Forces hold the molecules together in this form of connection. These secondary bonds are the product of dipole or intermolecular attraction. Dipoles are produced by the asymmetric electron distribution in molecules and atoms. Dipoles cause molecules to be drawn to other molecules with opposing dipoles. Atoms with similar asymmetric electron distributions have dipoles. It is important to keep in mind that atomic dipolar bonds are weaker than molecular dipole bonds, and they also fluctuate as the electron distribution in atomic outer shells changes. Vander Waals bonds and hydrogen bonds are typical instances of secondary bonds[3], [4].

## DISCUSSION

### Forces Between Atoms: Mechanism of Bond formation and Bond energy

We have also stated that there are two different types of forces that can act between atoms: (i) attraction forces, which hold atoms together, and (ii) repulsive forces, which take effect when a solid is crushed. Atoms are drawn closer to one another by the force of attraction until the individual electron clouds start to overlap and, in accordance with Pauli's exclusion principle, a strong repulsive force develops. The system's potential energy is decreased by attracting forces while it is increased by repulsive forces. It follows that the algebraic sum of these two energies represents the system's net energy. Any two atoms should be in a stable state with a low potential energy when the attractive force and the repulsive force between them are equal. The forces that exist between two atoms or ions in a solid in relation to their separation,  $r$ .

Since potential energy is inversely proportional to some power of the distance of separation, let's suppose two atoms in their ground states that are infinitely distant from one another such that they do not interact to form a solid. In this case, the potential energy is zero. One of the two events listed below may occur when the atoms get closer to one another, assuming that the atoms are made up of moving electric charges. Atoms either pull together or pull apart. Since atoms do the work of attraction, the potential energy resulting from attraction is negative. Since external work must be done to bring the atoms together, the repulsive energy between them is positive and inversely proportional to some power of the interatomic distance  $r$ . The net potential energy is the sum of the two variables, it is important to notice. Until energy equivalent to the bond energy is given, the bond energy between atoms tends to remain, as well. When atoms separated by an infinite distance are brought together at equilibrium distance, the energy decrease is known as the bond energy. Typically, the bond energy is given on a mole basis. The dissociation energy, however, will have the opposite sign from the binding energy and be equal to it[5], [6].

Energy is generally not accurately represented by a power function. However, it is helpful to draw a few significant qualitative inferences concerning atom bonding in solids:

Cohesive energy (i) The binding energy or molecular cohesion energy is the energy corresponding to the equilibrium position ( $r = r_0$ ), represented as  $U(r_0)$  or  $U_0$ . This is the amount of energy needed to split the molecule's two atoms apart infinitely. This energy, which is provided by Eq. (4), is known as the energy of dissociation. A diatomic molecule's atoms need this much energy to be separated from one another by an infinite distance. Typically, this is in the range of a few electron volts. The energy generated when two atoms are placed close to one another at an equilibrium distance,  $r_0$ , can alternatively be thought of as the cohesive energy. The bond established is more stable the more energy released, and the crystal structure is consequently more stable.

Repulsive forces between like charges begin to take hold when the atoms in a molecule are only a few atomic diameters apart. The potential energy is at its lowest point ( $U_0$ ) and the forces of attraction and repulsion are about equal at the equilibrium separation. This is the molecule or system's bonding energy, which is roughly equivalent to the heat of molecular dissociation. Since there are many additional atoms around each atom in a crystal, the straightforward equation for attracting and repulsive energies provided by Eq. (1) does not apply. One must thoroughly research these energy concepts' origins in order to get a clear image of them. It also necessitates an understanding of charge distributions, notably valence electrons in atoms. When bonds are formed in some crystals, the valence electrons move from one atom to the next. While in certain crystals the nearby atoms share electrons, in others the valence electrons act like free electrons and travel from one region of the crystal to another. The crystals have a variety of different electric interactions[7], [8].

The type of these interactions or bonds determines the type of crystals that are created. The amount of energy needed to break a bond serves as the strongest indicator of a bond's strength. It is the amount of heat required to vaporize the material and then split its atoms. The bond energy is the amount of energy needed to create one mole of a substance from its ions or atoms. The strength of the binding was also discovered to affect the melting points of the elements; the stronger the bond, the higher the melting points. Five major categories can be used to classify these connections.

### **Bond Length**

Bond length is the separation distance ( $r$ ) between the centers of the two bonding atoms that results in the stable bond.

Naturally, the bond length ( $r$ ) will be shorter the stronger the force of attraction between the two bonding atoms. We must keep in mind that primary bonds are more powerful than secondary bonds.

### **Ionic Bonding**

Perhaps the easiest type of chemical bonding to visualize is ionic or hetero-polar bonding, which is created by the actual transfer of electrons from one atom to another so that each atom acquires a stable configuration similar to the nearest inert gas atoms. This type of bonding is almost entirely electrostatic in nature. Electropositive (metals; those elements on the left side of the periodic table) and electronegative (non-metals; those elements on the right hand of the periodic table) elements form ionic bonds.

These bonds are mostly generated in inorganic substances, such as the common salt sodium chloride ( $\text{NaCl}$ ),  $\text{MgO}$ ,  $\text{CuO}$ ,  $\text{CrO}_2$ , and  $\text{MoF}_2$ . In  $\text{MgO}$ , the ions are doubly ionized, resulting in a stronger interatomic connection and a melting point that is higher (around  $2800^\circ\text{C}$ ) than that of  $\text{NaCl}$  ( $800^\circ\text{C}$ ). Any metal can get ionised by losing its valence electrons, as shown by the study of the creation of ionic bonds, such as those between cupric oxide, chromous oxide, and molybdenum fluoride. The metallic element need not be from Group I or II.

## Ionic Solids

These are made up of atoms of various sizes that are connected by directed bonds. NaCl, CsCl, and FeO crystals are good examples of this category. Iron ions are positively charged and negatively charged in the FeO lattice. Because the atoms' sizes differ, ionic solids cannot form close-packed structures like FCC and HCP. Since each ion wants to attract as many ions of the opposite sign as possible, the coordination number in these materials relies on the ratio of the radii of the metallic and non-metallic ions. Ions are organized in spheres with varying sizes that resemble a lattice. Because a metallic ion's radius is greater than a non-metallic ion's, metallic ions fill in the gaps created by non-metallic ions in the crystal lattice. The coordination numbers of the ions of opposite signs surrounding a specific ion in ionic solids.

### Characteristics of Ionic Solids

- (i) Ionic solids are typically hard and crystalline in form.
- (ii) Ionic crystals' bond energies are higher than those of metallic and, even more so, molecular crystals, and are roughly equivalent to those of covalent crystals. Because of this, they have low linear expansion and compressibility, high elasticity, high melting and boiling temperatures, and low coefficients of compressibility.
- (iii) In the process of forming an ionic bond, an atom of a metallic element loses an amount of electrons equal to its valency (numerical) from the outer electron shell. Between positive and negative ions, there is undoubtedly an electrical attraction.
- (iv) The link itself in an ionic crystal is non-directional, with each positive ion attracting all nearby negative ions and vice versa.
- (v) In general, ionic solids are not electrical conductors.
- (vi) Ionic solids are very soluble in water but insoluble in organic solvents
- (vii) A portion of a covalent bond may also exist in many ionic crystals. A mixed ionic-covalent bond is created when ions become polarized as a result of the electromagnetic fields they generate. Ions lose their spherical symmetry due to polarization, which deforms the electron zones. The characteristics of ionic crystals change with a change in the covalent bonding percentage. In crystals made up of elements from different groups, such as AI BVII, AII BVI, AIII BV, and AIV BIV, the percentage of covalent bonds rises from first to last. The percentage of covalent bonds is 90%, making the compounds made up of elements from the fourth group (AIV BIV) practically covalent crystals. Since the electric conductivity increases with the covalent bond fraction, AIV BIV crystals become semiconductors while AI BVII crystals become dielectrics[9], [10].

### Covalent Bond

Two nearby atoms with incomplete outermost shells join together to establish this kind of link by sharing electrons equally. In order to achieve a stable electrical configuration that complies with the octet rule, the atoms take this action. The atoms involved in covalent bonds, unlike ionic bonds, have electrical configurations that prevent them from completing their octets by the actual transfer of electrons from one atom to another. Evidently, each atom in the crystal has no associated charge. Most solids with covalent connections also have ionic or Vander Waals bonds tying them together. Between atoms that are similar or distinct and have an equal amount of missing electrons, a covalent connection is created. The original atomic charge distributions of atoms are distorted and each atom transfers its unpaired electron to the common space between the atoms when two atoms, each lacking one electron, are sufficiently close to one another that their electronic shells begin to overlap. A pair of electrons that belong equally to both atoms and complete the outermost shell of each atom are

evidently present in the common space. This is referred to as electron sharing. If the exchanged electrons have the opposing spins, sharing is successful. The atoms are drawn to one another in this situation, and a covalent bond is created. This bond is also known as a "valence bond" since the atoms involved in it have the same valence state. The chlorine molecule provides a fantastic illustration of covalent bonding. Each chlorine atom has seven electrons in its outer shell. It goes without saying that each chlorine atom wants to pick up an electron to complete a stable octet. Two electrons can be shared between couples to accomplish this.

Groups IV, V, and VI, subgroup B elements are responsible for creating covalent bonds. Due to their high ionization potential, these elements are electronegative and take up valence electrons from elements of other groups to complete their valence zones. When these elements interact with one another, the valence electrons are shared by the nearby atoms to complete the valence zone. Since each atom can interact with a specific number of atoms nearby, a covalent connection is characterised by directivity. As a result, atoms in covalent crystals do not form tightly packed crystal structures and have a low number of coordinations. For instance, the diamond cubic lattice has the coordination number 4.

### **Characteristics of Covalent Compound**

- (i) The majority of covalent compounds are gases and liquids.
- (ii) They typically act as electrical insulators
- (iii) They have a directed quality
- (iv) They are soluble in non-polar solvents such as benzene, chloroform, alcohol, paraffins, etc. but insoluble in polar solvents such as water.
- (v) Covalent compounds are homo-polar, meaning that the valence electrons are attached to specific atoms or pairs of atoms and that they are unable to move freely inside the substance, as they can in the case of metallic bonds.
- (vi) Covalent compounds are soft, rubbery elastomers that can be used to create a range of structural materials that are typically referred to as plastics. Low melting and boiling points characterize these substances.
- (vii) Diamond is a unique situation where covalent bonding is extremely strong because of the extremely high cohesive energy. The binding energy typically falls between 1 and 5 eV. Diamond has a high melting point and is extremely hard due to the strong covalent bonding.

### **Covalent Solids**

The directed nature of the covalent connections must be preserved since they are highly strong and stiff. Covalent solids do not form densely packed formations because of this. The most basic covalent structure is that of diamond, which is also seen in germanium and silicon and is not tightly packed. The number for coordination is 4. The diamond lattice is a complex cubic lattice having two atoms at each of the cubic lattice sites, such as (000) and (1/4, 1/4, 1/4), for example.

Graphite, which is distinct from diamond in many ways, is the low-pressure crystal form of carbon. The layers themselves are relatively weakly joined by Vander Waals interactions in the vast structure of graphite, where the atoms are only covalently bound to their closest neighbors. There is a large supply of free electrons in graphite because each atom has one electron that is not used in the covalent bonding. Because of this, diamond is a nearly perfect insulator, whereas graphite is a good electrical conductor. However, in graphite, free electrons find it difficult to move between layers.



## Metallic Bond

A metallic bond is created when nearby atoms share some of their valence electrons. All the components of subgroups A, I–III, and B combine to make them. The sharing in a metallic link is not localized, in contrast to a covalent bond. As a result, a metallic bond can alternatively be thought of as an unsaturated or delocalized covalent link. Electropositive bonds are found in metals. Atoms in a metallic crystal can readily release their valence electrons and transform into positive ions when interacting with elements of other groups.

Atoms' valence energy zones overlap when they come into contact with one another, creating a shared zone with open sublevels. As a result, the valence electrons get the ability to travel freely throughout the zone. Valence electrons are obviously spread over the entire crystal's volume. In a metal, the valence electrons cannot be thought of as being lost or gained by atoms. In contrast to covalent crystals, where sharing of electrons is restricted to a single pair of atoms, they are shared by all the atoms in the volume of a crystal. The metallic bond is substantially less directed than a covalent link because of the delocalized nature of valence electrons. Metal crystal formations as a result have a high coordination number and dense packing. FCC and HCP lattice crystal formations typically have high coordination numbers. Many metals have an FCC lattice, including Ni, Ag, Cu, Au, Fe, Pt, Al, and Pb. Only Mg and Co among the several metals with an HCP lattice have the axial ratio  $c/a = 1.633$ , which corresponds to the spherical symmetry of the atoms.

The presence of incomplete covalent bonds, which results in an asymmetrical symmetry of the atoms, can be used to explain deviations from the  $c/a$  ratio of 1.633. In that scenario, covalent interaction is added to the metallic interaction in the direction of atom stretching. When non-spherical atoms are positioned in a crystal with their major axes parallel to the  $z$ -axis, the  $c/a$  ratio (for Zn and Cl) exceeds 1.633. However, the  $c/a$  ratio is smaller than 1.633 if their minor axis is placed along the  $z$ -axis.

Partial covalent bonding and non-spherical atomic symmetry both contribute to the development of crystal formations with a BCC lattice. A closer packing of atoms is not seen in these formations. Fe, Cr, Mo, W, V, Ta, Ti, Nb, and Zr, and a few other metals frequently have BCC lattices in their crystal structures. Many metals and some non-metals are polymorphous, meaning that depending on temperature, they may have different types of crystal formations in the solid state. These crystal formations are referred to as allotropic modifications. When the nature of bond varies, the stability of allotropic alterations may also differ. For instance, due to the high energy of the covalent bond and consequently low enthalpy, the tin modification with diamond type lattice Sn is stable at low temperatures. It transforms into the Sn modification upon heating, which has a weaker metallic bond.

About 30 metals, including Titanium, Zirconium, Tin, Uranium, Iron, and Cobalt, exhibit the temperature polymorphism phenomena. Fast cooling at 20–25 °C allows for the long-term retention of a high-temperature alteration in a metal because the atoms' poor diffusion mobility at these temperatures prevents the lattice from being rearranged. Additionally, some polymorphous changes take place as a result of pressure and temperature. For instance, when heated to 2000°C and placed under a pressure of around 1010 Pa, carbon that has undergone graphite alteration re-crystallizes into diamond. Iron undergoes a low-temperature alteration with HCP lattice under extremely high pressures.

At low temperatures, a rise in pressure can transform less densely packed alterations into densely packed structures. High pressure can transform Ge, Si, and Sn's covalent crystals into metallic crystals with a tetragonal body centered lattice ( $C = 8$ ), as has been observed for these three elements. Because the entropy of metallic bonds is a little lower than that of covalent bonds, most metals have greater temperature coefficients of linear expansion than covalent crystals, but lower melting and boiling temperatures and elastic moduli. The melting

point, elastic modulus, and the activation energy of self-diffusion are typically increased with a rise in bond energy, whereas the coefficient of linear expansion is typically decreased. These patterns have a few outliers and have been observed experimentally. In particular, beryllium has an abnormally high elastic modulus, which contributes to the enhanced stiffness of beryllium alloys. The elastic modulus and self-diffusion activation energy of Ti and Zr are too low. This last factor accounts for their low heat resistance. Metallic crystals are more malleable and less rigid than covalent crystals due to the non-directivity of metallic bonds and the close-packed structures. They have a high electric conductivity because the valence energy zone contains free sublevels.

### **Characteristic of metallic crystals**

- (i) Metallic compounds are crystalline in nature as a result of the positive ions being arranged symmetrically in a space lattice.
- (ii) Metallic compounds are effective heat- and electricity-conductors. Both their thermal and electrical conductivities are high.
- (iii) Because metallic bonds are weak, metals have moderate to high melting temperatures, meaning that their melting points are lower than those of electrovalent crystals.
- (iv) Metals are opaque to light because they absorb light energy with their free electrons.
- (v) Metallic crystals have a high reflectivity and good luster.

### **Secondary Bonds**

There are other secondary bonds in addition to the three primary bonds mentioned above. Molecular bonds, sometimes known as secondary bonds, are secondary in the sense that they are weaker than the three major bonds. Secondary bonds have bond energies that range from 4 to 42 kJ/mole. When the electron configuration of two elements or compounds is such that there is little electron transport between them, secondary bonds are created. Secondary bonds are produced by the electrostatic attraction of dipoles, which emerge when the distribution of electrons in asymmetrical molecules is not balanced. Weak Vander Waals forces of attraction between atoms or molecules that have their outermost shells fully occupied and, as a result, have no inclination to gain, lose, or share valence electrons with other atoms or molecules in the solid, lead to the formation of secondary bonds. The electrostatic attraction between the nucleus of one atom and the electrons of the other results in Vander Waals forces. Molecular crystals are the crystals that are created as a result of this kind of connection. Examples of these solids include the crystalline forms of inert gases like He, Ne, and Ar, as well as other gases like O<sub>2</sub>, Cl<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, and others. At sufficiently low temperatures, the rare gases, such as helium and argon, condense to form solids and produce secondary bonds that are not created by the sharing or transfer of electrons (covalent or metallic, respectively). Compared to primary bonds, these bonds are weaker.

It is difficult to defeat the Vander Waals forces. At room temperature, atoms or molecules have accumulated enough thermal energy to render these forces ineffectual. Therefore, at normal temperature, molecular solids are in a gaseous form. However, at low temperatures, these forces predominate over the thermal forces and play a big part in changing a gas into a liquid or solid. Only about 0.1 eV of energy per bond is released during the creation of Vander Waals bonds. The very low melting and boiling temperatures, low mechanical strength, and ease of deformation of molecular solids are due to this. Additionally, the heat and electricity conduct poorly through these substances. Except for water (H<sub>2</sub>O), molecules are typically transparent to light and excellent insulators. Many non-metallic materials, like plastics, paraffins, and graphite, depend heavily on secondary bonds to determine their

structure and properties. The three forms of secondary bonds, often known as mixed bonds, are as follows:

Dispersion bonds, dipole bonds, and hydrogen bonds are among them.

**Dispersion bonds** The electrons in a symmetrical molecule are evenly spaced around the nucleus and are in continual motion. Positive charge centres and negative charge centres naturally coincide in symmetrical molecules. However, it has been noted that the molecule's distribution of electrons around its nucleus occasionally is not symmetrical. The centres of positive and negative charges are displaced as a result. It causes an electrical charge imbalance known as polarisation. The dispersion effect describes the fluctuating nature of this polarisation. A weak force of attraction exists between two molecules of the same element because of the dispersion effect. This force causes a bond between the two molecules that is known as a dispersion bond.

When noble gas molecules, such as helium and argon, consisting of a single atom, solidify at extremely low temperatures, dispersion bonds hold them together. This condensation makes it clear that the forces drawing the atoms together are weak interatomic forces. These are what are referred to as Vander Waals forces and Vander Waals bonding.

**Dipole Bonds** A covalent bond is created when two or more atoms share the outermost electrons of an atom. The distribution of electrons between two atoms might be uneven at times. Only those compounds in which one atom in a molecule has a higher attraction to attract electrons than the other experience unequal electron sharing. This asymmetrical distribution of electrons has the overall result of giving the parent atoms opposing charges. Permanent dipoles are as a result created. Such dipoles are attracted to one another, and a bond known as a dipole bond is created. Dipole bonds are more powerful than dispersion bonds but less powerful than ionic binds.

The hydrogen atom has an atomic weight of 1 and an electronic configuration of  $1s^2$ . Fluorine has an atomic number of 9 and an atomic configuration. Fluorine possesses seven electrons in its outermost energy level ( $2s^2 2p^5$ ) compared to the hydrogen atom's single electron. Thus, in order to achieve a stable configuration, the hydrogen atom needs an additional electron, but the fluorine atom likewise needs an additional electron. To achieve a stable state, the hydrogen and fluorine atoms share a pair of electrons. As a result, a covalent bond forms, and the resulting molecule is known as hydrogen fluoride.

We must be aware that the fluorine atom has a higher affinity than the hydrogen atom in this covalent interaction. The shared electron pair moves in favour of the fluorine atom for this reason. A dipole is created by the electron pair moving. Hydrogen cyanide,  $SO_2$ ,  $HBr$ , and hydrogen chloride are more examples. Hydrogen bonds Although it is a unique kind of dipole bond, this one is more stronger. It is a unique instance of intermolecular attraction caused by specific hydrogen atoms that are covalently bound to one pair of electrons on another atom. A potent permanent dipole is created when a hydrogen atom forms a covalent connection with a relatively big atom, such as nitrogen, oxygen, or fluorine. The hydrogen is surrounded by a positive field, while the electron pair is surrounded by a negative field. This force is found to be crucial in biological compounds like DNA and plastics. The hydrogen bond is well represented by the water molecule. Covalent bonds hold the hydrogen and oxygen atoms in water together in the arrangement.

The oxygen atom in this covalent bond has a stronger affinity for the shared electron pair than the hydrogen atom, it is important to note. The shared electron pair naturally moves closer to the oxygen atom. A dipole is the result of this movement. The other compounds also produce dipoles that are similar to these. As a result of these dipoles' mutual attraction, liquid water is created. The nature of hydrogen bonding is directed. Animal life contains them in a variety of tissues, organs, blood, skin, and bones. Proteins have hydrogen bonds of the form  $N \dots H \dots O$ , which are crucial for establishing their structural details.

## Mixed Bonds

There are many substances in which the bonding between atoms takes the form of a combination of these bondings rather than one of the primary or secondary types of ideal bonding listed above. The materials in which mixed ionic covalent bonding occurs are quartz, glass, or silica. The lattice of materials has many structural flaws caused by ionic and metallic bonding. It is discovered that a variety of metal alloys, including copper-zinc, copper-nickel, and copper-tin, exhibit a constant shift in bonding nature. Despite the presence of non-metallic bonding, some metallic properties are still present.

(i) An atom with a closed electronic shell is basically made up of a positive nucleus that is encircled by a spherical cloud of negatively charged particles. There would be no force between two such atoms if their electron clouds were static and unmoving. However, as different electrons move around the nucleus, electron clouds form. This means that an atom may occasionally not have an electrical dipole moment but may occasionally have one that fluctuates quickly. The nucleus is not always where the centre of the negative charge distribution is; instead, it oscillates quickly around it, this changing charge on one molecule has a tendency to interact with the fluctuating charge on a nearby molecule, creating a net attraction. Inert gas molecules, which are made up of a single atom, are held together by dispersion forces as the gases solidify.

(ii) As two atoms get close to one another, the quickly changing dipole moments of each atom affect the motion of the electrons in the other. If the fluctuations occur in asympathy with one another, a lower energy is created. Each atom in the picture is depicted as a tiny electric dipole. Unsurprisingly, an electric dipole is created when the centres of the positive and negative charges do not line up. This demonstrates a strong pulling force that acts as a mechanism for molecule bonding. Additionally, the Vander Waals forces of attraction are also at blame for this. We are aware of the non-directional nature of Vander Waals bonding. When molecules without permanent dipoles come together, these bonds are created. Examples of polar chemicals in which this type of binding occurs frequently are HCl and PVC.

(iii) As we just mentioned, atomic groups without any spare electrons can form hydrogen bonds, a specific kind of dipole bond. These bonds resemble Vander Waals bonds but only form when a hydrogen atom is present. In organic materials, hydrogen frequently plays a significant role and hydrogen bonds regularly arise. Hydrogen bonding are the cause of the peculiar physical characteristics of ice and water. Because oxygen has a higher electronegativity than hydrogen, the electrons shared by the oxygen and hydrogen atoms in an H<sub>2</sub>O molecule, or water molecule, tend to stick closer to the oxygen atom than the hydrogen atom. Because of this, hydrogen atoms serve as the dipole's positive ends and oxygen serves as its negative end. The negative end of another water molecule is drawn to the positive end, which serves to join the molecules together. We have already mentioned that a hydrogen bond, which is also known as a hydrogen bridge, is crucial for many biological molecules, including DNA.

## Properties of Solid Materials

The classification of solid materials into ionic, metallic, covalent, and molecular groups has been covered thus far. One must focus on the bond's strength in order to understand the qualities of chemical bonding. The energy needed to break the bond, or the amount of heat required to vaporize the solid, or to separate the constituent atoms, is the greatest indicator of the bond's strength. It is clear that Vander Waals and hydrogen connections are the weakest, followed by metallic, ionic, and covalent chemical bonds, all of whose strengths are about equal. Bond strength can also be determined by the melting points of various substances. We are aware that melting takes place when thermal vibration reaches a certain level, breaking

bonds and making atoms mobile. It has been found that ionic bond valency enhances bond strength. We can easily see why magnesium oxide has a higher melting point than salt chloride.

Knowing the bond strength makes it simple to ascertain the strength of materials and their crystal structure.

Materials with ionic or covalent bonds are not conductors because their electrons are securely confined within the bonds. Due to the fluctuation of the electron cloud caused by the application of a potential difference, we can understand why metals are great conductors. Metals have ductility because electrons can move around in them. Metallic bonded materials are opaque and glossy because valence electrons can readily absorb the impinging light energy.

### CONCLUSION

Understanding solid-state bonds is crucial for comprehending the characteristics and behavior of solids. The many bond types in solids have been examined in this essay, which also highlighted their importance in materials science. Electrons are transferred when positively and negatively charged ions form ionic bonds. Ions are held together in a crystal lattice by powerful electrostatic forces. The high melting temperatures, brittleness, and electrical conductivity features of ionic solids are caused by ionic bonding. Sharing electrons between atoms creates covalent bonds, which result in a web of interconnected atoms. Covalent solids' directionality, strength, and stability are all a result of covalent bonding. These substances can either be electrically insulating or semiconducting and have high melting points. When electrons are delocalized and shared among a lattice of positively charged metal ions, metallic bonds can form. Properties like malleability, high electrical and thermal conductivity, and metallic luster are brought about via metallic bonding. The mechanical characteristics of metals are governed by the strength of their metallic connections.

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## CHAPTER 6

### AN ELABORATION OF ELECTRON THEORY OF METALS

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#### ABSTRACT

The free electron model, commonly referred to as the electron theory of metals, is a key idea in solid-state physics that describes how electrons behave in metallic materials. This hypothesis states that the positively charged ion lattice of metals is encircled by a "sea" of delocalized electrons. These electrons can flow freely throughout the metal since they are not attached to any one atom. The electron theory of metals, its fundamental ideas, and its importance for comprehending the characteristics of metallic materials are all covered in this abstract. The free electron theory, commonly referred to as the band theory or the electron theory of metals, is a key idea in solid-state physics that describes how electrons behave in metallic materials. The electron theory of metals is elaborated in this abstract, with special attention paid to its fundamental ideas, ramifications, and importance for comprehending the electrical, thermal, and optical properties of metals. Metals are said to be made up of a lattice of positively charged ions submerged in a body of delocalized electrons, in accordance with the theory of metals' electrons. These valence electrons are unrestrictedly free to roam over the entire lattice and are only weakly attached to the corresponding atoms. Due to the loose coupling of electrons to their parent atoms in semiconductors and insulators, the distinctive property of metals sets them apart from these materials.

#### KEYWORDS

Band, Electrons, Energy, Free, Theory, Temperature, Zone.

#### INTRODUCTION

Numerous essential characteristics of solids, such as their electronic structure-dependent electrical and thermal conductivities, magnetic and optical properties, etc. In terms of the solid-state electron theory, we can comprehend a variety of solid-state physical characteristics. Beginning in the early 20th century, the electron theory of solids underwent development. Today, it serves as the foundation for categorizing all solids. Free electron theory, when applied to metals, unifies the energy levels and behavior of conductors, insulators, and magnetic materials. It explains forces of cohesion and repulsion. This concept states that the constituent atoms' valence electrons transform into conduction electrons and move around freely within the metal's volume. Early in the 20th century, P. Drude presented the first iteration of the free electron model, and H.A. Lorentz soon after made refinements [1], [2]. The Drude-Lorentz free electron theory is the current name for this. Other hypotheses include:

- (i) Sommerfeld free-electron theory
- (ii) Zone Theory

#### Metallic Bonding

The metal's valence electrons, also known as free electrons, flow within it with just the sample's surface acting as a physical barrier. Electron collisions are not taken into consideration. Electrostatic attraction between the positive ions and the negative cloud or diluted gas of electrons causes the binding forces in metals. P. Drude first proposed such a free electron model in the early 1900s, and H.A. Lorentz quickly improved on it. We now have a current illustration of metallic bonding. This illustration shows how the metallic bond

resembles the ionic bond and is more closely connected to the covalent or electron pair bond. The metallic bond is essentially an unsaturated covalent connection that enables many atoms to be held together by reciprocal exchange of free electrons. In addition, the metallic bonding has a far lower electron density than is permitted by the Pauli exclusion principle. As a result, the electrons can travel freely from one location to another without experiencing a major energy gain. According to what we've read, the cohesive and repulsive forces that keep atoms at specific distances from one another form the bonds that hold them together in solids. It is appropriate to grasp the forces that underlie the electron structure of atoms. Mutual repulsion is primarily caused when two atoms are too close to one another and too many electrons end up in interaction regions. The equilibrium position is obtained when the cohesive and repulsive forces are equal.

### **Drude Lorentz theory**

Drude proposed in 1900 that positive ion centers make up the cores of metals, and that valence electrons can freely move around these cores. However, because of electrostatic attraction between the positive ion cores and the electrons, the electrons are constrained to move within the metal. These ion cores' potential field, which is responsible for such an interaction, and the mutual repulsion between the electrons is disregarded, is assumed to be constant throughout the metal. Free electrons travelling inside of metals are thought to behave similarly to atoms or molecules in a perfect gas. As a result, the theory is also known as Drude and Lorentz's classical free electron theory and the free electrons are also referred to as free electron gas. The classical kinetic theory of gases' equations governs how electrons flow. Using the following two presumptions, Lorentz applied Maxwell-Boltzmann statistics to the electron gas in 1909:

- (i) There is hardly any mutual repulsion between negatively charged electrons.
- (ii) It is possible to suppose that the positive ion-induced potential field throughout the crystal is constant. The ratio of the electrical conductivity, to the thermal conductivity,  $k$ , should be constant for all metals at a constant temperature since electrons travel freely inside metals regardless of their crystal structure.

The electrical, thermal, lustre, and opacity properties of metals, among others, were all described by this hypothesis. The significant flaws in this theory include:

- (i) The theory properly predicted the resistivity of different metals at room temperature; however the temperature dependence of resistivity could not be accurately proved. Contrary to what the theory predicted; resistivity is observed to vary linearly with temperature.
- (ii) The specific heat and paramagnetic susceptibility of metals were estimated by the theory with inaccurate magnitudes.

### **Somerfield Free-electron theory**

The valence electrons of a metal are free, according to the fundamental premise of this theory.

- (ii) In a crystal, valence electrons are constrained to move only within the crystal's confines. The electrons inside the crystal have a lower potential energy than those outside, obviously. It is important to remember that an electron's potential energy is constant or uniform across a crystal (Drude theory).
- (iii) The crystal's surface has extremely high potential energy barriers, which restrict the electrons from leaving the crystal's boundaries even though they are free to flow throughout the crystal.



- (iv) A single atom-bound electron's permitted energy levels are quantized.
- (v) Metals have very low electronic specific heats[3], [4].

## DISCUSSION

### Fermi-Dirac distribution function

We are aware that in a system, valence electrons tend to inhabit the lowest energy states. The Pauli exclusion principle states that only two electrons can occupy a given state. However, it is important to take into account all of the electrons in the single system because of the mutual interactions that all of the electrons forming the electron gas have with one another. Only by using the Pauli exclusion principle is this possible. We are aware that only two electrons—one with spin up and the other with spin down or the opposite spin—can occupy a particular state as defined by the three quantum numbers ( $n_x$ ,  $n_y$ ,  $n_z$ ) in accordance with the Pauli exclusion principle. When the metal is in its ground state, which happens at absolute zero, all electrons are at the lowest energy levels that are consistent with the exclusion principle. The electrons will occupy all energy states up to a maximum, denoted by  $E_{\max}$ , if the total number of electrons per unit volume (let's say  $n_0$ ) is fewer than the total number of energy levels available in the band. How many free electrons there are affects the value of  $E_{\max}$ . All quantum states in the energy levels above the Fermi level, which is the highest energy level ( $E_{\max}$ ), are empty. The Fermi level, abbreviated  $E_F$ , is the point at which the probability of occupation is 50%. Energy is needed to remove an electron from the Fermi level and take it out of the metal. This is referred to as the "work function" and is typically represented by the symbol, which is equal to the energy typically measured when an electron is extracted from a metal's surface.

Even at normal temperature, very few electrons are excited above the Fermi energy because thermal energies pale in comparison to that energy. Because of this, the work function is essentially constant across a broad temperature range. We must keep in mind that an electron at the Fermi level has the highest energy of all the metal's electrons and is the simplest to remove at absolute zero. We'll now talk about how temperature affects the energy levels of electrons. Since some of the electrons from the filled energy levels may be excited to the higher levels, it is clear that for temperatures higher than 0K, the Fermi level may not be the topmost filled level. At  $T = 0^\circ\text{K}$ , the probability that an electron will occupy a state at a level of energy  $E$  is constant, equal to 1 (unity) up to the Fermi level  $E_F$ , and zero above it. Excited electrons flow into the new energy levels when the system's temperature rises. Therefore, some of the levels beneath  $E_{\max}$  would be vacant while others above it would be filled with people[5], [6]. The so-called Fermi function determines the likelihood that a specific quantum state of energy  $E$  will be occupied at a given temperature  $T$ .

### Band theory of solids

The many electronic and thermal properties of metals, including specific heat, paramagnetism, electrical conductivity, electron emission, etc., were successfully explained by Sommerfeld's free electron theory. However, this theory is unable to account for a number of additional features. For instance, the theory was unable to explain why some materials behave as good conductors because they have many free electrons, but other solids have few electrons and behave as insulators as a result. Additionally, it was unable to explain how the resistivity of the latter class of materials varied with temperature. Furthermore, this theory was unable to explain the characteristics of semiconductors.

The oversimplified assumption that a conduction electron in a metal experiences a constant or zero potential due to the ion cores and is, therefore, free to move around in a crystal with just

the surface of the crystal limiting its motion is the reason the free electron theory fails. In actuality, the potential caused by the ion cores might vary depending on where the electron is located in the crystal. The other electrons in the crystal could potentially contribute to potential in some way. It goes without saying that the actual potential under which an electron flows in a crystal is extremely complex. By assuming that the electrons flow in a region of constant potential, the band or zone theory of solids explains this with the idea of a periodic potential field. The periodic potential field created by the crystal lattice governs how the electrons flow. The periodic nature of the atomic organization in all solids—i.e., the periodic arrangement of positively charged ions through which the electrons move—was already discussed in the discussion of the periodic table of elements. The ion cores may be approximated as being at rest, and the potential that an electron encounters in a crystal is assumed to be periodic with period equal to the lattice constant  $a$ . The locations of the positive ions are shown by the deep, appealing wells. When the potential  $V$  fluctuates regularly with distance  $x$ , we observe that each ion has a deep potential well because of the Coulomb forces.

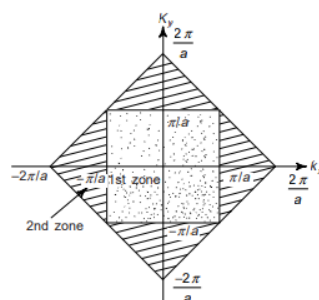
### Brillouin zones

The wave number  $K$  is represented in relation (11) by. The magnitude of  $K$ , a vector whose direction the electron is travelling in, is inversely correlated with the magnitude of the momentum of the electron. A momentum, or  $K$ -space, is represented by the components of vector  $K$ , which are  $K_x$ ,  $K_y$ , and  $K_z$  along the  $x$ ,  $y$ , and  $z$  directions, respectively. The travelling electron is diffracted by the lattice plane when the Bragg condition (10) is met. For a one-dimensional lattice where  $n = 1, 2$  for the critical value of  $K$ , we need  $K_x = n d$  (12) for this to occur.

Let's have a look at a straightforward two-dimensional cubic lattice. We can observe that the (100) and (010) planes of this lattice satisfy the Bragg's condition. Additionally, we observe that the Bragg's condition for another set of planes (110) is met at a certain point as the energy of the electrons rises. The Brillouin zone is the region in wave-number space that is bounded by a line that corresponds to  $K$ -vectors.

The first Brillouin zone is defined as the range of  $K$  values between  $-a$  and  $+a$ . The second Brillouin zone for  $K$  is that region between  $2/a$  and  $-2/a$ ,  $2/a$  and  $-2/a$ , and so on. For the first zone, we observe that one number is 1 and the other integer is 0. Each integer in the second zone is 1.

It is evident that the  $K$ -space is segmented into zones. When an electron meets a lattice boundary within a zone, it encounters an energy barrier that prevents wave number from increasing further until more energy is provided to excite the electron past the potential barrier. The energy gap is another name for the potential barrier. The energy gaps and Brillouin zones for a straightforward cubic lattice. The arrow indicates how the wave number and energy of the electron change within the zone when an external force is applied[7], [8]. Fig. 1 Brillouin zones for a two dimensional crystal lattice.



**Fig. 1 Brillouin zones for a two dimensional crystal lattice.(newagepublishers.com)**

### Distinction between conductors, insulators and semiconductors

The solids can be divided into the following three groups according to Zone theory: Conductors, Insulators, and Semiconductors

**Conductors** (i) The magnitude of the energy gap between zones and the extent to which the Brillouin zones are filled are crucial in determining a solid's electrical conductivity. There is an electron flow in the electric field's direction when the solid is exposed to an external field. When electrons are sufficiently excited, they can move to the second Brillouin zone and occupy empty energy levels or states. We are aware that in a metal, empty states are always present at energies just a little higher than the highest energies of filled states, and that electrons can be elevated by adding an external field. Let's look at the situation with monovalent metals, like sodium, potassium, etc. Theoretically, there can be no more than two electrons in each atom of these monovalent metals. We can plainly see that only half of the first zone could be filled with the available electrons because each metal atom has a single valence electron. The energy level in the second Brillouin zone is noticeably higher. Any tiny applied electric field can accelerate electrons to migrate into the second zone or higher energy levels or states because half of the energy levels are unoccupied. Fig. 2 shows Brillouin zones for conductors.

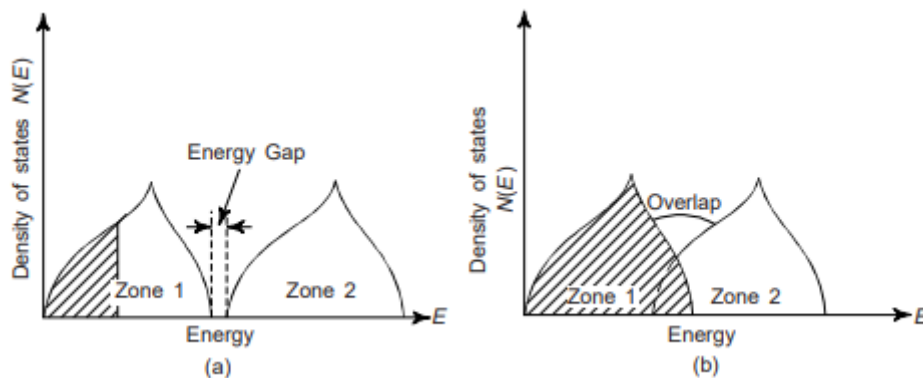


Fig. 2 shows Brillouin zones for conductors(newagepublishers.com)

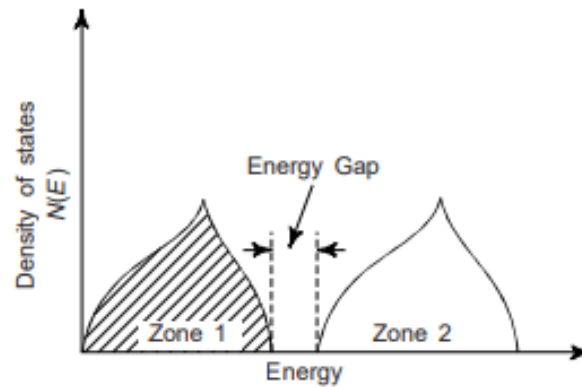
### Insulators

The energies of the lowest levels in the second zone should be significantly greater than those of the top levels in the first zone in these materials, where there is a significant energy difference between the first zone and the second zone.

Let's take a look at a monovalent metal that has just enough electrons to entirely fill the first zone. We are aware that each zone can only accommodate two electrons per atom. Since there are two electrons in each atom in the first zone and a large energy gap between them, the charge cannot transfer from the first to the second zone in the solid.

Since all the energy states in the first zone are occupied, electrons there are unable to travel to higher energy levels since a regular electric field cannot excite them to go to the next permitted energy level.

Obviously, electrical conduction cannot occur in insulators. According to a report, some electrons do leap into the second zone when an insulator's temperature is elevated, which might lead to electrical conduction. Examples include rubber, bakelite, mica, and more. An great insulator is diamond. Each zone in diamond has four valence electrons per atom, just enough to fill the first zone entirely. The energy differential between zone 2 and zone 1 is substantial. Fig. 3 shows Brillouin zones for insulators.

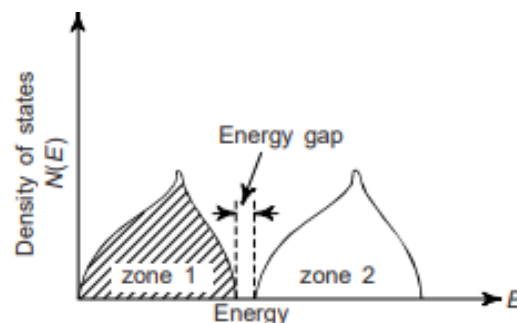


**Fig. 3 shows Brillouin zones for insulators(newagepublishers.com).**

### Semiconductors.

These materials fall into a category where the energy difference between full and empty zones is very tiny and there is no zone overlap. At absolute zero temperature, or  $0^{\circ}\text{K}$ , no electron can travel from the first zone to the second zone (which is empty), due to the minimal energy gap between the two zones.

When temperature is increased, let's say to room temperature, electrons have enough thermal energy to jump across the narrow gap and into the unoccupied zone 2. Evidently, when temperature rises, semiconductors' electrical conductivity or the flow of electrons, or current increases as well. Because there is no thermal energy available to bridge the energy at absolute zero, a semiconductor acts as an insulator. Semiconductors' electrical conductivity falls between that of conductors and that of insulators[9], [10].



**Fig. 4 Energy Gap.**

### Electrical Resistance of Materials

The following factors have an impact on a material's electrical resistance:

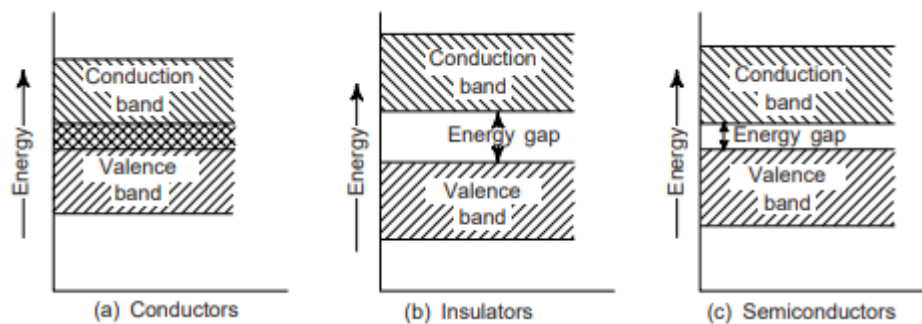
In comparison to pure metal, adding impurities or alloying elements increases lattice defects and decreases electrical conductivity. With an increase in temperature, metallic conductors' electrical resistance likewise rises. It is important to keep in mind that metals have positive temperature coefficients. The thermal vibrations of atoms in the lattice are more pronounced at higher temperatures. This results in less regular atomic spacing, which reduces the mobility of electrons in metals. A material's nature, composition, and surface quality all have an impact on how resistant it is to electricity. Several dislocations can be created in a material by mechanical processes like cold working and enhanced strain hardening, which raises the electrical resistance. It has been noted that electron mobility is constrained as a result of age hardening. The metal's electrical resistance rises as a result. The reverse effect of annealing is discovered to exist.

## Energy Bands

The fact that the band theory of solids provided a straightforward explanation for the noticeably diverse electrical behavior of solids (i.e., conductors, semiconductors, and insulators) was one of the key factors in its initial success.

### Conductors

If the uppermost energy band is partially filled or if the uppermost filled band and the following unoccupied band overlap in energy, a crystalline solid is referred to as a conductor or metal. In this situation, the electrons in the highest band shift into nearby empty states and function as free particles. A metal is a good conductor of electricity because when an electric field is applied, these electrons absorb energy from the field and generate an electric current. The conduction band is the band that is only half filled. Free electrons or conduction electrons are the names for the electrons involved in conduction. Several examples of effective conductors are silver, copper, aluminum, and others. Fig. 5 Energy band structure conductors, insulators, semiconductors.



**Fig.5 Energy band structure conductors, insulators, semiconductors.(newagepublishers.com)**

### Insulators

The prohibited energy gap in some crystalline materials between the uppermost filled band, known as the valence band, and the lowermost empty band, known as the conduction band, is quite enormous. Only a small number of electrons in such substances can obtain sufficient thermal energy to transition from the valence band into the conduction band at room temperature. Insulators are those kinds of solids. An insulator is a poor conductor of electricity because the conduction band has a limited number of free electrons. It has been noted that some electrons do move into the conduction band when the temperature of an insulator is raised.

Consequently, a minor electrical conduction might occur. Insulators make up the majority of covalent solids, which are made up of atoms with an even number of valence electrons. Good examples of insulators are rubber, bakelite, mica, etc.

### Semiconductors

A substance is referred to as a semiconductor if the forbidden energy gap between the valence and conduction bands is reasonably narrow (1 eV). Typical semiconductors include germanium and silicon, which have forbidden energy gaps at 0K of 0.78 and 1.2 eV, respectively.

Some of the valence electrons gain enough thermal energy to enter the conduction band since the prohibited gap is not particularly broad. Once liberated, these electrons can move about in response to an applied electric field. A hole is the result of an electron being missing from the

valence band. The perforations also act as electrical conductors. A semiconductor has a higher electrical conductivity than an insulator but a lower conductivity than a metal.

### Mean Free Path

A metal is a substance made up of a lattice of positively charged ion cores that are held together by valence electrons that are loosely bonded, also known as gas of electrons or delocalized electrons. We are aware that as they move throughout the metal, these electrons exhibit wave properties. Waves move with the least amount of interruption when passing through a periodic structure, or a structure with regular repetition. The wave will be deflected by any abnormality in the periodic, or repeated, structure that it travels through. It stands to reason that an alien or displaced atom could reflect an electron that is moving towards the positive electrode in the direction of the negative electrode.

We must keep in mind that as they go towards the positive electrode, electrons continue to gain momentum and speed. Additionally, electrons continuously lose momentum and subsequently velocity as they migrate in the direction of the negative electrode. The distance between reflections and deflections thus governs the electrons' net or drift velocity. Mean free path, as is obvious, is the average distance an electron travels while exhibiting a wavelike pattern without reflection or deflection.

### Thermoelectricity

This suggests that heat is directly converted into electricity. A current flows in the circuit in a direction that depends on the temperature differential between the two junctions and the type of the metals when two dissimilar metals are connected and the junctions are maintained at different temperatures. The discoverer, Seebeck, gave this phenomena the name "Seebeck effect." The thermoelectric current, so named because it results from an e.m.f. in the circuit brought on by the temperature differential between the junctions, is a type of electric current. The thermal emf is the name given to this emf. The thermocouple is a circuit made up of two distinct metals whose junctions are at two different temperatures. Fig. 6 shows thermocouple.

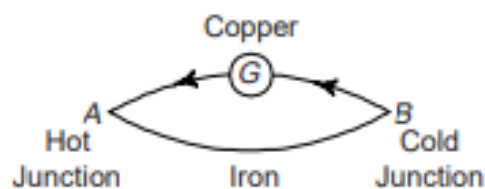


Fig.6 shows thermocouple (newagepublishers.com)

### Origin of thermoelectricity

The free electron theory can be used to explain how the thermoelectric effect came about. A conductor has a significant amount of free electrons, whose concentration varies depending on the metal. Due to the gradient in concentration, when two distinct metal wires are in touch with one another, electrons from one metal wire diffuse to the other metal wire. This causes one metallic wire to become positively charged and the other to become negatively charged. As a result, a potential difference across the contact is set up. Contact potential is what we refer to as. It is important to remember that temperature has a significant impact on the contact potential.

The potential difference created at the hot junction of a thermocouple is comparatively greater than that of the cold junction when one of the junctions is heated while keeping the other junction cool. As a result, the thermocouple generates a net electromagnetic field known as the thermo emf. Thermoelectric current is caused by the thermo emf.

### Magnitude and direction of thermo emf

It has been noted that the following parameters affect the strength and direction of the thermoe.m.f. generated in a thermal couple:

(i) Metal composition of the thermocouple: In order to ensure that the thermocurrent flows from the metal that appears earlier in the series to the one that appears later in the series over the hot junction, Seebeck created a series of metals known as the Seebeck series. Here are the see-back episodes: the following elements: Bi, Ni, Co, Pd, U, Cu, Mn, Ti, Hg, Pb, Sn, Cr, Mo, Rh, Ir, Au, Ag, Zn, W, Cd, Fe, As, Sb, and Te. For a given temperature differential between the connections, the thermoe.m.f. increases with the distance between the two metals in the series. The thermal e.m.f. for the Ni-Fe couple is obviously higher than for the Cu-Fe couple. Through the cold junction, the current will flow from a metal that appears earlier in the series to a metal that appears later in the series. In the Cu-Fe thermocouple, for instance, the current passes through the hot junction from Fe to Cu and the cold junction from Cu to Fe. The thermoelectric field's strength is on the order of a few microvolts for every degree of temperature difference between the two junctions. The magnitude of the thermal e.m.f. relies on the Seebeck series' separation of the metals.

(ii) Temperature difference between two junctions of thermocouple: One of the thermocouple's connections is kept warm by being submerged in an oil bath and heated with a hob. By submerging the other joint in ice cube powder, it is kept cold.

A thermometer submerged in the hot oil bath can be used to measure the temperature ( $T$ ) of the hot junction. A galvanometer ( $G$ ) that is connected to the circuit is used to measure the amount of thermoelectric current flowing through it.

By altering the heat output from the hob, the temperature of the hot junction ( $t_h$ ) can be changed. The cold junction's temperature in  $t_c$ , which is  $0^\circ\text{C}$ . The deflection of the galvanometer is directly proportional to the thermoelectric current and consequently the thermal e.m.f. as the temperature of the hot junction is raised above  $0^\circ\text{C}$ . The temperature at which the thermoelectric effect reaches its maximum, known as the neutral temperature ( $t_n$ ), is attained as the hot junction's temperature rises further. We must keep in mind that the neutral temperature for a specific thermocouple has a set value and is independent of the cold junction temperature. Cu-Fe thermocouple's  $t_n$  value is  $270^\circ\text{C}$ . The strength of the thermoe.m.f. gradually diminishes until it is zero as the hot junction's temperature rises more. The e.m.f. is now generated in the other direction if the temperature of the hot junction is raised further. As was previously mentioned, the temperature of inversion is the temperature of the hot junction at which the direction of the thermoelectric field reverses.

### Uses of thermocouples

Temperature measurement is the thermoelectric effect's most well-known practical use. The range of temperatures involved determines which thermocouple wires should be used. Platinum combined with a platinum rhodium alloy is utilised for temperatures between  $1000^\circ\text{C}$  and  $1700^\circ\text{C}$  since these metals do not melt or exhibit an inversion effect at such high temperatures. A Cu-Fe couple can be employed for temperature variations of one or two hundred degrees. Since  $275^\circ\text{C}$  is the neutral temperature, it cannot be used at higher temperatures. Because a copper-constantan thermocouple provides a significant e.m.f. for the same temperature differential, it is more useful. The general criteria is that the temperature must vary steadily enough to be measured while avoiding neutral and inversion points. The thermocouples have the following major benefits: (i) they respond quickly to temperature changes due to their small heat capacity and high conductivity; (ii) they can be placed in areas that are inaccessible to ordinary temperatures; (iii) they can measure temperatures as accurately as the e.m.f.; and (iv) they can be made of temperature-resistant metals, allowing

for the investigation of temperatures that would be impossible to study using regular materials like glass. Thermocouple pyrometer, thermopile, thermo-galvanometer, and other applications are some of the others.

## CONCLUSION

The behavior and characteristics of metallic materials have been clarified in large part because to the metals' electron theory. This theory has shed light on a variety of phenomena, including electrical conductivity, thermal conductivity, and optical characteristics of metals, by viewing metals as a collection of free electrons travelling through a lattice of ions. The great electrical and thermal conductivity of metals, their capacity for plastic deformation, and their reflectivity and luster may all be successfully explained by this theory. Furthermore, the advancement of cutting-edge technology and applications has been made possible by the electron theory of metals. It serves as the framework for the electronic components and circuits that make use of metals' capacity to conduct electricity. In materials science, it has been crucial in directing the design and manufacturing of metallic alloys with particular qualities suited for various purposes.

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## CHAPTER 7

### AN ELABORATION OF THE PHOTOELECTRIC EFFECT

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#### ABSTRACT

When a material is subjected to enough light energy, a phenomenon known as the photoelectric effect takes place, resulting in the emission of electrons. The notion of photoelectric current was developed as a result of the considerable study of this effect. We give a general review of the photoelectric current, its underlying theories, and its uses in a variety of fields in this abstract. When light interacts with matter, the photoelectric effect is a physics process that results in the emission of electrons from a material's surface. This abstract elaborates on the photoelectric effect by emphasizing its fundamentals, ramifications, and importance for comprehending light behavior and the nature of electrons. Albert Einstein received the Nobel Prize in Physics in 1905 for his original explanation of the photoelectric phenomenon. The conventional theory of light asserts that light is a wave. However, the wave-particle duality of light provided by quantum mechanics is necessary to fully understand the photoelectric effect, which cannot be explained by the wave nature of light alone. In a nutshell, the photoelectric effect is as follows: A metal surface will emit electrons when exposed to light with a high enough frequency (or energy). Photoelectrons are the name given to these released electrons. For electrons to be liberated, the incident photons' energy must be higher than the material's work function.

#### KEYWORDS

Cell, Current, Energy, Incident, Light, Photoelectric.

#### INTRODUCTION

We have indicated that the wave-corpusele (wave-particle) duality of light is its distinguishing feature.

While light is a wave-like phenomenon that exhibits interference, diffraction, and polarization phenomena, it is also a stream of tiny particles called photons that have no rest mass and move at the speed of light in a vacuum. In the processes of transitioning excited atoms, molecules, ions, and atomic nuclei into less energetic states, as well as in the acceleration and deceleration of charged particles, as well as in particle decay and annihilation, photons are created (emitted).

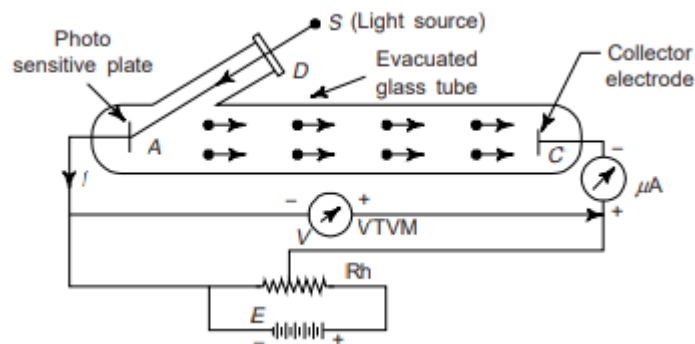
The mechanism by which electrons are emitted from a metal surface when it is exposed by high frequency electromagnetic radiation is known as the photoelectric effect (photo effect).

Heinrich Hertz made the discovery of the effect in 1887. When he saw that allowing ultraviolet light to shine on the cathode greatly facilitated the flow of an electric current via a gas discharge tube. When exposed to ultraviolet radiation, a zinc plate was found to become positively charged, indicating that the surface had shed its negative charges. In 1888, Hallahs began further experimental research. In 1899, Lenard demonstrated that electrons were the electricity's primary carriers when they were emitted from metal surfaces by high frequency radiations. The emitted electrons are called photoelectrons, and the phenomenon is known as the photoelectric effect. The electromagnetic spectrum's visible and ultraviolet parts are most frequently involved; however, the infrared and X-ray sections are also of importance.

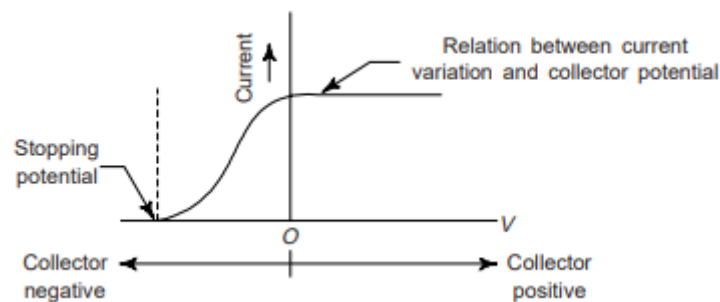
Alkali metals like sodium, potassium, and others are sensitive to visible light, whereas metals like zinc, cadmium, and selenium are only susceptible to ultraviolet light. Photosensitive devices like photo tubes or electric eyes, photo-conducting devices like automated door openers and closers, and photovoltaic cells like solar batteries or solar cells are only a few examples of technologies based on this phenomenon[1], [2].

### Experimental arrangement to study photoelectric effect

Fig.1 depicts a straightforward experimental setup for the investigation of the photoelectric effect. In a highly evacuated glass tube C, the emitting surface, which is a photosensitive plate A, is positioned opposite a metal plate B. A variable potential difference can be provided to the two electrodes, which are formed by the two plates A and B. In order to transmit ultraviolet or visible light from the source S and allow it to fall on the plate A, the evacuated glass tube is fitted with a quartz window D (if the cell is to operate in ultraviolet light), whereas if it is to be used in visible light, it is made of ordinary glass. The photoelectrons released from plate A are accelerated towards plate C when the applied potential difference between the two plates is such that A is at negative potential with respect to plate C. Microammeters ( $\mu\text{A}$ ) are used to measure the resulting photoelectric current  $I$  flowing in the circuit, and vacuum tube voltmeters are used to detect the accelerating potential difference  $V$ . Fig. 2 displays the fluctuations between the current value and collector potential  $V$ [3], [4].



**Fig.1 shows experimental arrangement to study the photoelectric effect.(newagepublishers.com)**



**Fig. 2 shows fluctuations between the current value and collector potential  $V$ .(newagepublishers.com)**

A photoelectric cell's window receives an incident light beam that completes the electrical circuit by acting as a switch. A flow of electrons moves from the photosensitive metal surface A to the collector electrode (C) when the incident light beam hits the surface. This makes the circuit's electric current flow. The quantity of photoelectrons grows in direct proportion to the increase in light intensity, which raises the circuit's current. When we turn off the incident light, the photoelectric reaction and current both come to an end. It is important to note that if the metal layer is positively charged, electrostatic repulsion prevents the electrons from

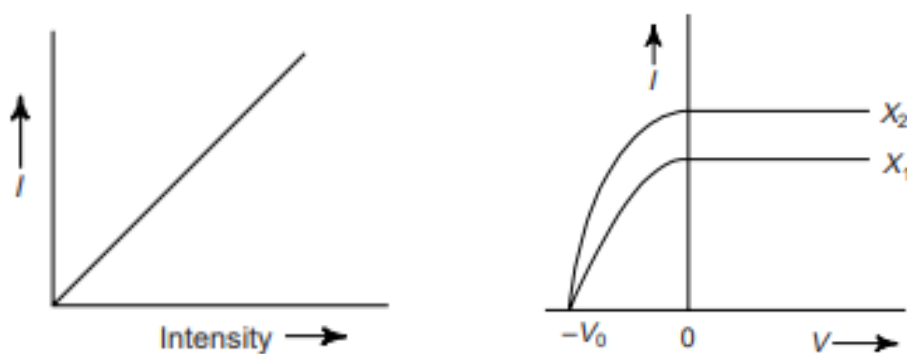
leaving the plate, rendering the cell inactive to light. It is discovered that the following variables affect photoelectric current: The nature or photosensitivity of the coated metal, as well as the frequency or wavelength of the incident light or radiation, the intensity of the light or radiation, the potential difference between the electrodes.

**The following are the key experimental findings:**

The collector plate B is appropriately made positive with respect to the emitter photosensitive plate A.

(i) The Effect of Frequency on the Photoelectric Current. Plate A's surface is lit up by monochromatic light of various frequencies. It has been discovered that the photoelectric current only manifests itself when the frequency of the incident light exceeds a specific minimum value of 0. The threshold frequency for the specified surface is this frequency's lowest possible value.

(ii) Effect of Incident Light Intensity: The Collector Plate B is sufficiently positive with regard to the Emitter Plate A in order to analyse the impact of the incident light intensity. The photoelectric current  $I$  is measured for a range of incident light intensities by maintaining constant the frequency of the incident light and the potential difference  $V$ . The relationship between photoelectric current and intensity is depicted in Fig.3. The photoelectric current is obviously inversely correlated with incident light intensity[5], [6].

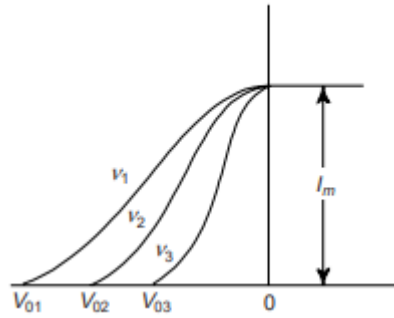


**Fig. 3 shows effect of incident light intensity. Fig.4 shows photoelectric current changes as a function of potential difference(newagepublishers.com)**

(iii) Effect of Potential Difference: The potential difference between the electrodes is changed while maintaining a constant frequency and intensity  $X$  of the incident light. A reversing key is used to reverse the initial modest positive potential, which is subsequently brought down to zero and turned negative.

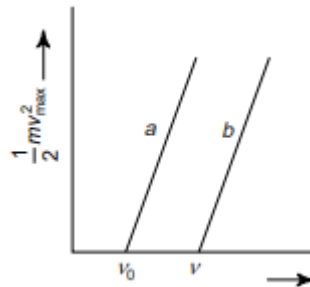
The photoelectric current is constant while collector plate B is positive. The photoelectric current continues to drop until it stops altogether when the collection plate is turned more and more negatively. The stopping potential is the retarding potential that terminates the photocurrent. Initial photocurrent for potential  $V_0$  is found to be the same for light of the same frequency if the incoming light intensity is increased to  $X_2$ .

(iv) Effect of Frequency on the Stopping Potential: The intensity of light of various frequencies is adjusted to create the same maximum ( $I_m$ ) value of the photoelectric current when collector B is positive in order to analyse the impact of the frequency of the incident light on the stopping potential. After being gradually zeroed out, the potential of collector B is then made more and more negative with the aid of the reverse key. The graphs created for the chosen photocathode are depicted in fig.4. It is clear from the graphs that the stopping potential rises as the frequency of the incident light increases.



**Fig. 4 Effect of Frequency on the Stopping Potential(newagepublishers.com)**

(v) Effect of Frequency on Maximum Kinetic Energy: Maximum kinetic energies are calculated using stopping potential magnitudes at various frequencies. In Fig. 5, the maximal kinetic energy is shown against the frequency. The result is a straight line. At a specific frequency of 0, the straight line (a) intersects the frequency axis. This demonstrates that the minimal frequency of 0 is the one where the greatest kinetic energy is equal to zero. The threshold frequency for the emitting surface is this frequency's lowest value[7], [8].



**Fig. 5 shows Effect of Frequency on Maximum Kinetic Energy(newagepublishers.com)**

## DISCUSSION

### Failure of Classical Theory

The aforementioned experimental electromagnetic wave findings cannot be explained by the classical theory, which makes the assumption that light propagates as electromagnetic waves. The shortcomings of classical theory include:

- (i) According to the classical hypothesis, electrons would be emitted with higher energies if the illumination of incident radiation were raised in intensity. Contrary to experimental observation, photoelectrons are expelled with the same kinetic energy as incident light intensity increases.
- (ii) The wave theory of radiation cannot be used to explain the presence of a threshold frequency for a specific material.
- (iii) Classical theory is unable to explain the instantaneous ejection of electrons from the metal surface. In contrast to the above actual results, the classical theory predicts that before a single electron is produced, several minutes must pass if the illumination is very dim observation.

In 1905, Einstein developed the photoelectric equation by using Planck's quantum theory to explain the photoelectric phenomenon.

### Einstein Photoelectric Equation

The following two equations serve as the foundation for Einstein's photoelectric theory:

(i) A stream of discrete particles known as photons makes up a frequency radiation. Each photon or quanta has an energy of  $h\nu$ , where  $h$  is the Planck constant. In space, photons travel at the speed of light.

(ii) A single electron instantly absorbs all of the energy of a photon when it strikes a metal surface as a quanta of energy, or photon. The likelihood of a metal surface absorbing two or more photons simultaneously is extremely unlikely. Assume that in a vacuum, frequency radiation is impinge on the surface of a metal. A metal's electron absorbs a photon's full amount of energy, or  $h\nu$ . It is important to keep in mind that the incident radiation penetrates the metal by a number of atomic diameters, and electrons at various depths absorb this energy from the incident photons. The metal's electron uses the energy it has taken in in one of two ways:

(i) In order to resist the attractive attractions of the metal's positive ions, the electron expends a portion of the photon energy  $h\nu$ . The photoelectric work function is the name for this minimal quantity of energy, which is typically represented by the metal's  $W$  symbol. The emitting surface's nature affects the work function ( $W$ ).

(ii) The photoelectron's kinetic energy is represented by the residual energy ( $h\nu - W$ ). The electron does not collide with another electron if it originates from the surface and has this kinetic energy.

In this case, it will emit with this energy as its maximal kinetic energy from the surface into vacuum.

Einstein's equation is used to explain the features of the photoelectric effect.

(i) The emission of more photoelectrons per second results from an increase in the number of photons in the incident radiation when the intensity of the radiation is increased. It is obvious that the photoelectric current is inversely proportional to the incident radiation. The maximal kinetic energy is unaffected by an increase in intensity.

(b) Photoelectrons simply emit with no kinetic energy for  $\nu = \nu_0$ .

(c) Photoelectrons with kinetic energies ranging from zero to a maximum value are released for  $\nu > \nu_0$ .

(d) If the incident light intensity is increased for  $\nu > \nu_0$ , then more photoelectrons will be released each second.

The following are some recent, significant findings about the photoelectric effect:

(i) While the majority of input photons are absorbed by the system as a whole and produce thermal energy, only a tiny percentage (about 5%) of them are successful in ejecting photoelectrons from photometals.

(ii) A process known as photo-ionization is also used to describe the photoelectric effect that is seen for isolated atoms that are present in a gas, such as Na or K vapor.

(iii) Heating the metal, which causes the electrons to be ejected through thermionic emission, can also supply the energy needed to do so.

(iv) Two or more photon photo-emission from lasers that may emit coherent radiation at high power levels has now been observed.

Contrary to the single quantum photo effect's roughly linear relationship, theory indicates that the double quantum photo current should be proportional to the square of the power of the incident light[9], [10].

## Photoelectric Cells

A photo cell is a device that transforms radiant radiation into electric energy. There are typically three types of photo cells:

(i) Photo-emissive cells photo-conductive cells and photo-voltaic cells, respectively.

(ii) Phototubes or photo-emissive cells: In photo-emissive cells, the energy of a light beam impacting a metallic surface with a low work function results in the emission of electrons. The released electrons are captured by a positive anode, which is placed in contact with either a vacuum, a gas-filled envelope, or quartz covering this sensitive surface. These cells come in two varieties:

(a) Phototube or vacuum photo-emissive cell

(a) A gas phototube or a gas-filled photo-emissive cell

(a) **Vacuum Photo-emissive cell** This phototube uses a tiny wire and a low work function material to treat the cathode surface. Essentially, it comprises of two electrodes: an anode (A) and a cathode (C). The semicircular cathode serves as the electron emitter and is constructed of a metal plate with a coating of a photosensitive substance, such as Cs. To avoid obstructing the incident light, the anode, which serves as the collector, is shaped like a straight wire or a loop. The light-sensitive cathode emits electrons that are collected by the anode. Anode voltages are high enough to reach current saturations, meaning that all of the electrons released at voltages higher than 40 V arrive at the anode.

The photo current is capped at around 10 A per lumen of the incident radiation in order to prevent cathode damage. The main benefits of this form of photo cell are that (i) the photocurrent is proportional to the light intensity and (ii) there is no delay between the incident light and the emission of photoelectrons. According to the characteristic curves of the photo cell, the variation in current with p. d. is linear, with the saturation current being proportional to the intensity. Because of its incredibly exact response, this type of photo cell is employed in photometry and television.

(b) **Gas phototube** Vacuum photo cells' current output and sensitivity can be improved for a given light flux by injecting an inert gas such as argon or neon at low pressure (a few mm of mercury or less) inside the tube. The current is increased five to ten times by ionisation, which occurs when electrons collide with gas molecules. Thermionic effect is another name for this phenomenon. Gas-filled photo cells are the name given to this type of photo cell. The produced photoelectrons ionise the gas atoms when the potential difference between the electrodes is greater than the gas's ionisation potential, which causes a significant current to flow. The p. d. should be around 100 V, nevertheless, to prevent excessive ion bombardment from harming the cathode.

Since it only takes the ions  $10^{-4}$  s to recombine and the current cannot keep up with the changes in illumination in that little time, the gas-filled photo cell cannot be utilised to record extremely rapid changes in illumination. As a result, the current is unable to remain proportionate to changes in light intensity. To follow the variations in light intensity from the music track, a film projector could make use of the gas-filled photo cells.

Photo-tube output can be as low as a fraction of an amp when utilised in extremely low light conditions. The current output of phototubes must be amplified for various practical uses, such as the reproduction of sound captured on film in television, etc. A photomultiplier tube or electron multiplier is a device that can directly amplify these currents. The secondary emission theory serves as the foundation for these tubes. A metallic plate's surface will typically emit additional electrons when a highly energy electron collides with it. The

electron that strikes the surface is referred to as the "primary electron," and the electrons that are released from it are referred to as "secondary electrons." The term "secondary electron emission" refers to this process. For every initial electron, up to four or even more secondary electrons can be released by treating the surface specially.

### **Photovoltaic cells**

It is a different kind of photocell known as a photovoltaic cell since it produces a little amount of e.m.f. The photovoltaic effect can be seen at the intersection of metals and semiconductors. The barrier layer cell is another name for this particular cell. Ane.m.f. is produced in this sort of photocell by the radiant energy impacting the photocell surface. You can use this emf with an external circuit. A linear relationship between the external current flow and light intensity can be achieved by designing the external circuit. A metallic plate is covered with chemicals or oxides to create this type of photocell. Photovoltaic cells made of copper and copper oxide are one category for these cells.

#### **(b) Photovoltaics made of iron and selenium.**

Photovoltaic cells made of copper and copper are either front-wall or back-wall cells. The semiconductor cuprous oxide is deposited on a copper-based plate in the back-wall type cell. The source of photoelectrons is the barrier, or blocking layer, that exists between the copper-based plate and the cuprous oxide. The oxide layer is covered by a metallic layer that is semitransparent. One electrode is the copper-based plate, and the other is the electrode that is in touch with the semi-transparent metallic layer. When illuminated, photoelectrons go through the barrier layer from the cuprous oxide to the copper, or from the semiconductor to the metal. This cell is referred to as a back-wall cell because the barrier layer is separated from the incident light.

When the barrier layer is located between the top electrode and cuprous oxide, the cell is referred to as a front-wall cell. Through the barrier layer, the semiconducting cuprous oxide is connected to the metal electrode as the current flows in that direction. Evidently, this cell's external circuit has electron flow in the opposite direction from the black-wall cell.

Photon cells are the common name for both front-wall and back-wall cells. The front-wall cell's sensitivity is higher than that of the back-wall cell because light passes through the barrier completely instead of being partially absorbed by the ineffective cuprous oxide. The iron-selenium front-wall cell is depicted. Iron forms the basal plate of this cell. In this cell, an iron-based plate is coated with a thin coating of iron selenide, which is subsequently covered by a layer of silver. This cell's base plate serves as one electrode and is attached to a copper ring. The second electrode of the cell is a copper ring in contact with the silver layer. When radiation is absorbed close to a P-N junction in a semiconductor, a photovoltaic effect is created. Fig. 6 shows Photovoltaic cells.

Excellent photovoltaic cells have been created using semiconductors like silicon, germanium, or indium antimonide. In artificial satellites, radio transmitters are powered by silicon photovoltaic cells. Photovoltaic cells are lightweight and portable and don't need an external power source. It has a far higher sensitivity than a photoemissive cell. The basic properties of photovoltaic cells are as follows: (i) Unlike photoconductive or photoemissive cells, photovoltaic cells do not require an external voltage.

(ii) Because only a modest dc voltage is produced, direct vacuum tube amplification is not feasible.

(iii) With modulated light, the reaction declines quickly due to large barrier-layer capacities.

(iv) By joining cells in series, the voltage sensitivity can be increased.

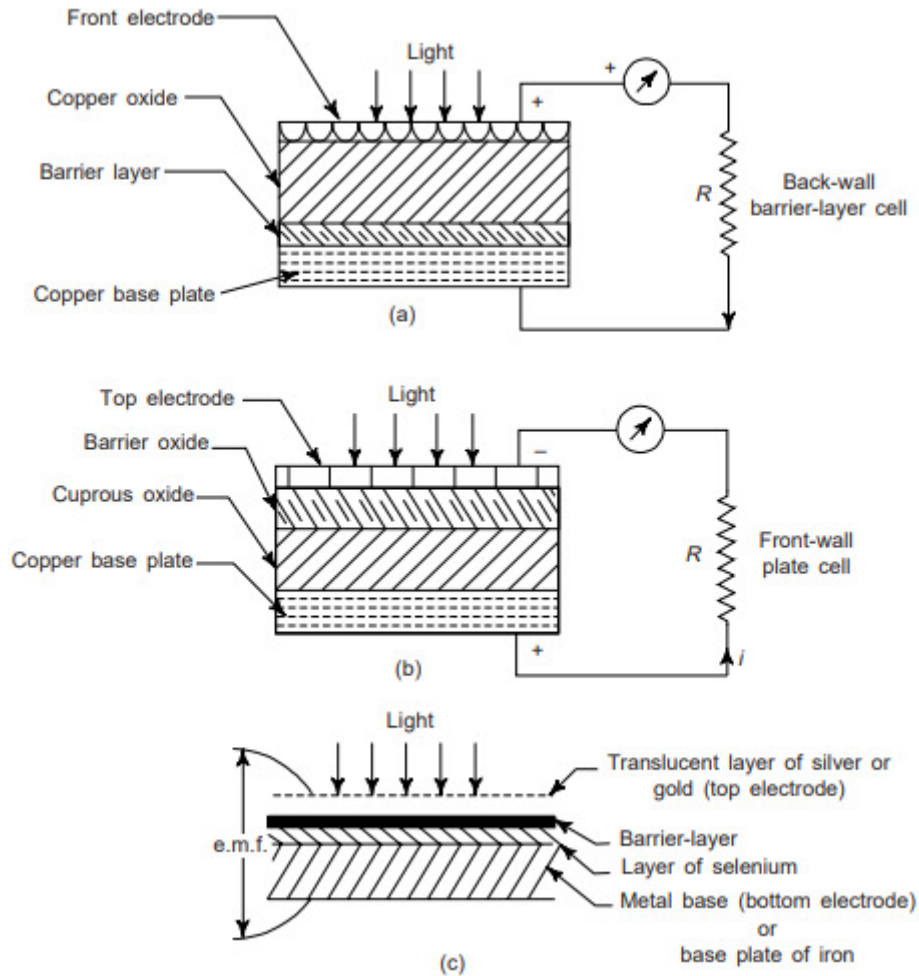


Fig. 6 shows Photovoltaic cells(newagepublishers.com).

### Solar cell or Battery

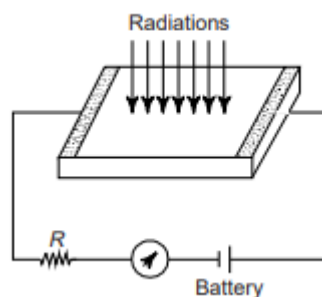
We refer to photovoltaic cells as solar cells when we want them to be a source of electrical energy. They perform the same purpose as a battery to generate power, however instead of the dry battery's chemical energy source, sunlight is used. Undoubtedly, a long stretch of pleasant weather is necessary. A p-n junction diode, the solar cell converts sunlight into electricity with a high conversion efficiency. Solar cells are made of razor-thin silicon wafers that have undergone thorough refinement and have had an impurity distributed into their faces as a minuscule layer close to the surface. A solar cell is made up of these newly produced strips, which make up a p-n junction. The energy in sunshine causes electrons to travel to one face of this p-n junction and holes to the other, creating polarity in the solar battery. As long as the p-n junction is exposed to sunlight, the current fluctuates according to the brightness of the sun and flows continuously.

**Photoconductive Cell:** A semiconducting material changes in resistance when radiation is impacted upon it. Photoconductivity is a general feature of semiconducting solids. When exposed to radiation, semiconducting substances like selenium, lead sulphide, cadmium sulphide, etc. lose some of their resistance. These materials, obviously, have low radiation resistance and dark resistance. When correctly produced as thin films, semiconducting substances like lead sulphide, lead selenide, and lead telluride respond well to infrared light and are presently utilised extensively. There are currently no known photoemitters at wave lengths beyond the near infrared part of the spectrum since it is claimed that relatively high photon energies were required for photo-emission to occur. However, in semiconductors,



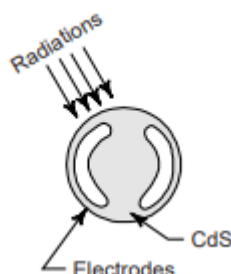
relatively low photon energy can generate internal electron-hole pairs, boosting the material's conductivity and carrier concentrations. This photo-induced conductivity can be used to detect light from the infrared to the ultraviolet spectrum. Visible light can stimulate the electrons in the valence band into the conduction band when the semiconductor's energy gap is in the proper range. In an approximate external circuit, the incident light produces more holes and electrons, which in turn causes the current to grow. We are aware that the current is a direct indicator of light intensity, and that photo conductors are the tools utilised to detect and measure light energy.

We observe that the semiconductor material comes with two electrodes. Since the photo cell's resistance is constantly high when it is dark, or not lighted, the amount of current flowing through the circuit is minimal. The circuit's resistance will drop as soon as the cell is lighted, causing the current to flow through it to increase significantly. The shape of the semiconductor must be correctly constructed in order to provide a high ratio of dark to light resistance. Typically, in high light, the resistance between the terminals drops from around  $10^7$  ohm in the dark to about  $10^6$  ohm. Fig. 7 shows photoconductive cell.



**Fig. 7 Shows photoconductive cell (newagepublishers.com)**

Fig. 8 depicts another widely used photoconductive cadmium cell. This cell has an extremely high dark-to-light ratio and a maximum response at 5000 thanks to its unique design. In order to expand the contact area, the two electrodes of the cell are often stretched in an inter-digital pattern. These cells are typically employed for telecommunication by modulated infrared light as well as for detection of ships and aircraft by the radiations given off by their exhausts or fuel gases. The device can be utilized in burglar alarms when combined with the appropriate amplifiers. But the gadget moves slowly. It takes some time for it to react to illumination completely. Furthermore, it responds differently to each variation in illumination.



**Fig. 8 Shows Cadmium sulphide photoconductive cell (newagepublishers.com)**

### Uses of Photoelectric cells

The most well-known practical application of the thermoelectric effect is temperature measurement. Which thermocouple wires should be used depends on the temperature range involved. For temperatures between  $1000^{\circ}\text{C}$  and  $1700^{\circ}\text{C}$ , platinum mixed with a platinum rhodium alloy is used since these metals do not melt or show an inversion effect at such high

temperatures. For temperature changes of one or two hundred degrees, a Cu-Fe couple can be used. It cannot be utilised at higher temperatures because 275 °C is the neutral temperature. A copper-constantan thermocouple is more beneficial because it produces a sizable e.m.f. for the same temperature difference. The main requirement is that neutral and inversion points must be avoided while the temperature must vary steadily enough to be monitored. The thermocouples have the following major advantages: (i) they can be placed in places that are inaccessible to ordinary temperatures; (ii) they can measure temperatures as accurately as the e.m.f.; and (iii) they can be made of temperature-resistant metals, allowing for the investigation of temperatures that would be impossible to study using regular materials like glass. The thermocouples also have the following minor advantages. Other applications include thermocouple pyrometers, thermopiles, thermo-galvanometers, and others.

### CONCLUSION

Our understanding of the relationship between light and matter has undergone a radical change as a result of the photoelectric current phenomena. Insights into the nature of electrons and the quantum behavior of particles have been gained as a result. The fundamental ideas behind the photoelectric effect, including the threshold energy and the direct relationship between light intensity and the quantity of released electrons, have been validated by experimentation and are now widely accepted. The photoelectric current has numerous and varied practical uses. The photoelectric effect is used in photo-detectors, such as photodiodes and photomultiplier tubes, to transform light impulses into electrical signals. These gadgets are used for scientific instrumentation, optical sensing, and telecommunications among other things. In solar cells, the photoelectric current serves as the fundamental mechanism for turning sunlight into usable electrical energy. A greater comprehension of this interesting phenomena is possible thanks to the explanation of the photoelectric effect, which sheds light on the complex interaction between light and electrons. When a material is exposed to light with enough energy, it will emit electrons, which is referred to as the photoelectric effect.

The essential concepts, experimental findings, and consequences of the photoelectric effect have been outlined in this abstract. Due to the ability of light to transmit distinct energy packets known as photons to electrons, the photoelectric effect serves as a demonstration of the particle-like nature of light. To expel electrons from the material, incident photon energy must be greater than a predetermined limit called the work function. Only the quantity of expelled electrons is impacted by the incident light's intensity; their kinetic energy is unaffected.

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## CHAPTER 8

### AN EXPLORATION OF THE DIFFUSION IN SOLIDS

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#### ABSTRACT

the movement of atoms or molecules from regions of higher concentration to regions of lower concentration is known as diffusion, and it is a basic phenomenon in solids. It is essential to the development of alloys, heat treatment, and impurity diffusion, among other elements of materials science. We give a general overview of diffusion in solids, its mechanisms, the variables affecting diffusion rates, and its relevance to material engineering and other related topics in this abstract. The movement of atoms, ions, or molecules from areas of high concentration to areas of low concentration is known as diffusion, and it is a crucial phenomenon in solid-state materials. This abstract explores diffusion in solids, stressing its mechanics, variables that affect diffusion, and the importance of diffusion in numerous applications. Vacancy diffusion, interstitial diffusion, and grain boundary diffusion are a few of the ways through which materials diffuse. In vacancy diffusion, atoms or ions migrate around a crystal lattice by swapping places with vacancies or empty lattice sites. Smaller atoms or ions move between the interstitial spaces in the crystal lattice, which is known as interstitial diffusion. Atoms or ions can move via grain borders during a process known as grain boundary diffusion, which occurs along the boundaries between several crystal grains.

#### KEYWORDS

Atoms, Diffusion, Energy, Interstitial, Mechanism, Surface.

#### INTRODUCTION

Atoms are transported through a crystalline or glassy solid by a process known as diffusion. Self-diffusion or diffusion is linked to a variety of phenomena that take place in metals and alloys, especially at high temperatures. The kinetics of microstructural changes during metallurgical processing and applications, as well as many solid-state phenomena, depend heavily on diffusion processes; typical examples include phase transformations, nucleation, recrystallization, oxidation, creep, sintering, ionic conductivity, and intermixing in thin film devices. Solid electrolytes for cutting-edge batteries and fuel cells, semiconductor chip and microcircuit fabrication, and surface hardening of steels through carburization are a few examples of direct technical applications of diffusion. For the introduction of a very small concentration of an impurity in a solid-state device, knowledge of the diffusion phenomenon is crucial [1], [2].

#### Types of Diffusion

- (i) Self Diffusion: This is the movement of a thermally stimulated atom from one interstice or site in a crystal lattice to another.
- (ii) Inter Diffusion: Binary metal alloys like the Cu-Ni system exhibit this phenomenon.
- (iii) Volume Diffusion: Atomic movement in bulk materials results in this type of diffusion.
- (iv) Atomic mobility along the grain boundaries alone is the only factor contributing to this sort of diffusion.
- (v) Surface Diffusion: Atomic movement along a phase's surface results in this sort of diffusion.

## Diffusion Mechanisms

Diffusion is the movement of dissimilar atoms along with a change in component concentration in specific areas of an alloy. The processes of diffusion have been explained by a number of different methods. The vibrational energy of the atoms in a solid serve as the foundation for almost all of these mechanisms. The common diffusion mechanisms include direct exchange, cyclic, interstitial, vacancy, etc. However, the mechanism of diffusion that has the lowest energy barrier (activation energy) required for moving atoms to cross it is really the most likely one. The forces of interatomic interactions and crystal lattice imperfections that promote diffusion transfer are what determine activation energy (the activation energy at grain borders is only half that in the bulk of a grain). The most likely mode of diffusion for metal atoms is the vacancy mechanism, while the interstitial mechanism applies to elements with tiny atomic radii (H, N, and C). We shall now research these mechanisms.

**Vacancy Mechanism:** In FCC, BCC, and HCP metals and solid solution alloys, this mechanism is a particularly important process for diffusion. The energy needed to create and shift a vacancy together make up the activation energy for this activity. The diffusion in a pure solid is caused by this mechanism. Atoms can enter unoccupied sites that are nearby to cause diffusion by the vacancy mechanism. We can assume that the vacancies move through the lattice and produce random shifts of atoms from one lattice position to another as a result of atom jumping. In a pure solid, during diffusion by this mechanism, the atoms surrounding the vacant site shift their equilibrium positions to compensate for the change in binding that occurs with the removal of a metal ion and its valence electron. Over time, concentration variations occur as a result of diffusion. At the surface, grain boundaries, and suitable internal sites, such as dislocations, voids are constantly being generated and removed. Naturally, as temperature rises, the rate of diffusion increases quickly.

**Interstitial Mechanism:** Although self-diffusion does not typically occur in metals, the interstitial mechanism, where an atom changes places by utilizing an interstitial site, is encouraged when interstitial impurities are present due to its low activation energy. Interstitial solutions may develop in solids made up of two or more elements with considerably different atomic radii. The smaller size atoms fit into the spaces (referred to as interstices) left by the larger atoms, while the larger atoms occupy lattice sites. The diffusion mechanism in this instance is comparable to vacancy diffusion with the exception that the interstitial atoms remain on interstitial sites. We must keep in mind that interstitial diffusion requires an activation energy because, in order to reach the vacant site, it must squeeze past nearby atoms with energy provided by the vibrational energy of the moving atoms. Interstitial diffusion is undoubtedly a thermally triggered phenomenon. The interstitial mechanism method is easier since the solute atom can migrate even in the absence of vacancies. The following situations need the use of this mechanism[3], [4].

- (a) The mechanical characteristics of metals are significantly influenced by the presence of very tiny atoms in the lattice's interstices.
- (b) Oxygen, hydrogen, and nitrogen can diffuse freely in metals at low temperatures.

**Interchange Mechanism:** In this kind of mechanism, the atoms switch positions by rotating around a central point. Because the process requires a significant level of activation energy, this mechanism is highly improbable in the majority of systems. The number of sites does not change even as two or more nearby atoms jump past one another and swap locations. For BCC, this exchange can be either two or four atoms (Zener ring). The exchange mechanism causes significant local distortion as a result of the movement of atoms near the jumping pairs. In this instance, substantially more energy is needed for atoms to jump. This mechanism results in a large number of undesirable diffusion partners with various

compositions. This is known as the Kirkendall effect. Kirkendall was the first to demonstrate diffusion inequity. Kirkendall demonstrated that Zn atoms diffused out of brass into Cu more quickly than Cu atoms diffused into brass using a -brass/copper pair. Brass exhibits voids as a result of a net loss of Zn atoms. From a theoretical perspective, Kirkendall's impact in diffusion is crucial. We should point out that the application of this effect to metal cladding, sintering, and metal deformation is important[5], [6].

## DISCUSSION

### Diffusion Coefficient: Fick's law of diffusion

When atoms (or molecules) in a phase change their locations in relation to their neighbors under the effect of thermal energy and a gradient, the process is known as diffusion. The gradient could be a gradient in concentration, a gradient in an electric or magnetic field, or a gradient in stress. We will solely take into account mass flow in concentration gradients. Given that during diffusion, atoms must hop from one location to another, we are aware that thermal energy is required for mass flow. The thermal energy manifests as atoms vibrating around their average locations within the material. Fick's laws, which apply to weak solutions and systems with a low concentration gradient of the diffusing substance, are the classical laws of diffusion.

(i) Fick's First Law: This law outlines the speed at which diffusion takes place. This statute declares

$$dn = -D (dc/dx) a \cdot dt$$

(ii) Fick's Second Law: This applies to non-steady flow and is an extension of Fick's First Law.

The instantaneous mass flow rate (flux) past any plane in a solid can be calculated using Fick's first law, but it doesn't tell us how the concentration changes over time. However, non-steady conditions are frequently encountered while using engineering materials. In non-steady diffusion, the solute atom concentration might fluctuate at any time with regard to time.

### Factors Affecting Diffusion Coefficient

We have already indicated that concentration has an impact on diffusion coefficient. In contrast to the impact of temperature, this effect is minimal. We have assumed that atoms leapt from one lattice site to another while considering diffusion mechanisms. The crystal structure, temperature, activation energy, and vibrational frequency of the atoms all play major roles in determining how quickly they leap.

### Self- Diffusion

It is the movement of a thermally excited atom from one interstice or location of the crystal lattice to another. The movement of the atom is referred to as self-diffusion if the solid is made up of a single chemical element, such as pure copper, in which case both the moving atom and the solid have the same chemical composition. Self-diffusion plays a crucial role in the annealing and creep processes. Self-diffusion coefficient can be determined relatively effectively by using radioactive tracers.

### Inter-Diffusion

This phenomenon occurs in binary metallic alloys, such as the Cu-Ni system, and is the opposite of self-diffusion. If copper had been coated with nickel, then over enough time and at high temperatures, atomic diffusion would cause nickel homogeneity inside the copper[7], [8].

### Diffusion with Constant Concentration

Case hardening is a process where one element, typically in gaseous form, diffuses into another, usually in solid form, but the diffusion only affects a small area close to the surface. The characteristics of this region change as a result. In general, it is seen that the core stays flexible while the surface portions harden and become more fragile. Fick's second law governs the case hardening process. One of the diffusion mechanisms causes the atoms of gas to diffuse into the solid. It is discovered that the interstitial mechanism is typically this diffusion mechanism. According to reports, as diffusion advances, the depth of interstitial alloy increases as does the depth to which the gas atoms can penetrate.

Now let's look at an illustration of nitrogen diffusion through iron, often known as nitriding. The Fe-N alloy that is created when nitrogen is dissolved in the interstitial spaces of an iron crystal is more brittle, harder, and stronger than the original iron. The nitrogen concentration would be higher close to the surface according to the concentration profiles because the interstitial atoms prevent dislocation motion. Steel gears and other steel objects are regularly carburized or nitrided to increase their surface hardness. Carbon is diffused into the steel object's surface layers during the carburizing process. In pack carburizing, the object is packed in solid carbon powder, whereas in gas carburizing, the object is surrounded by a carbon-rich environment of methane gas.

When the steel object is annealed in the carburizing liquid at a high temperature, carbon diffuses into the steel from the surface along a gradient of concentration. It is important to highlight that surface hardening enhances wear resistance of parts like gears without degrading the bulk mechanical characteristics, such as toughness. Decarburization is the opposite of carburization. Due to an oxidizing environment reacting with the carbon in the steel to form CO or CO<sub>2</sub>, the carbon is lost from the steel's surface layers in this instance. Because of this, utilizing a protective environment while heating steel should be avoided because it reduces the steel's fatigue resistance.

### The Kirkendall effect

The speeds at which A and B diffuse are not always the same when we think of them as a binary solution. It has been noted that the lower melting component typically diffuses significantly more quickly than the other. This had several intriguing side effects, which Kirkendall was the first to notice. Prior to the diffusion of anneal, thin rods of a material with a high melting point that is insoluble in the diffusion matrix are positioned at the couple's weld junction as inert markers. The markers change during the anneal in the same direction as the slower moving species, it has been discovered. According to reports, this shift's size is related to the square root of the diffusion time. This kind of movement demonstrates that a bulk flow of matter in the opposite direction is compensating for the net mass flow caused by the difference in diffusivities inside the diffusion zone. It is obvious that lattice planes are formed on one side of the diffusion zone and destroyed on the other, and the ensuing bulk flow transports the markers. The bulk flow happens in relation to the ends of the diffusion couple, it is important to remember. The fact that it is a quite different phenomenon from the diffusion process itself is interesting to note. Porosity on the side of the lower-melting component is seen in a number of instances, suggesting that the bulk flow does not adequately make up for the difference between the diffusivities of the two species.

The concept of gaseous inter-diffusion can be used as an example to comprehend the Kirkendall effect. Let's imagine that hydrogen and argon are held in two chambers connected by a tube at the same pressure, and that a frictionless piston inside the tube separates the gases. The gases diffuse when an opening in the piston is opened. Since the lighter hydrogen will diffuse more quickly, there will naturally be a pressure difference that tends to move the piston in the same direction as the argon's slower diffusion[9], [10].

## Diffusion in oxides and ionic crystals

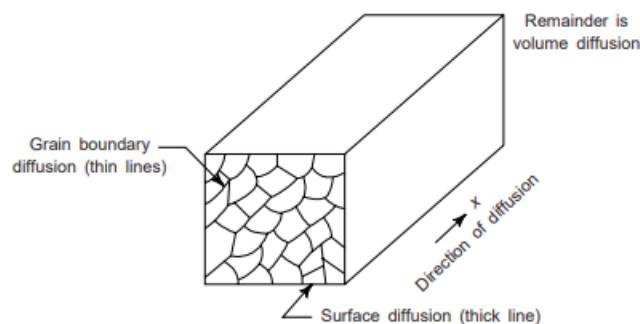
Diffusion processes can cause ionic or partial ionic bond-containing oxides and other crystalline compounds to diffuse. Due to the demand for electrical neutrality, the diffusion process in the current situation is a little problematic. The formation of vacancies must prevent the crystal from picking up charge. This requires that the vacancies arise in pairs, each pair consisting of a vacancy in an anion (-ve charge) and a vacancy in a cation (+ve charge).

We might observe that diffusion in ionic crystals is aided by Schottky and Frankel defects. The cation (+ve) interstitial carries the flux in the Frankel diffusion processes, whereas the cation vacancy carries the flux in the Schottky diffusion mechanisms. Anions diffuse through anion vacancies, while cations do the same through cation vacancies. However, the activation energies for these two processes are different. It has been claimed that the concentration of impurities, which affects the number of vacancies, has a significant impact on the diffusion in ionic crystals and oxides. Let's imagine that a NaCl crystal has a trace amount of cadmium added to it as an impurity. We are aware that Na has a valence of 1, and Cd has a valence of 2. To maintain electrical neutrality and create a cation vacancy, a single Cd ion would need to replace two Na ions in the crystal. This implies that the diffusion rate will rise with the addition of Cd cations.

Metallic oxides frequently contain impurities, and the presence of impurities that occupy anion sites frequently accelerates the rate of oxygen diffusion through an oxide. When using the powder metallurgy approach to create parts out of high temperature ceramics, diffusion in oxides and ionic crystals is particularly helpful. Diffusion would cause the powdered particles to adhere to one another during the sintering process.

## Surface Diffusion

Diffusion occurs through a material's volume as well as along the surfaces of a solid and in the poly-crystal's grain boundaries. One can anticipate lower activation to surface diffusion than volume diffusion because atoms at a solid's surface make fewer bonds than atoms at its interior. Atomic migration that occurs during the solidification process is known as solid diffusion. Fig. 1 shows area of volume, grain boundaries and surface diffusion.

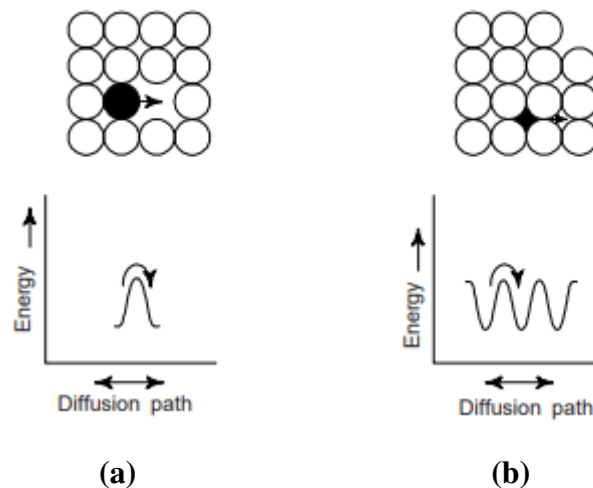


**Fig.1 shows area of volume, grain boundaries and surface diffusion.(newagepublishers.com)**

## Activation Energy of Diffusion

The diffusion process is caused by atomic movement, as we have already mentioned. In order for the atoms to move or leap from one point in the lattice to another, energy is obviously needed. The energy needed by the atom to cross this energy barrier is known as the activation energy of diffusion. Fig. 2 shows Activation Energy For Diffusion (a) vacancy mechanism (b) interstitial mechanism.



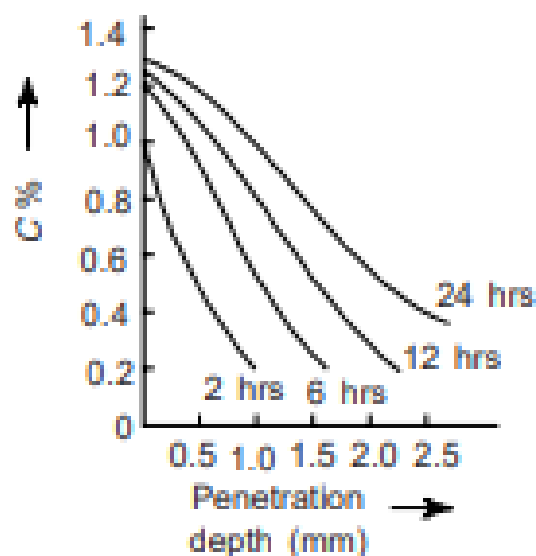


**Fig. 2 shows Activation Energy For Diffusion (a) vacancy mechanism (b) interstitial mechanism(newagepublishers.com).**

In the vacancy mechanism, the energy is needed to draw the atom away from the atoms that are closest to it. Along with moving along them in interstitial diffusion, energy is also needed to bring the atom closer to its neighbors. Additional energy is needed if the typical interatomic distance increases or decreases. We should be aware that the activation energy changes depending on the size of the atom, the strength of the bond, and the type of diffusion process. According to reports, firmly bound materials with large-sized atoms, such as corundum and tungsten carbide, require a high activation energy because interstitial diffusion uses more energy than vacancy processes.

### Application of Diffusion

The fundamental mechanisms behind crystallization, recrystallization, phase change, and the saturation of alloy surfaces by additional elements are diffusion processes. Several significant diffusion uses include: Metal oxidation, semiconductor doping, diffusion bonding, such as welding, soldering, galvanizing, brazing, and metal cladding, are examples of these processes.



**Fig. 3 C gradient in 1022 steel carburized in 1.6% CH, 20% CO and 4% H(newagepublishers.com).**

Sintering, or powder metallurgy, produces strong bodies; case hardening is a surface treatment for steels; homogenizing treatment of castings, recovery, recrystallization, and phase precipitation are important heat treatments. Fig. 3 C gradient in 1022 steel carburized in 1.6% CH, 20% CO and 4% H.

## CONCLUSION

A common occurrence that profoundly affects the characteristics and behavior of materials is diffusion in solids. For a variety of applications, including the creation of materials with desired properties, it is crucial to comprehend and manage diffusion processes. Diffusion research has provided crucial insights into the processes that underlie atomic motion and the variables that control diffusion rates. The three main categories of diffusion mechanisms in solids are vacancy diffusion, interstitial diffusion, and grain boundary diffusion. Each process involves a unique atomic motion and is controlled by a variety of variables, including temperature, concentration gradients, and crystal lattice defects. Using mathematical models, such as Fick's equations of diffusion, which offer a framework for projecting and analyzing diffusion behavior in solids, the diffusion rates can be quantitatively defined.

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## CHAPTER 9

### MECHANICAL PROPERTIES OF MATERIALS AND MECHANICAL TESTS

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#### ABSTRACT

The behavior and applicability of materials for different purposes are greatly influenced by their mechanical properties. These qualities are assessed mechanically, and the results are useful for material selection, design, and performance analysis. The mechanical properties of materials and the most frequent mechanical tests used to evaluate them are summarized in this abstract. Material's response to applied forces or loads is largely determined by its mechanical properties. In a variety of technical and manufacturing applications, these characteristics are extremely important in the selection, design, and performance assessment of materials. The mechanical characteristics of materials and the mechanical tests used to evaluate them are discussed in this abstract. Various behaviors exhibited by materials under various mechanical circumstances are covered by mechanical characteristics. The most typical mechanical characteristics include Mechanical evaluation of these attributes yields data that are helpful in material selection, design, and performance analysis. This overview provides a summary of the mechanical properties of materials and the most common mechanical tests performed to assess them. The mechanical characteristics of a material play a significant role in determining how it responds to applied forces or loads. These qualities are crucial for the selection, design, and evaluation of materials' performance in a range of technical and manufacturing applications. This abstract discusses the mechanical properties of materials and the mechanical tests that are performed to assess them.

#### KEYWORDS

Elongation, Load, Material, Plastic, Stress, Strength, Strain.

#### INTRODUCTION

The mechanical characteristics of materials, such as their strength, stiffness, and ductility, are crucial in defining the fabrication and potential practical uses. Elasticity, plasticity, strength, ductility, hardness, brittleness, toughness, stiffness, resilience, malleability, fatigue, creep, and other key mechanical properties of materials include these. BIS has standardized the full range of mechanical characteristics and chemical make-up of different materials. Materials have a wide range of mechanical characteristics, including the ductility of pure copper, the hardness of diamond, and the surprisingly elastic behavior of rubber, for example. Many materials respond to stress in rather different ways. For instance, cast iron, cement, and bricks are significantly stronger in compression than tension, but steel and wood are stronger in tension. Of course, stresses can result in a material breaking or fractured, as well as a change in shape. The melting point is also significant for materials that must tolerate high temperatures[1].

Steel is a great structural material due to its strong yield strength and exceptional fracture toughness or ductility. Modern high strength low alloy (HSLA) steels have both high strength and good crack development resistance or fracture toughness by having very tiny grain sizes of roughly 10 micrometers. Duct ion length can be as per the nature of the topic. Hence it can be prepared as per the discretion of the author.

An engineer must consider the following characteristics of materials in addition to their mechanical properties in order to choose the best metals for different tasks:

- (i) **Physical Properties:** The shape, size, colour, lustres, specific gravity, porosity, structure, finish, etc. of a material are examples of its physical properties.
- (ii) **Technological Properties:** It's important to note that a metal's mechanical properties, such as malleability, machinability, weldability, formability or workability, castability, etc., make up all of its technical properties.
- (iii) **Thermal qualities:** This category of qualities includes things like specific heat, thermal conductivity, thermal expansion, latent heat, thermal stresses, thermal shock, and more.
- (iv) **Electrical Properties:** These include dielectric strength, conductivity, resistivity, and relative capacity.
- (v) **Chemical Properties:** These characteristics include acidity, alkalinity, chemical composition, corrosion, atomic weight, equivalent weight molecular weight, atomic number, and others.

We will talk about mechanical and technological properties in this chapter. Subsequent chapters will address other qualities. First, we give a quick overview of a few definitions of typical mechanical properties[2], [3].

## DISCUSSION

### Isotropy

When a body's physical characteristics are independent of direction in the body along which they are measured, the body is said to be isotropic. For example, a polycrystalline material in which the grains or crystals are randomly oriented exhibits isotropic behaviour. Crystal distribution in cast iron, steel, and aluminium is random. Engineers are interested in solid materials from a design perspective if they can withstand applied force when they are subjected to it. When exposed to a load or strain, many solid materials exhibit elastic behaviour. This means that when a solid material is loaded, it deforms, but when the load is released, it recovers to its original shape. An isotropic body has just one refractive index, one dielectric constant, etc. R. Hooke conducted research on the elastic behaviour of metals and came up with the law that is now known as Hooke's law. Elongation occurs when a specimen of length  $l$  and cross-sectional area  $A$  is loaded with a force  $P$ , causing the length to rise by an amount  $l$ . Up to a certain limit, the elongation also rises as the load is increased.

### Anisotropy

As an example, the resistivity of some single crystals measured with the electric field along a specific crystallographic direction may be higher than along directions perpendicular to it. This is due to the quality of variation of a physical property with the direction in a body along which the property is measured. As a result, these crystals are resistivity-anisotropic. Anisotropy is undoubtedly a situation in which certain characteristics vary depending on the direction. Examples of materials with high anisotropy include various composite materials, aggregates of poly-crystals with a preferred orientation, wood, laminated plastics, etc.

### Elasticity

As an example, the resistivity of some single crystals measured with the electric field along a specific crystallographic direction may be higher than along directions perpendicular to it. This is due to the quality of variation of a physical property with the direction in a body along which the property is measured. As a result, these crystals are resistivity-anisotropic. Anisotropy is undoubtedly a situation in which certain characteristics vary depending on the

direction. Examples of materials with high anisotropy include various composite materials, aggregates of poly-crystals with a preferred orientation, wood, laminated plastics, etc.

### **Plasticity**

It is a material's capacity to remain permanently distorted (without breaking) even after the load has been lifted. All materials are somewhat plastic. In determining manufacturing procedures like forming, shaping, extruding operations, etc., this feature of a material—which is the complete opposite of elasticity—is crucial. High temperatures increase the flexibility of metals. The flexibility of a material often increases with temperature, and this is significant in determining the subsequent procedures[4], [5].

Whether a metal is formed in a red-hot or cold environment relies on the metal's composition and the surrounding conditions. Lead and clay are both plastic when left at room temperature. When steel is brilliant red hot, it turns into plastic and can be sculpted. In the forming, shaping, and extruding of metals, this feature is used. Only after the elastic range has been exceeded does plastic deformation occur. Since materials can deform under continual, sustained stress when they are in the plastic state, the time rate of strain would be a general description of plastic action. The idea of the limit of deformation before to rupture would also be involved. Yield, plastic flow, and creep are examples of plastic activity in structural materials. As was already mentioned, plasticity plays a crucial role in the forming, shaping, and extruding processes. Some materials are formed cold, such as when sheets are deep drawn, while others, particularly metals, are shaped hot, such as when structural steel shapes are rolled and some material components are forged[5], [6].

### **Ductility**

It is described as a metal's characteristic that allows for elongation or drawing into wires without rupture. It is the deformation that a material undergoes at the point of rupture and is quantified by the amount of elongation and the amount of area decrease before the test piece ruptures. Most commonly, percentage elongation is employed to quantify ductility and its value is expressed as elongation. The maximum length increase stated as a percentage of the original length is referred to as percentage elongation.

Ductility, or strain at fracture, is a term frequently used in tensile tests. Ductility is measured in the same unit as strain. As previously mentioned, the shape of test curves and the percentage elongation and percentage reduction in the area of the test piece at the neck provide important information regarding a material's ductility. When a material hits its breaking point, the degree of permanent distortion that has taken place is measured by ductility. We can see that brittle materials, like cast irons, do not exhibit ductility since they exhibit little to no plastic deformation prior to fracture. A little thought reveals that a metal's high ductility is explained by a material with a good proportion of elongation or reduction in cross-sectional area. Metals are regarded as ductile if their elongation is greater than 15%. Metals with an elongation of 5 to 15% are regarded as having intermediate ductility. However, brittle metals are those that have less than 5% elongation. Cast irons and other brittle materials exhibit little to no plastic deformation prior to fracture, i.e., they are not ductile. Due to its high ductility, copper is a ductile material that exhibits significant plastic flow before fracture. This attribute enables one to draw cables. Glass may be drawn in a variety of shapes when it is heated due to its strong ductility[7], [8].

### **Strength**

It might be described as a material's ability to support or withstand an external force or load without rupturing. It is measured in terms of force per unit of cross-sectional area. This is a metal's most significant characteristic and it is crucial for designing different components and structures.

Different types of loads, such as tensile, compressive, and shear loads, must be withstood by a material. As a result, one can broadly divide strength into the two main categories:

- (a) A metal's strengths can be elastic or plastic depending on the amount of stress.
- (b) The strengths of a metal can be tensile, compressive, shear, bending, and torsional depending on the type of stress. We are currently researching all of these strengths.

### **Ultimate Strength**

It is the force necessary to cause a unit cross-section of material to fracture.

### **Elastic Strength**

It is the strength value that corresponds to the transition from the elastic to the plastic range, or when a material shifts from an elastic to a plastic behavior. It is impossible to quantify precisely. This is referred to as the optimum stress value, and it's used to describe a material's elastic strength.

### **Plastic Strength**

The material's strength value corresponds to the plastic range and rupture. It also goes by the name "ultimate strength." In actual use, a specimen is always put under a stress that is lower than the working stress. The term "factor of safety" or "factor of ignorance" refers to the ratio of a metal's working stress to ultimate stress. This is very dependent on the types of pressures or loads.

### **Tensile Strength**

It is the highest tensile stress that a material can experience up until rupture when loaded at that point.

The maximum load in a tension test correlates to the tensile strength, which is the maximum strength under tension. The highest point on the typical stress-strain curve is used to measure it. This strength offers the fundamental design data on the material's suitability for engineering tests.

Due to necking, the load in ductile materials decreases after the ultimate load, which is an indication of plastic instability. In brittle materials, the ultimate tensile strength makes sense as a basis for working stresses. We might observe that, similar to yield strength, tensile strength is applied with a safety factor.

### **Compressive Strength**

The amount of force needed to crush a piece of metal is its compressive strength.

Compressive Stress = Maximum Compressive Load/ Original Cross-Sectional Area.

### **Shear Strength**

The amount of stress that must be applied tangentially to shear a metal off across the resisting part determines the metal's shear strength.

Shear Stress = Maximum tangential load/ Original cross-sectional area

### **Bending strength**

For a metal, it is the amount of load that can cause it to bend across the resistant part and break off.

Bending Stress = Maximum bending load/ Original cross sectional area

**Torsional strength**

The amount of force required to twist across the resistant part and shatter a metal is known as its torsional strength. Mathematically,

Torsional stress = Maximum twisting load/Original cross-sectional area

**Stress and Strain**

Strain is the fractional change in length, area, or volume, and stress is the force per unit area. This is, of course, the body's resistance to deformation brought on by the application of an external force.

Stress is a term used to describe the strength of a force acting on a given area. Its unit, N/mm<sup>2</sup> or N/m<sup>2</sup>, is known as Pascal in SI and is represented by the letter Pa.

$$\text{Stress} = \text{Force} / \text{Area}$$

$$\text{Strain} = \text{change in length} / \text{original length}$$

We have two classes of strain that correspond to the elastic and plastic qualities of materials:

(a) Elastic Strain: This is the change in a body's dimensions caused by being loaded. This is a reversible occurrence, meaning that when the applied stress is withdrawn, the elastic strain goes away. This is proportional to the amount of stress.

(b) Plastic Strain: This is the long-term alteration that occurs in the body as a result of a load. Even after the imposed load is withdrawn, the alteration is still present.

The percentage elongation is the amount of elongation represented as a proportion of the initial gauge length:

$$\text{Percentage elongation} = \text{Final length} / \text{Initial length} * 100$$

**Hooke's law**

For the first time, Robert Hooke asserted in 1678 that stress is proportional to strain within elastic limits, i.e., stress equals a constant strain. A constant property of a material is the ratio of stress to strain, and this proportionality constant is known as the material's modulus. It varies depending on the material and the type of stressors. Young's modulus of elasticity is the term for the constant when tensile or compressive stress is being applied. Young's Modulus of Elasticity is the slope of the stress-strain diagram up to the limit of proportionality[9], [10].

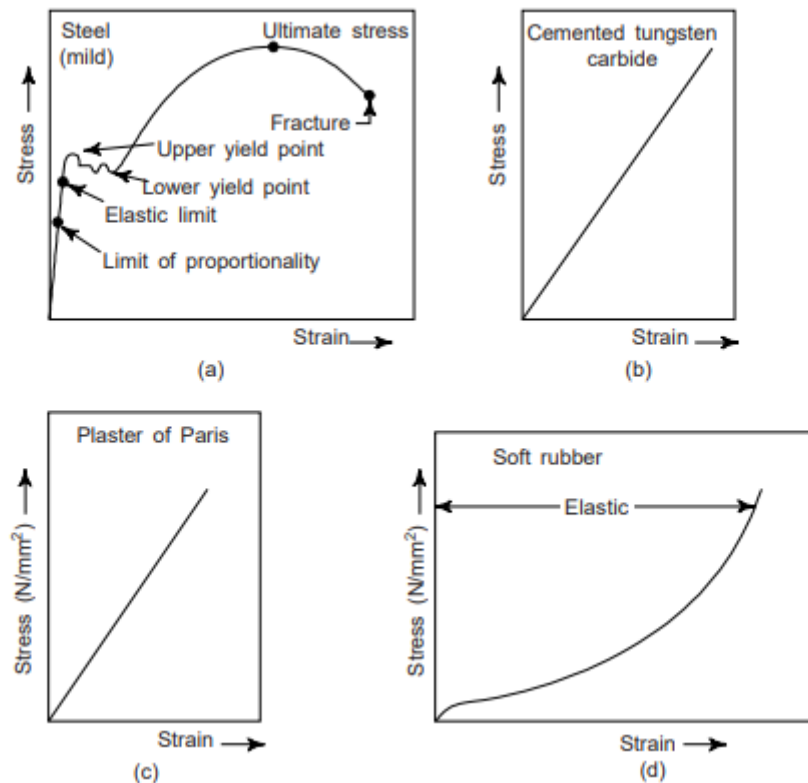
**Poisson Ratio**

A specimen is strained in the force's direction as well as in a direction perpendicular to the force when it is stressed by a uniaxial force. Longitudinal strain and lateral strain are terms used to describe strain that is parallel to the direction of force. Lateral strain and the link they have Poisson's ratio is used to describe axial strain.

$$\text{Poisson's ratio} = \text{Lateral strain} / \text{Longitudinal strain}$$

**Stress- strain Relation**

A stress-strain diagram is a common tool for illustrating the relationship between stress and strain. These diagrams are created by creating a graph or curve using the data from a tensile test, in which a specimen is subjected to increasing tensile stress. By using strain measuring tools, it is possible to see and record the length changes that result. Various engineering materials' stress-strain relationships are displayed.



**Fig. 1 shows stress-strain curve for different materials.(newagepublishers.com)**

In the case of ductile materials, the material stretches elastically at the start of the test. When the tension is removed, the sample or specimen returns to its original length. At initially, the strain (both longitudinal and lateral) grows according to the stress. The stage at which the specimen, or material, perfectly complies with Hooke's law is known as the limit of proportionality (stress strain) (Fig. 1 (a)). Beyond the elastic limit, or by applying further stress, it causes plastic deformation, which results in persistent extension even after the given load, or stress, has been removed. At this moment, the resultant strain starts to grow faster than the corresponding stress and keeps growing until the yield point is reached. We must keep in mind that the material quickly extends near the yield point.

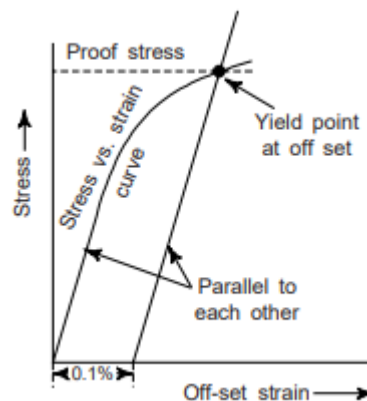
The normal stress is defined as the ratio of the applied load to the initial cross-sectional area. This stress rises with elongation as a result of work hardening or strain hardening until the tensile stress reaches its maximum. By multiplying the maximum load by the initial cross-sectional area, one can get the stress value at maximum load. The ultimate tensile stress is the stress in question (Fig. 1 a)). It is clear from Fig. 1 (a) that the strain remains slowly at a given load value in the absence of additional stress or loading. Creep is the name given to the phenomena of gradual extension that grows over time while under persistent stress. At this time, a neck starts to form along the specimen's length, and more plastic deformation is localized within the neck. During elastic elongation, the cross-sectional area shrinks proportionally to the lengthening. It is important to note that the specimen, or test bar, maintains a constant volume. A stress-strain diagram for mild steel is shown in Fig. 1 (a). The yield point, elastic limit, maximum tensile stress, and fracture stress at the breaking points are all clearly displayed in this diagram. We observe that the yield point in this diagram is clearly defined.

Fig.2 depicts a poorly defined yield point, as would be the case for brittle materials. According to standard procedure, one must draw a straight line parallel to the elastic region



of the stress-strain curve at a predetermined strain ordinate value (let's say 0.1%), in order to determine the yield strength in such materials. The yield point at off-set, also known as the yield strength at 0.1% or 0.2% of set strain, is where this line meets the stress vs. strain curve. For hard steels and non-ferrous metals, a specific amount of permanent elongation is designated as the stress. This tension is known as the proof tension. It is important to keep in mind that the proof tension is applied for 15 seconds, after which the specimen shouldn't lengthen permanently by more than 0.1%. Fig. 2 illustrates the process for determining the proof stress from the stress-strain curve.

Curves of stress against strain can also be used to explain the characteristics of ductile materials. We discover that a metal is more elastic the more inclined the line of stress vs. strain proportionality is to the ordinates. Greater hardness of the metal is indicated by a higher yield point. Maximum stress point measurements that are higher indicate stronger metals. Similar to this, the distance from the ordinates of the breaking stress or load point indicates the toughness and brittleness of metal. When the distance is smaller, the metal becomes more fragile. We discover that before fracture, fragile materials exhibit little to no persistent deformation. Brittle behavior is displayed by several metals and magnesium oxide. The slight elongation before fracture demonstrates that the material does not show signs of impending fracture and that brittle fracture often happens quickly. There are reports that this frequently occurs with loud sounds.



**Fig. 2 shows stress vs strain curve for brittle materials. (newagepublishers.com)**

### **Engineering and True stress-strain Diagram**

The above-mentioned types of stress and strain are commonly referred to as conventional, nominal, or engineering stress and strain. They are merely a measurement of the load deformation on a standard specimen, in actuality. It is preferable to apply the ideas of true stress and true strain when studying the plastic flow of materials. Any engineering material that has been put through a tensile test will notice that as the test goes on, one area of the specimen deforms significantly more quickly than the rest. The dilemma of which area should be taken into account for calculating stress, the initial area or the actual area of the specimen at any instant of the load, is thus raised by the reduction in area. The engineering or nominal stress is the result of computing the stress based on the original area. True stress is what results from calculating the stress based on the instantaneous area at any instant of load. The strain is known as the engineering strain if the original length is used to compute it. Brittleness is the quality of a metal that causes it to shatter easily and with little noticeable deformation. The ductility of a metal is directly opposed by this characteristic. Cast iron, glass, and concrete are a few examples of fragile materials. This metal feature is crucial for the design of machinery that is subject to abrupt loads. Brittle metals are those that have less than 5% elongation.

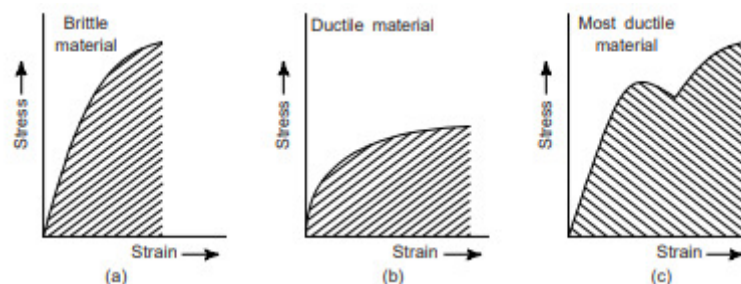
The ability of a metal to absorb the greatest amount of energy possible before fracturing is known as toughness. It measures a material's maximum energy strength and is given as work units/unit volume, or  $\text{kg fm/m}^3$ . Area under the stress-strain curve is another way to measure toughness. The whole area under the stress-strain curve, it should be noted, represents the work required to deform one  $\text{m}^3$  of material until it cracks. This project is also known as toughness modulus. Toughness is measured by a metal's tenacity and hardness. Toughness is roughly calculated as the sum of strength and elongation; this calculation is used to compare materials and is known as the merit number.

The ability of a material to be twisted, bent, or stretched under a high stress before rupturing is known as toughness. As temperatures rise, toughness value decreases. When designing structural and mechanical components that must tolerate stress and vibration, toughness is a highly desired quality. When the load goes past the elastic limit or yield point, as in the case of power press punches and pneumatic hammers, for example, it is crucial to choose the right material. Few materials are as durable as brass, mild steel, manganese, and wrought iron. A ductile material is more difficult to break even though it has the same strength as a non-ductile material because it requires more force.

(xi) Stiffness: A metal's ability to resist deformation is characterised by this quality.

The indicator of stiffness is the modulus of rigidity. Flexibility is the complete opposite of stiffness. High degrees of stiffness are found in materials that deform less when loaded. We may observe that a material becomes stiffer the more stress is needed to create a particular strain. When choosing a metal for a part or component of a machine or construction, stiffness of the metal is crucial. Let's use two beams as an example, one made of steel and the other of aluminium, to clarify. The specified weight may be carried by any of the two beams, but the aluminium beam will sag or deflect more than the mild steel beam. The steel beam is obviously more rigid than the aluminium beam. Graduating spring balances and spring-controlled measurement devices both use stiffness. The relationship between stiffness and flexibility depends on the material's dimensions, shape, and properties.

(xii) Resilience: A metal's capacity to retain energy and withstand impacts or shocks is referred to as this attribute. When a material is stressed to the point of elastic failure, it is quantified by the amount of energy absorbed per unit volume. When choosing a material for different types of springs, this characteristic is crucial. Fig. 3 shows stress-strain curves.



**Fig. 3 shows stress-strain curves.(newagepublishers.com)**

The maximum amount of energy that a body can store up to its elastic limit is referred to as proof resilience. The word "modulus of resilience" refers to the proof resilience per unit volume. Evidently, the modulus of resilience is the amount of energy stored per unit volume at the elastic limit. Since annealed copper has a very low elastic limit, springs are rarely made a much higher elastic limit (and robustness) and is used for springs. This demonstrates that resilience and high elastic limit are related. We should be aware that materials needed to withstand vibrations and shocks must be resilient.

(xiii) **Endurance:** This is the characteristic of a metal that allows it to tolerate different stresses (of the same or opposing nature). The utmost amount of stress that can be applied without leading to a failure is referred to as the endurance limit. The endurance limit for typical steel is approximately half the tensile strength. This metal feature is crucial for the design and manufacture of parts for reciprocating machines and other vibrating components. It is always preferable to keep a material's working stress well within its elastic limit.

### **An elastic behavior**

Elastic deformation is defined as recoverable deformation that develops over time. Even after applying a load, the material continues to bend elastically because of a relaxation process within it. When the load is removed, portion of the elastic deformation is only partially restored over time due to the relaxation process being reversed.

### **Relaxation Processes**

In reaction to an imposed stress from the outside, a material goes through a number of relaxation processes. We discovered that the stress-strain relationship is essentially time independent when the time scale of a relaxation process is excessively rapid or excessively slow in comparison to the time span over which the stress is imposed. The stress-strain connection is time sensitive and leads to anelastic behavior, though, if the time scale of the process is comparable to the time interval of stress application. The temporal spectrum of relaxation processes in materials ranges from  $10^{-13}$  s for atomic vibrations to more than  $10^6$  s for the viscous flow of grain boundaries. A given process's relaxation time is greatly influenced by temperature and reduces exponentially as temperature rises.

### **Viscoelastic behavior**

This is present in materials that exhibit time-dependent recoverable and permanent deformations in response to an applied stress. Organic polymers that are not crystalline display this characteristic. Viscous flow is a word used to describe time-dependent persistent deformation. It is similar to the creep phenomenon in crystalline materials, we may observe.

### **Fundamental Mechanical Properties**

The following are the fundamental mechanical properties of materials: (i) Tensile Strength (ii) Hardness (iii) Impact Strength (iv) Fatigue and (v) Creep

#### **Hardness**

The ability of a material (metal) to withstand abrasion, indentation (or penetration), and scratching by harder bodies is what gives it this feature. It is a material's resistance to the surface's long-term deformation.

In other terms, one may define it as the metal's resistance to indenter piercing. Interatomic forces acting on a material's surface are, of course, the primary cause of that surface's hardness. The combination of compressive, elastic, and plastic qualities in relation to the mode of penetration, shape of the penetrator, etc. results in hardness, which is not a fundamental feature of a material. It is possible to utilise hardness as a practical non-destructive test to get a rough notion of the value of that property and the condition of the metal close to the surface because it appears to have a reasonably constant relationship to the tensile strength of a specific material.

There are various ways to test for hardness, depending on whether the metal surface is directly penetrated by some type of penetrator, the surface is ploughed as a stylus is drawn across it under a controlled load, or the elastic rebound of an impacting hammer with known energy is measured. Hardness measurements are the simplest to take and are frequently

utilised in research and industrial design. All hardness testing are conducted on or very near the surface. It's important to understand that mechanical testing require a lot of stuff. Brinell hardness number is determined by applying a standard load while pushing a hardened steel ball (indenter) into a test specimen.

Brinell, Rockwell, and Vickers hardness tests are used to evaluate the hardness of metallic materials, the level of product quality, the homogeneity of metal sample sets, and the consistency of heat treatment results.

## CONCLUSION

For materials to respond to external forces and operate as expected in various applications, it is essential to understand their mechanical properties. To quantify and assess these qualities, mechanical tests are useful instruments. Mechanical tests give useful information about the strength, stiffness, ductility, hardness, and other mechanical properties of materials by exposing them to controlled forces and deformations. Tensile testing, compression testing, bending testing, and hardness testing are a few of the frequently used mechanical tests. A material's response to stretching pressures is determined through tensile testing, which measures qualities like yield strength, ultimate tensile strength, and elongation. A material's response to compressive stresses is assessed through compression testing, which sheds light on both its deformation properties and compressive strength.

A material's flexural characteristics and resistance to bending loads are evaluated by bending testing. A material's resistance to indentation or scratching can be determined using a hardness test, which also reveals details about the material's wear resistance and capacity to withstand localized stresses.

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## CHAPTER 10

### ALLOY SYSTEMS, PHASE DIAGRAMS AND PHASE TRANSFORMATIONS

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#### **ABSTRACT:**

Phase diagrams, phase transformations, and alloy systems are essential ideas in materials science and engineering. When two or more metallic or non-metallic elements are combined to create a solid solution, this is referred to as an alloy system. The link between temperature, composition, and the many phases that can exist in an alloy system is shown in phase diagrams. Phase transformations refer to the alteration of a material's microstructure and properties during the transition from one phase to another. We give an overview of alloy systems, phase diagrams, and phase transformations in this abstract, emphasizing their importance for comprehending and creating materials with desired qualities. Alloys are substances made of two or more elements, usually metals, that are mixed together to provide specific qualities. To grasp the behavior of alloys and regulate their properties requires a thorough grasp of alloy systems, phase diagrams, and phase transformations. The significance of alloy systems, phase diagrams, and phase transitions in materials science and engineering is highlighted in this abstract. Binary alloys (two elements), ternary alloys (three elements), and multicomponent alloys are only a few examples of the many different combinations that make up alloy systems. Based on the composition and interactions of its constituent elements, each alloy system displays distinct features. Engineers and scientists can adjust an alloy's qualities, such as strength, corrosion resistance, electrical conductivity, and thermal stability, to match particular application needs by choosing particular components and their proportions.

#### **KEYWORDS:**

Alloy, Atoms, Metals, Phase, Solid, Solution.

#### **INTRODUCTION**

Since it is possible for the design engineer to realize an unlimited range of physical qualities in the product by modifying the metallic composition of the alloy, metals in practical commercial use are nearly exclusively alloys and not pure metals. An alloy is created when a homogenous mixture of two or more metals or a metal and a non-metal is fused together at a specific temperature and solidifies to form a new metal. The highly purified single crystal of a metal is very soft and malleable with high electrical conductivity, whereas alloys are typically harder than their constituent parts, less ductile, and/or may have a significantly lower conductivity. Because of this, only a few applications call for the usage of pure metals. The alloy often has greater resistance to corrosion and is less susceptible to atmospheric effects. The degree of order in an alloy affects its conductivity, and the specific heat treatment affects its hardness.

The fundamental understanding of alloy structural properties is still largely based on empirical knowledge, and it is likely impossible to derive formulas that will predict which metals to combine in what proportions and with what heat treatment to produce a given property or set of properties. But there is a set of guidelines that describes the qualitative behavior of a certain class of alloys. The relative sizes of the constituent atoms for alloy formation and the types of phases to anticipate in terms of the valence of the constituent atoms are both addressed by these principles. The laws were established strictly empirically,

and the majority of the theoretical knowledge about alloys at this time is comprised of elementary theories that explain how the laws result from fundamental laws of physics. An alloy may exist in one or more of the following types in the solid state: As a solid solution, an intermediate phase, an intermediate chemical compound, a finely divided mechanical mixture of the metals, a solid solution, an intermediate phase, an intermediate chemical compound, a finely divided mechanical mixture of the metals, etc. As a mechanical mixture of metal chemical compounds, individual metals, and solid solutions that has been finely split. Alloys can be divided into multicomponent alloys, ternary alloys, or binary alloys, each of which has three components. Multicomponent alloys are the norm in industry. Giving the percentage (either by weight or by atoms) of each element in an alloy helps to describe its composition [1], [2].

- (i) By virtue of their chemical makeup, metal alloys are frequently divided into two classes: (i) ferrous and non-ferrous. Steels and cast irons are examples of ferrous alloys, which contain iron as their main component. All alloys with a non-iron base are referred to as non-ferrous alloys.
- (ii) Because their physical and chemical characteristics may be easily changed to meet the precise requirements of each individual, alloys are frequently utilized in industry. This can be accomplished by creating alloys out of several metals.
- (iii) Usually alloys rather than pure metals are used to make metallic items. One or more of the following qualities are enhanced by the alloying elements: Tensile strength, hardness, toughness, corrosion and oxidation resistance, machinability, elasticity, hardenability, creep strength, fatigue resistance, etc. are only a few of the qualities that materials can have.
- (iv) With the aid of alloy phase diagrams, any succession of alloys' characteristics can be quickly investigated. When an alloy has attained thermodynamic equilibrium, a phase diagram is a graphical representation of the types and quantities of the phases that can be anticipated in that alloy as a function of its composition, temperature, and pressure.
- (v) The phases can have different ordered and disordered crystal formations and can be liquid, vapour, or solid. How quickly equilibrium can be attained is not information that a phase diagram can give. When a phase diagram is created experimentally, it's important to confirm that the alloy is in a stable equilibrium condition in addition to learning which phases are present. When the system's Gibbs free energy reaches its minimum level, equilibrium has been achieved. The phase diagram's potential shapes are constrained by the thermodynamic principle of minimal Gibbs free energy, and even a complex diagram with numerous phases is made up of just a few geometrical elements.

The phrases listed below are frequently used while discussing phase diagrams and solid phases.

- (i) System: Metals and non-metals may be present independently or in any combination in a system, which may be made up of solids, liquids, gases, or any combination of these. It is described as a comprehensive complex of phases involving one or more components at various pressures and compositions. A system is sufficiently separated from its environment to be unaffected by solids, liquids, gases, or their mixtures. It is only subject to changes in the overall composition, temperature, pressure, or total volume to the extent that the investigator permits.
- (ii) Components: These are the elements or chemical compounds whose existence is both necessary and sufficient to create a system. One-component systems are used to describe pure metals, binary or two-component systems are used to describe alloys of two metals, etc.

(iii) Phase: It is a homogenous area of a system with constant physical and chemical properties. When a system is homogenous, the amount of various chemicals it contains determines how many phases it has.

(iv) Phase diagram: A visual representation of the interactions between composition, regions of phase stability, and environmental restrictions (such as temperature and occasionally pressure), typically under equilibrium conditions[3], [4].

The majority of phase diagrams are created under conditions of gradual cooling where the phases are in equilibrium.

The phase diagrams can provide the critical information listed below.

- (a) Phases at various compositions and temperatures
- (b) The solubility of an element or compound in an equilibrium with another element.
- (c) The melting points of the various alloy phases.
- (d) The range of temperatures at which an alloy solidifies.
- (v) Phase equilibrium: The situation in which a system's phase properties remain constant for an endless amount of time. The free energy is at its lowest level at equilibrium. Liquid is one phase in an equilibrium diagram, and solid solution is another.
- (vi) Phase Transformation: A modification of the quantity and/or nature of the phases that make up an alloy's microstructure.

## DISCUSSION

### Alloy Systems

The following variables affect how an alloy system's characteristics can be improved:

- (i) The way that the two or more metals are combined.
- (ii) Amounts of various alloying metals or elements.
- (iii) Cooling temperature for these, etc.

In the liquid state, two or more metals may dissolve in one another, although they may or may not do so in the solid form. Even if they are soluble in a liquid state, substances could still preserve their identity. For instance, cadmium and bismuth are soluble in a liquid state but insoluble in a solid form. Additionally, it is possible that the two or more metals may be soluble in one another in both the liquid and solid states. For instance, copper and nickel are soluble in one another in both the liquid and solid states. No one can tell copper from nickel, of course.

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The atoms of the constituent are dispersed at random throughout the liquid when an alloy is in a liquid state. Many possibilities become apparent when solidification occurs. Solutions of the following various categories could form:



(a) **Simple Eutectic Type** In this instance, the two alloy system components (binary) are soluble in the liquid state but separate out in the solid state while each keeping its own identity. The two elements are said to be insoluble in one another in the solid form. The remedy is referred to as eutectic kind.

(b) **Type of Solid Solution** The two constituents of a binary alloy are said to be soluble in each other when they remain totally mixed in both the liquid and solid states, and a distinct kind of solution may result from this. It's referred to as a solid solution.

(c) **Combination Type** - A binary alloy's two constituents may only partially dissolve one another as it solidifies. This kind of solution blends the qualities of the two halves.

(d) **Inter-metallic compounds** - When the elements' affinities are high, it has been observed that during solidification, they may join to produce inter-metallic compounds. These kinds of compounds could be present between the chemical compound and the solid solution. A well-known illustration is the copper-zinc system. When the copper-to-zinc solubility is exceeded, a zinc-rich phase coexists with the Cu-rich phase. Inter-metallic compounds can be employed as bearing metals because they are often hard and brittle. These materials consist of wear-resistant, low-friction pads embedded in a matrix of a hard solid solution [7], [8].

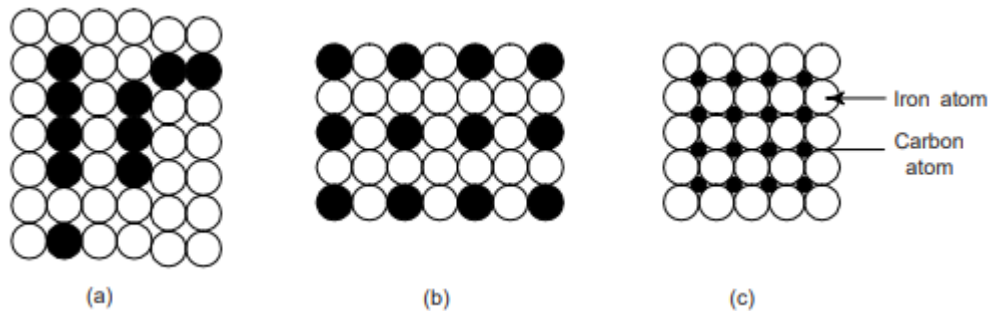
### **Solid Solutions**

When the host material's crystal structure is maintained when the solute atoms are added and no new structures are created, a solid solution is created. In other terms, the final phase is referred to as a solid solution when elements entirely dissolve in each other in a liquid or solid state. When the atom sizes and electron structures of the solvent and solute are comparable, a solid solution can easily develop. This homogeneous composition or chemical state prevents the component atoms of the elements from being physically or mechanically discriminated. The components are distributed uniformly throughout the solid state to create a single phase or solid solution. Basically solid solutions are of two types:

**Solid Substitution Solution:** Substitutional solid solution is one in which the solute or impurity atoms replace or act as a substitute for the host atoms when the two metals in the solid solution form a single face-centered cubic lattice. Solid solutions can also be thought of as crystalline phases with a range of compositions. By either substituting for some of the solvent A's atoms in the crystal lattice or by occupying the interatomic gaps, or interstices, between the atoms, a solute B's atoms can be organised in the crystal lattice of a solvent A. We can see that the two metals' atoms are nearly the same size, with less than 15% of a variation between their atomic radii. Otherwise, significant lattice deformation and the formation of a new phase will be caused by the solute atoms. The crystal structures of the metals in both atoms must match for there to be noticeable solid solubility.

An intermetallic complex rather than a substitutional solid solution is more likely to form if one element has more electro-positivity and the other higher electronegativity. Additionally, it has been found that, all other things being equal—atomic size, crystal structure, and electronegativity—a metal will tend to dissolve another metal with a greater valency rather than one with a lower valency. The formation of monel from copper and nickel is a well-known illustration of substitutional solid solution. At all ratios, these two elements are entirely soluble in one another. Another illustration is brass, an alloy of copper and zinc that readily forms solid solutions because the atoms of these two elements have similar sizes and electrical structures. Unlimited solubility in the solid state may also be seen in alloys of copper with gold and germanium with silicon. Within a single alteration of the space lattice, polymorphous metals may have infinite solubility. For instance, Fe may combine with Cr to generate a continuous series of solid solutions (BCC lattices), and Fe can combine with Ni to form a continuous series of solid solutions (FCC lattices). Increases in electric resistance and

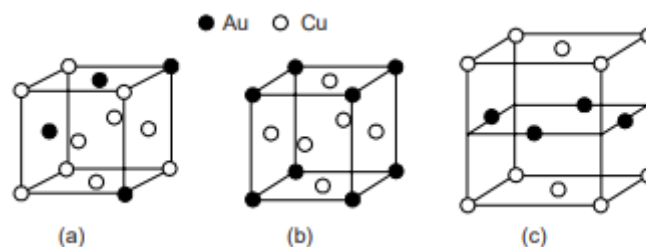
drops in the temperature coefficient of electric resistance are invariably linked to the production of solid solutions. Except for copper-based solid solutions, solid solutions are often less plastic, harder, and stronger than pure metals. Two forms of substitution solid solutions exist. (i) Random substitutional solid solutions (ii) Ordered substitutional solid solutions.



**Fig.1 shows (a) solid solution (b) substitution solid solutions (c) Interstitial solid solution.(newagepublishers.com)**

The probability of one metal element occupying any specific atomic site in the crystal when there is no order in the replacement of the two metal elements is equal to the atomic percent of the element in the alloy (Fig. 1(a)). It goes without saying that in such a circumstance, the solute atom concentration can vary significantly across the lattice structure. A random or disordered substitutional solid solution is the name given to this kind of solid solution that is produced. In contrast to the fact that atoms of two different elements are distributed across the sites of the space lattice not statistically but in a fully specified order, many substitution solid solutions can exist in an ordered form at very low temperatures. These stable solutions are referred to as ordered, however "superstructure" is also a valid term. Such ordering is typical at low temperatures since it tends to be destroyed by increased thermal agitation. [Fig. 1(b)].

The transition from an unorganized to an organized state occurs at a specific temperature or within a specific temperature range. The Kurnakov point (K) is the temperature at which a solid solution entirely decomposes. Ordering typically occurs when a solid solution is gradually cooled from the temperature zone above K. Systems with substantial or unrestricted solubility in the solid state can have ordered solid solutions; in these cases, full ordering can happen with concentrations of the solid solution elements corresponding to simple atomic ratios of the components of the type, let's say AB or AB<sub>3</sub>. In systems with concentration ratios near to those suggested, partial ordering may be seen. Fig. 2 depicts the atomic configuration of two Cu and Au alloys, AuCu<sub>3</sub> and AuCu, in ordered solid solutions[9], [10].



**Fig.2 shows crystals lattice of Cu alloys (a) disordered solid solution (b) ordered solid solution( Au Cu<sub>3</sub> alloy) (c) ordered solid solution (Au Cu alloy)(newagepublishers.com)**

Changes in an alloy's characteristics are related to the appearance and disappearance of an order in the atoms' arrangement in solid solutions. An alloy's ductility is reduced by ordering, while its electrical conductivity, temperature coefficient of electric resistance, hardness, and

strength are all increased. It alters the magnetic characteristics of ferromagnetic alloys; for example, the magnetic permeability of perm alloys (magnetic iron-nickel alloys) can decrease upon ordering to a tiny portion of its initial value. Particularly at high temperatures, substitution solid solutions typically exhibit a random arrangement of the constituent atoms on the atomic sites. This is true because, according to  $G = H - TS$ , configurational entropy contributes more to lowering the free energy as temperature rises. If ordering significantly reduces the enthalpy of the crystal, this random arrangement of the constituent atoms in a solid solution may transform into an ordered structure upon cooling to lower temperatures.

**Interstitial solid solution:** These may develop, for example, during the melting of transition metals and non-metals (H, N, C, or B) with small atomic radii.

The size of a solute atom must be equal to or slightly smaller than the size of an interstitial void in order for there to be a chance of creating an interstitial solution. Interstitial solid solutions are inherently insoluble and form best in solvents with an HCP or FCC lattice and interstices that are 0.41 R in radius, where R is the radius of an atom in the solvent. Since the size of the interstices in BCC lattices does not exceed 0.29 R, the solubility is minimal. Fe<sub>γ</sub>, which has an FCC lattice, may dissolve up to 2.14% (by mass) of carbon, while Fe (alpha) (BCC lattice) does not effectively dissolve carbon, with the greatest solubility being around 0.02 (by mass). These interstitial solid solutions have economic applications. Other factors include hydrogen introduced during welding operations, nitrogen for keeping stainless steel in an austenitic state for nitriding, and nitrogen for maintaining austenitic conditions in stainless steel. Acid cleaning and plating also results in hydrogen embrittlement, which sharply reduces ductility. Because interstitial solid solution production results in higher lattice distortions than substitution solid solution formation, the characteristics of alloys can be substantially altered.

Interstitial solid solutions typically have very limited solubility and are typically regarded as of secondary importance. As the concentration of a solute in a solid solution increase, this increases noticeably the electric resistance, coercive force, hardness, and strength but decreases the ductility and toughness. More than two elements in an alloy can result in either a substitution or an interstitial solution. For instance, when iron is melted with manganese and carbon, the carbon and iron produce an interstitial solid solution rather than a substitution solid solution.

### **Families of Engineering Alloys**

Engineering alloys often fall into one of the three categories listed below: (i) The light alloys, which are based on aluminum, magnesium, and titanium. Alloys of aluminum: Cast items consume about 20% of the aluminum produced worldwide. Alloys made of aluminum have a low melting point but experience significant shrinkage during solidification. To attain dimensional accuracy, it is necessary to account for shrinkage of between 3.5 and 8.5% while designing the mold. In this category are cast aluminum alloys, wrought aluminum alloys, aluminum-silicon alloys, aluminum-copper alloys, aluminum-magnesium alloys, and aluminum-zinc-magnesium alloys. Under the category of non-heat-treatable alloys, there are two significant families of aluminum alloys: the aluminum-manganese alloys (3 XXX series) and the aluminum-magnesium alloys (5 XXX series). Under the category of "heat-treatable alloys," there are three significant families of aluminum: the aluminum-copper alloys (2 XXX series), the aluminum-magnesium-silicon alloys (6 XXX series), and the aluminum-zinc-magnesium alloys (7 XXX series).

### **Application of Phase Transformations**

In castings, amorphous structures (solidification phenomenon in glassy structures), heat treatment, or in the binary phase diagram of the Fe-Fe<sub>3</sub>C system and TTT diagrams for

eutectoid steels, phase transformations are typically observed in microstructural changes. Recrystallization and grain development during mechanical working are some examples of phase changes that can be seen. Phase transformations are obviously quite important in terms of technology.

- (a) Dendrite formation and Structure of Ingots- The pace and direction of heat removal, the temperature of the molten metal, and the concentration of impurities are the key factors that affect the shape and size of crystallised grains as they increase during solidification.
- (b) Dendritic (tree-like) growth takes place in freely growing crystals. It is known that crystals form most quickly along the planes and directions where atoms are packed closely together.
- (c) Long branches, known as the first-order dendritic axes, so emerge first. They then give rise to second-order axes, which in turn give rise to third-order axes, and so forth. The metal that is still present between dendritic axes finally solidifies.
- (d) Dendrites continue to develop until they start to clash. After that, the dendrites transform into continuous crystals with irregularly shaped exterior surfaces as the interaxial voids are filled in. These crystals are referred to as crystallites or grains. Some crystals may maintain their dendritic shape if there is enough liquid metal to fill in the interaxial spaces (for example, at the opening end of a mould where a shrinkage cavity arises). Impurities concentrate at grain boundaries during solidification between dendritic axes, and this is also where voids are most likely to form due to shrinkage and impeded access of liquid metal to the solidification front.
- (e) The concentrations and characteristics of impurities in pure metals or of alloying elements in an alloy; the temperature of casting; the rate of cooling during solidification; and the shape, temperature, thermal conductivity, and condition of the internal surface of the casting mould are just a few of the many variables that affect ingot structure.
- (f) By rapidly cooling ingots and castings, gravity segregation is minimised. Since the gravitational forces in space are so tiny, this flaw can be completely removed with space technology.

## Casting

From a practical standpoint, this process is crucial. In this procedure, a liquid or viscous substance is poured into a hollow and allowed to set or solidify into a predetermined shape. The process can lead to complicated thermal gradients and temperature variations. The microstructure of the cast metal or casting may be impacted by these. Casting is sometimes referred to as establishing. The foundry is a location where all casting equipment, primarily for casting metals, is gathered. The cavity in a mould into which molten material is poured is known as a mould. Moulding is the practise of creating the mould.

Alloys of the Al-Si system (silumins) exhibit the best casting qualities, such as high fluidity, little shrinkage, little (if any) liability to hot cracking, and excellent gas tightness, which can be attributed to a high eutectic component in their structural makeup. The process of creating a mould from sand, plaster, or metal for casting molten metal is known as patterning. The mould is at the centre of foundry work. The casting's ultimate dimensions, form, and hole placement are determined by the mould, which also serves as support for the casting while it is being poured and solidified. There are provisions for both opening the mould and removing the design. The mould is typically much cooler than the melt flowing for the majority of casting procedures.

We might observe that the mould frequently exists at room temperature. Wood is the most typical material used to create patterns. Plaster and plastic are the other materials that are

frequently used. Additionally recommended in evaporative casing procedures are wax and foamed polystyrene. The simplest pattern of them all has a flat side or bottom, making it the flat pattern. For a pattern to be removed from a mould without being damaged, certain properties are required, such as a fillet, a draught, and a round shape. In order to make the moulding process easier, split patterns are created in two parts. Each piece of the pattern can be removed from the sand mould because it is so divided.

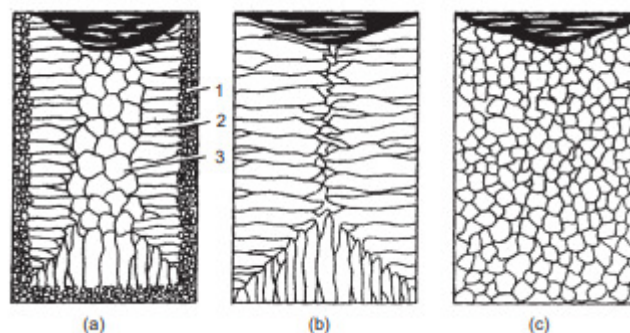
Together, flat and split patterns are referred to as loose patterns. A mounted pattern is a pattern that is permanently attached to a plane and passes through the middle of it.

(c) Amorphous (or glassy) structures during the glass transition Glass transition occurs in amorphous and semi-crystalline polymers and is caused by a slowing down of long molecular chain segments with cooling. The progressive change from a liquid to a rubbery substance and then to a stiff solid is represented by the glass transition when a material cools. The glass transition temperature ( $T_g$ ) is the temperature at which a polymer changes from a rubbery to a rigid state. However, when hard glass heated to a temperature below  $T_g$ , this sequence of events takes place in the opposite order.

Additionally, this glass transition is accompanied by sudden changes in other physical characteristics, such as stiffness, heat capacity, and coefficient of thermal expansion.

By electrolysis, cathode sputtering with a high rate of deposition, and rapid cooling from the gaseous (vapour or ionised) state, metallic materials with an amorphous structure can also be created. In Fe-C Systems, phase transformation is (d) The study of steels and cast irons centres on a group of alloys made of iron and carbon that comprise a variety of steels and cast iron. Both carbon and iron can take on several forms. Cast iron contains carbon in the range of 2.3% to 4.2% while steel is an alloy with up to 1.2% carbon. Carbon content in alloys above 4.6% is undesirable due to their poor characteristics. Due to the numerous uses of ferrous metallurgy in fabrication, casting, and production processes, Fe-C alloys are crucial to modern industry. Theoretically, it is based on the phase transformations that occur in metals, such as when liquid iron is cooled to become solid during the manufacturing process of iron; heat treatment processes where different mechanical properties can be obtained by altering the crystal structure.

We should remark that the Fe-C system, which is based on polymorphic transformations and eutectoid decomposition, provides the most significant knowledge on heat treatment. Fe-C alloys can contain a variety of phases, but the liquid solution, ferrite, austenite, cementite, and free carbon (as graphite). Fig. 3 Macrostructure of ingots.



**Fig.3 Macrostructure of ingots(newagepublishers.com)**

## CONCLUSION

The behavior and properties of materials can be understood and controlled using tools like alloy systems, phase diagrams, and phase transformations. Materials with specialized

qualities, such as higher strength, improved corrosion resistance, or improved electrical conductivity, can be produced by combining several elements in alloy systems. Engineers can meet unique performance requirements for diverse applications by carefully choosing and modifying the composition of alloys. The relationships between temperature, composition, and phases in an alloy system are graphically depicted in phase diagrams. They offer useful knowledge regarding the stability of certain phases, the circumstances under which phases change, and the composition ranges in which specific phases exist. Foreseeing and managing the microstructure and characteristics of materials throughout processing, heat treatment, and cooling requires the use of phase diagrams.

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## CHAPTER 11

### AN OVERVIEW OF THE HEAT TREATMENT

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#### ABSTRACT

In order to change a material's microstructure and properties, heat treatment—a crucial step in materials science and engineering—involves carefully heating and cooling the material. It includes a variety of processes, such as solution heat treatment, quenching, tempering, and annealing, among others. The goals of heat treatment procedures, as well as their significance in enhancing the mechanical, thermal, and electrical properties of materials, are described in this abstract. The controlled heating and cooling of materials to change their microstructure and properties is known as heat treatment, and it is a crucial step in materials science and engineering. The ideas, methods, and importance of heat treatment are highlighted in this abstract along with how it affects the mechanical, physical, and chemical properties of materials. A variety of procedures are included in heat treatment, such as annealing, quenching, tempering, and aging, among others. By modifying the material's microstructure, such as grain size, phase composition, and defect density, each method is intended to accomplish particular goals. A material is heated to a specified temperature, held there for a predetermined amount of time, and then slowly cooled as part of the heat treatment process known as annealing. It is used to lessen the material's hardness, increase ductility, and relieve internal tensions. Additionally, annealing can enhance grain development and homogenize the microstructure.

#### KEYWORDS

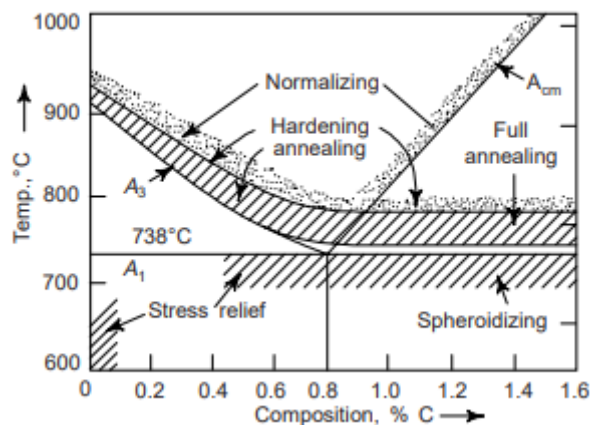
Temperature, Annealing, Heat, Steel, Treatment, Cooling, Hardness.

#### INTRODUCTION

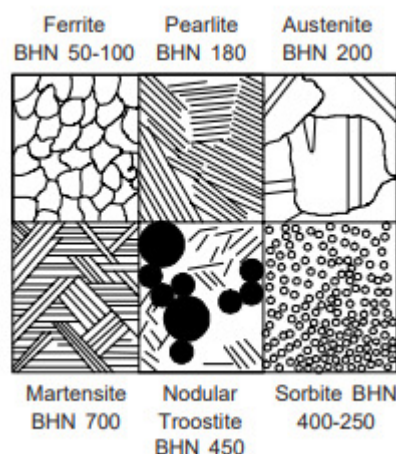
Heat treatment is the term used to describe the heating and cooling processes necessary to change the properties of materials such as metals, alloys, polymers, and ceramics. Modifications to the material's microstructure cause changes in its properties. Ingots, castings, semi-finished goods, welded joints, and numerous components of machines and instruments can all undergo heat treatment. Changes in the metal's micro-constituents occur when a metal item is heated to a specific temperature and then cooled at a reasonable rate during heat treatment. The type, form, size, and distribution of the metal's micro components may alter, as well as how they are distributed throughout the metal piece. Of course, the primary determining variables of changes in micro-constituents are the temperature of heating and the rate of cooling. The changes in the physical and mechanical characteristics of heat-treated metal specimens are therefore governed by these changes in the micro-constituents. Heat treatment is a crucial step in many fabrication and manufacturing processes [1], [2]. Heat treatment is used to accomplish any one or more of the following goals:

- (i) To reduce strain hardening and increase ductility in a cold-worked metal.
- (ii) To reduce internal stresses generated during casting, welding, and hot-working processes.
- (iii) To eliminate gases from castings, to soften a metal to make it easier to work with, to boost wear, heat, and corrosion resistance.

- (iv) To improve the grain structure after hot working a metal, to increase a steel tool's cutting capacity (i.e., hardness), and to eliminate the impacts of previously completed heat-treatment operations.
- (v) To enhance the magnetic characteristics, particularly of steels, in order to produce permanent magnets.
- (vi) To polish the grain structure of a metal following heat working.
- (vii) To toughen and soften a piece of high carbon steel.
- (viii) To create a single-phase stainless-steel alloy and to create a strong, wear-resistant shell for a robust steel part core.
- (ix) To make a single-phase alloy in stainless steel and to harden non-ferrous metals and alloys, especially aluminum alloys.
- (x) To toughen a hardened steel component at the expense of its hardness and to create a strong, wear-resistant case on a hard, tough core of a steel part.



**Fig.1 shows heat treatment range for carbon steels.**



**Fig. 2 shows microstructures of steel depicts the typical steel microstructure that results from heat treatment. It also depicts the iron-iron carbide phase diagram at the eutectoid (newagepublishers.com).**

According to the theory of heat treatment, when an alloy is cooled to room temperature after being heated above a specific temperature, it goes through a structural modification or stabilization. A key factor in this process is the cooling rate. The cooling rate is the primary



factor in the structural alteration. Hypo-eutectoid carbon steels typically receive the thermal treatments. The iron-carbon diagram's eutectoid reaction for steel involves austenite's transformation and disintegration into pearlite, cementite, or martensite. The temperature ranges and heat treatment procedures are depicted in Fig.1[3]. Fig. 2 shows microstructures of steel depicts the typical steel microstructure that results from heat treatment. It also depicts the iron-iron carbide phase diagram at the eutectoid.

### Heat treatment process

The principal kinds of heat treatment are: (i) Annealing (ii) Normalising (iii) Hardening (iv) Tempering (v) Case hardening (vi) Surface hardening and (vii) Ageing. Each of them has a number of varieties.

### Annealing

A metal or alloy can undergo this type of heat treatment to give it a structure that is similar to the equilibrium one. The prolonged exposure to a substance at a high temperature is followed by a delayed cooling process.

In most cases, annealing is done to (i) reduce relative stresses (ii) boost ductility, softness, and toughness; and/or (iii) create a particular microstructure.

The rate of cooling from the annealing temperature is often not high (between 30-200°C/h); the temperature of heating in annealing depends on the composition of an alloy and the specific sort of procedure. There are several possible annealing heat treatments. These are distinguished by the induced modifications, which are frequently microstructural and are in charge of changing the mechanical properties. Three steps make up the annealing process: heating to the appropriate temperature, staying at that temperature, or "soaking," and cooling, usually to room temperature. Time is a crucial factor in these annealing processes. During heating and cooling, there are temperature differences between the piece's exterior and interior. The size and geometry of the component affect the magnitudes of temperature gradients. Temperature gradients and internal tensions may be created if the rate of temperature change is too high, which could cause warping or even cracking. The actual annealing period also needs to be sufficient to accommodate any essential transformation reactions. Another crucial factor is the annealing temperature. Because diffusional processes are typically involved, annealing can be sped up by raising the temperature. There are several different annealing processes, including full annealing, process annealing, spheroidize annealing, and diffusion annealing[4], [5].

## DISCUSSION

### Annealing operations

**Full annealing:** Through a process called full recrystallization, this operation eliminates all structural flaws. Low- and medium-carbon steels that will be machined or that will undergo significant plastic deformation during a forming operation frequently use this operation. The following steps are involved in this process: (i) heating the hypo-eutectoid steel to a temperature that is between 50 and 70 °C above the upper critical temperature (for hypo-eutectoid steels) and a temperature that is a similar amount above the lower critical temperature (for hypereutectoid steels) until equilibrium is reached. This guarantees that the metal has been heated sufficiently and that phase change has occurred over the entire volume (ii) After that, the alloy is furnace cooled, meaning the heat-treating furnace is shut off and the steel cools to room temperature over a period of several hours. In addition to any pearlite phase, the microstructural byproduct of full annealing is coarse pearlite, which is soft and ductile.

**Process Annealing:** This heat treatment softens and improves the ductility of a previously strain-hardened metal in order to mitigate the consequences of cold work. Process annealing is frequently used in fabrication operations that call for significant plastic deformation in order to continue the deformation without fracture or excessive energy use. It is the recrystallization of cold work, which permits the recovery and recrystallization processes. Since a fine-grained microstructure is typically preferred, the heat treatment is stopped before significant grain growth has taken place. To put it another way, the precise temperature relies on the degree of cold working, grain size, composition, and duration spent at heat. By annealing at a relatively low temperature (but above the recrystallization point) or in an environment without oxygen, surface oxidation or scaling may be prevented or minimized. Process annealing is highly beneficial for low carbon and mild steel [6], [7].

**Process annealing**, also known as sub-critical annealing, is used to soften and relieve internal tensions in cold-worked low carbon steel sheet, wire, and tube. Here is how it works:

- (i) The steel is heated to a temperature between 550 and 650 °C, which is only slightly beyond the lower critical temperature on the iron-carbon curve for steel.
- (ii) Stresses are reduced throughout the metal, and new grains start to form and expand as a result of recrystallization.

A slow cooling stage follows the heating phase. The cementite in pearlite "balls up" or spheroidizes after prolonged annealing. Growth of ferrite grains also happens. Evidently, precise temperature and time control during annealing is crucial for effective process annealing. Fig. 3 shows full annealing.

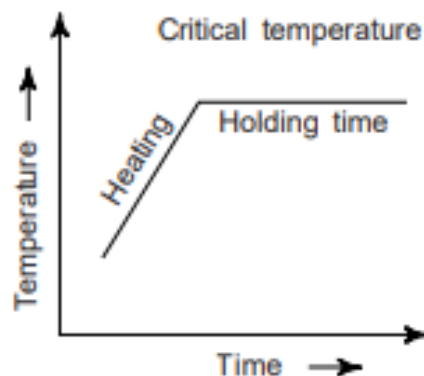


Fig. 3 shows full annealing.(newagepublishers.com)

### Patenting

Typically, it is used on medium- to high-carbon steels in between draughts or before wire drawing. This mainly makes wire drawing more ductile. Here is how it works:

- (a) Heating the steel to a temperature over the transformation range.
- (b) Subsequently cooling the steel to a temperature below that range in air, a bath of molten lead, or salt that has been kept at a temperature adequate to the steel's carbon content and the qualities needed for the completed product.

### Stress-Relief Annealing

Internal residual stresses can appear in metal pieces as a result of the following factors: (i) plastic deformation techniques like grinding and machining; (ii) uneven cooling of a piece that was processed or made at a high temperature, like a weld or a casting; and (iii) a phase transformation that is induced during cooling where the parent and product phases have

different densities. If residual stresses are not eliminated, distortion and warpage may happen. The component is heated to the necessary temperature, maintained there long enough to reach a uniform temperature, and then cooled to room temperature in air to get rid of them. Note that castings, forgings, weldments, and other work pieces may have residual stresses since the annealing temperature is often quite low, preserving the effects of cold working and other heat treatments.

The work components in this procedure are heated to a temperature that approximates their recrystallization temperature before being progressively cooled. Similar to process annealing, any metal can undergo this stress-relief procedure [8], [9]. Two-stage annealing Steel castings can benefit from it quite a little. It gets rid of the tensions. The sulphide layers, which weaken steel, consolidate in the ferrite, and rapid diffusion results in homogeneity. In the end, steel is produced using refined grains and in a soft state. In this procedure, steel is heated for a while to a temperature that is much over the A3 point, or above the critical range. Then the temperature is quickly cooled to a level below the lower critical temperature. Reheating is now carried out promptly for a short length of time to a point slightly above the upper critical temperature. Lastly, gradual cooling permitted to room temperature.

### **Normalizing**

This is applied to carbon steels as a finishing process to give them greater strength than annealing. No significant ductility loss has occurred either. Similar to full annealing, this method involves heating and soaking, but just part of it is allowed to cool in air, resulting in a substantially faster cooling rate. Normalizing, a type of annealing heat treatment, is used to refine the grains (i.e., reduce the average grain size) and create a more consistent and preferable size distribution. Pearlite steels with finer grains are more durable than those with coarser grains. The yield and ultimate strengths, hardness, and impact strength are all increased by the fine grain structure. Heating at a range of 55 to 85 °C above the highest critical temperature which, of course, depends on composition is how normalizing is performed.

Normalizing is a stress-relieving procedure frequently used on castings and forgings. It increases the strength of medium carbon steel to some extent. When used on low carbon steel, it enhances machinability.

Alloy steels with extremely stable austenite can be normalized to generate hard martensitic structures. This process is known as austenizing. High cooling rates caused by cooling in the air can degrade austenitic structures in these steels, producing martensite. This significantly increases the toughness.

These are the benefits of this approach:

- (i) Normalizing results in stronger material than fully annealed material.
- (ii) The grains are refined by normalizing
- (iii) Normalization results in homogenized structure.
- (iv) Rather than hardening and tempering steel castings, normalizing is utilized to enhance their qualities.
- (v) Hardness and strength are improved.
- (vi) When machining, a better surface polish is produced.
- (vii) Hot-rolled steel has greater resistance to brittle fracture.
- (viii) The spread of cracks is monitored.

## Spheroidising

The high carbon content (0.7-2%) of tool steels used to create cutting tools, measuring devices, and cold forming dies results in great hardness but also makes them difficult to machine. By annealing, tool steels' hardness can be decreased. Additionally, spheroidizing annealing of hypereutectoid steels prepares the structure of those steels for hardening. Instead of producing plates like pearlite, this sort of heat treatment results in spherical or globular (spheroidal) carbide. This structure provides improved formability, high ductility, and good machinability.

When a steel's structure is made of granular pearlite with inclusions of rounded-off (spherical) cementite grains, the steel's hardness is at its lowest. This leads to the name "spheroidizing" annealing. The alloy is heated to a temperature just below the eutectoid phase diagram, or at about 700°C) in the + Fe<sub>3</sub>C region of the phase diagram in order to spheroidize it. Spheroidizing timeframes typically range between 15 and 25 hours if the precursor microstructure contains pearlite. The Fe<sub>3</sub>C coalesces to form spheroid particles during this thermal annealing [10], [11].

## Hardening

It is a type of heat treatment that creates an alloy with a non-equilibrium structure. Only when the alloy being treated goes through specific transformations in solid solutions, such as the disintegration of a high-temperature solid solution by eutectoid reaction, etc., can non-equilibrium structures be generated by heat treatment. The creation of a non-equilibrium structure in an alloy requires heating it above the temperature at which the solid state phase transition occurs, followed by rapid cooling (chilling). Rapid cooling is necessary to avoid the equilibrium transformation during cooling.

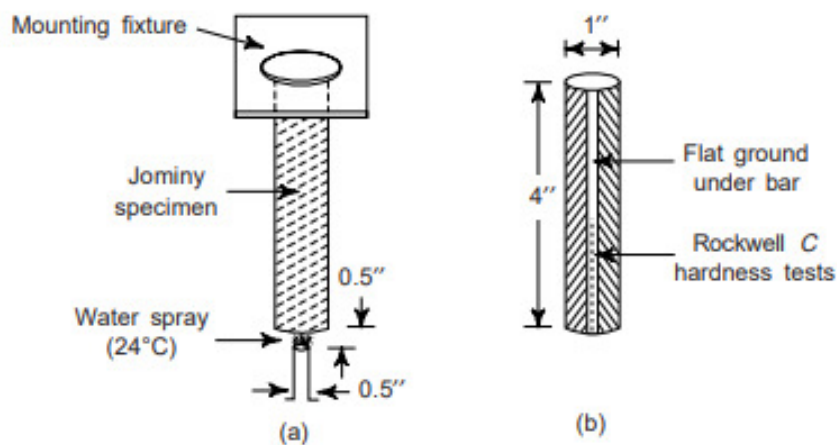
Alloys used for construction and tool-making are hardened to increase their strength. Under equilibrium conditions, alloys undergoing a eutectoid transformation can be significantly strengthened through hardening. Their strength increases either as a result of the eutectoid reaction's temperature being lowered or as a result of the eutectoid mixture undergoing a martensitic phase transition. The strengthening effect is minimal immediately following hardening if the hardening procedure left the metal in a fixed state of high-temperature solid solution at room temperature (20–25°C). Instead, it will be most noticeable after several low-temperature heating cycles or after holding at 20–25°C. Hardening enables the modification of structurally-sensitive physical and chemical properties in alloys with particular properties, such as an increase in electrical resistance, coercive force, or corrosion resistance. Important steel properties include hardenability and hardening capacity. A hardened object's surface hardness is known as its hardening capacity and is mostly determined by the steel's carbon content.

We should be aware that the parameter hardenability is connected to the effect of alloy composition on a steel alloy's capacity to transform to martensite for a specific quenching treatment. Additionally, there is a distinct correlation between the mechanical characteristics and the cooling rate for each particular steel alloy. The capacity of an alloy to be hardened by the development of martensite as a result of a certain heat treatment is referred to as "hardenability." It is important to note that hardenability is not the same as "hardness," which is the resistance to indentation; rather, it is a qualitative indicator of how quickly hardness decreases as one moves further into a specimen due to a decrease in martensite composition. Two tests can be used to determine a steel's ability to be hardened: the cylinder series test and the Jominy end-quench test. The first approach provides a single hardenability value. When quenched in a specific way, the value is expressed as a percentage of martensite at the centre. An index that quantifies the quenching state is the severity of the quench.

## The Jominy End-Quench Test

The easiest and most used laboratory test for hardenability is this one. With the exception of alloy composition, all variables that could affect how deeply a piece hardens (such as specimen size, shape, and quenching treatment) are kept constant in this test. Austenitization is carried out on a standard specimen that is 25.4 mm in diameter and 100 mm long at a certain temperature for a specified period of time. It is quickly placed in a fixture after withdrawal from the furnace (Fig. 4a). A normal water jet is then used to quench the specimen's lower end, causing a variable rate of cooling.

About  $300^{\circ}\text{C/s}$  of cooling occurs at the jet end while only  $3^{\circ}\text{C/s}$  occurs at the other end. Rockwell hardness measurements are made for the first 50 mm along each flat after the piece has cooled to room temperature (Fig. 4b); for the first 12.8 mm, hardness observations are noted at 1.6 mm intervals, and for the remaining 38.4 mm, at 3.2 mm intervals. A large variety of hardness is produced along the length of the Jominy specimen as a result of the changing cooling rate. When hardness is plotted as a function of position from the quenched end, a hardenability curve is produced.



**Fig.4 shows Jominy-end quench (a) mounted during quenching (b) hardness is measured along the length of the specimen.(newagepublishers.com)**

## CONCLUSION

The primary method for changing the microstructure and characteristics of materials is heat treatment. Engineers and metallurgists can customize the mechanical, thermal, and electrical properties of materials using heat treatment procedures by meticulously managing the heating and cooling conditions. The key to heat treatment's effectiveness is its capacity to bring about structural alterations at the atomic and microscopic levels, which enhance a material's strength, hardness, ductility, toughness, and other desirable properties. A typical heat treatment procedure called annealing is used to reduce internal tensions, clean up the grain structure, and improve the ductility and toughness of materials. In order to create a microstructure with a harder microstructure and increase strength and hardness, quenching entails rapidly cooling from a high temperature. After quenching, tempering is done to keep the desired hardness while lowering brittleness and increasing toughness. Alloys are given a solution heat treatment to dissolve and distribute the alloying elements more uniformly, increasing their strength and corrosion resistance.

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