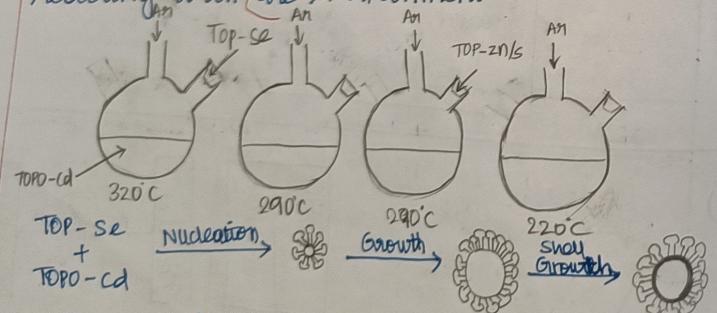


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CAT-2 PTA for CHD X04

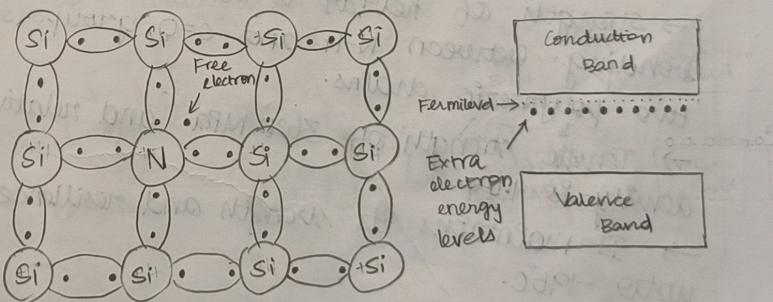
- 1) Describe the synthesis of CdSe (core) quantum dots. Find its applications in electronic gadgets.

A cadmium compound is heated to 320°C and dissolved in an organic solvent. At room temperature selenium compound dissolved in a different organic solvent is injected into the reaction vessel, causing supersaturation of the resultant core solution. As the temperature drops to around 290°C, nucleation of new crystals starts and existing crystals grow. After a period of growth, the length of which determines the size of the QDs, the solution is cooled to 220°C, stopping growth. A small amount of zinc sulphide is injected into the reaction vessel to coat the QDs and prevent them from reacting with the environment.

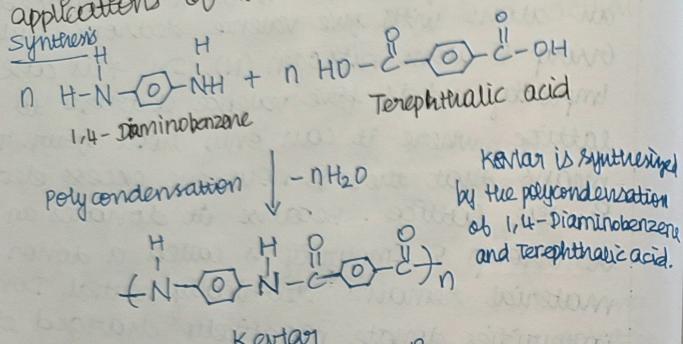


It is used in photodetectors, solar cells, LED's, lasers, radiation detection, Field Emitters, catalysts, biological imaging, etc.

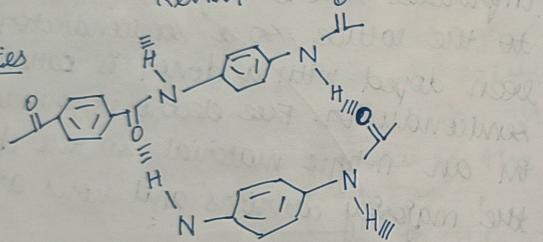
- 2) Write a note on nitrogen doped silicon when one of the silicon atom is replaced by an atom with five valence electrons, such as the group 5 atom nitrogen (N). In this case, the impurity adds five valence electrons to the lattice where it can only hold four. This means that there is now one excess electron in the lattice. Because it donates an electron, a group 5 impurity is called a donor. The material remains electrically neutral. Donor impurities donate negatively charged electrons to the lattice, so a semiconductor that has been doped with a donor is called an n-type semiconductor. Free electrons outnumber holes in an n-type material, so the electrons are the majority carriers and holes are the minority carriers.



3) Describe the synthesis, properties and applications of kevlar.



## Properties



→ Strength of Kevlar is due to hydrogen bonding between N-H and C=O groups of two polymeric chains.

→ Tensile strength of 3620 MPa and relative density is 1.44

→ It maintains its strength and resilience upto -19°C.

## Applications

→ Because of its cryogenic character and high strength, it is used as personal protective armors, etc.

(like combat helmets, bulletproof vests, ballistic

face masks, etc.)

→ Kevlar is also used as protective sheet for optical fibres.

→ Motorola RAZR, OnePlus, Poco backplate is made up of Kevlar instead of polycarbonate.

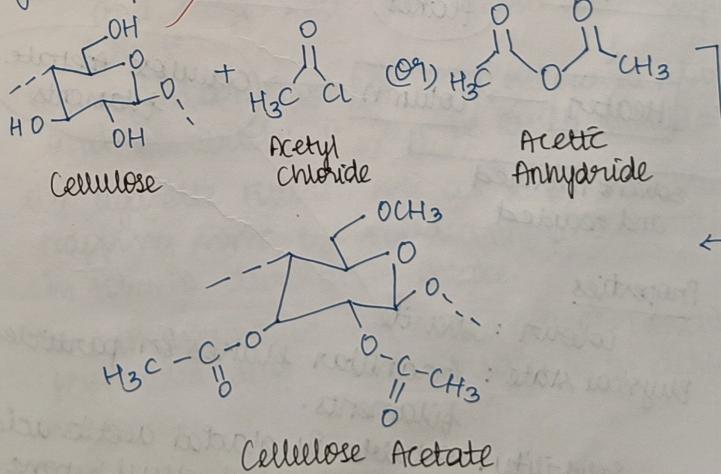
→ also used in aircraft.

4) Describe the synthesis, properties and applications of cellulose acetate.

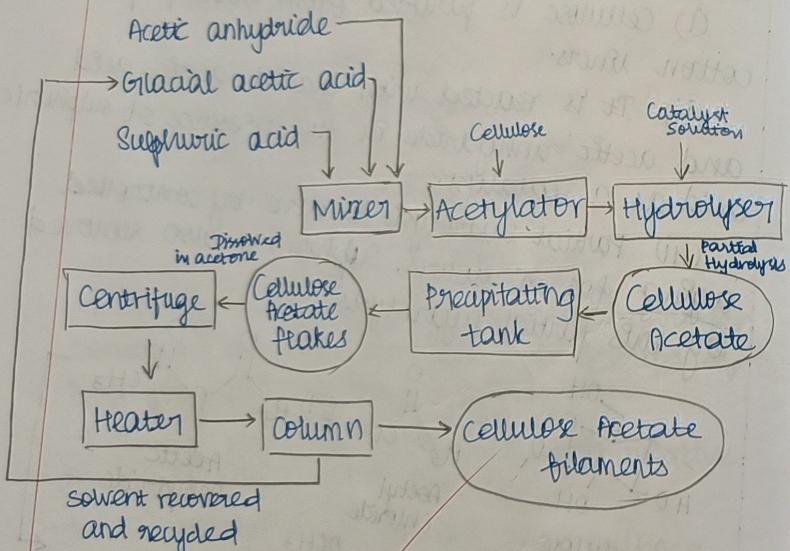
(i) Cellulose is purified from wood pulp or cotton fibers.

(ii) It is reacted with glacial acetic acid and acetic anhydride in the presence of sulphuric acid as a catalyst.

(iii) Partial hydrolysis is done by controlled aging for 20 hours. Sulphates are also removed by this partial hydrolysis.



- (iv) cellulose acetate is then precipitated as acid-resin flakes.
- (v) flakes are first dissolved in acetone so that solution is filtered or centrifuged.
- (vi) This spinning solution is extruded in column of warm air. solvent is recovered.
- (vii) Filaments are stretched and wound onto beams, cones or bobbins ready for use.



### Properties

Colour: white

Physical state: Granular flakes or particles or filaments.

Solubility: Soluble in glacial acetic acid, acetone, methyl ethyl ketone etc. Insoluble in water and ethanol.

- cellulose acetate → It wets easily, with good liquid fiber properties: transport and excellent absorption.
- It can usually be wet cleaned or dry cleaned and generally does not shrink. It can be dyed.
  - It is resistant to mold and mildew.
  - It is made from a renewable resource, so it is environmentally friendly.
  - It is very comfortable because it breathes, wicks, dries quickly and there is no static cling.

### Applications

- (i) Films and coatings: Due to its excellent transparency, high gloss and good adhesion properties.
- (ii) Textiles and fibres: Luxurious appearance and drape well. Also known as "acetate fibres".
- (iii) Eyewear: Due to its light weight, durability and flexibility, it can be easily moulded.
- (iv) cigarette Filters: Acts as a porous material, trapping some of the harmful substances in tobacco during its intake.
- (v) Adhesives: Due to its excellent bonding properties and compatibility with different materials.

- 5) Describe the composition, properties and applications of duralumin.  
It is one of the best light-weight alloys which has widespread utility in aircrafts and automobile sectors.

#### composition

95% Al, 4% Cu, 0.5% Mn, 0.5% Mg

#### Properties

- Strength comparable to steel but density only one third.
- Good conductor of heat and electricity
- Tough, ductile, easily castable and possesses high machinability.
- High Tensile Strength (about 2000 kg/cm<sup>2</sup>) if suitably heat treated.

#### Applications

- Duralumin finds extensive application in aircrafts, automobiles, and locomotion industry in the form of clad.
- Surgical instruments
- Cables
- Fluorescent tube caps, etc.

- 6) What is steel? Describe the composition, properties and applications of low-carbon, medium-carbon and high-carbon steel.

Steel is an alloy, which is a combination of iron and carbon, along with small amounts of other elements. It is one of the most widely used materials in construction, manufacturing and various industries due to its strength, versatility and relatively low cost. The main component of steel is iron, which is extracted from iron ore through a process called smelting. Carbon is added to iron in varying amounts, typically between 0.2% and 2.1%, depending on the desired properties of the steel. The carbon content affects the hardness, strength and other mechanical properties of the steel.

#### Low-carbon steel:

composition: 0.15 - 0.3 % of carbon.

#### Properties:

Strength: 40 kg/mm<sup>2</sup>  
Weldability by forging: Possible

Ability to withstand shock & impact: Good

Possibility of hardening and tempering: Yes but with difficulty

Structure: Fibrous

Toughness: Quite tough.

### Applications:

- \* Used for reinforcement in reinforced cement concrete.
- \* Used for roof covering.
- \* Used for the manufacture of bolts, nuts, rivets, screws, etc.
- \* Used in manufacture of rail tracks.
- \* Industry, building structure, etc.

### Medium-carbon steel:

Composition: 0.3 - 0.8 % of carbon

#### Properties:

Strength :	50 kg/mm <sup>2</sup>
Weldability by forging :	Difficult
Ability to withstand shock and impact :	Better
Possibility of hardening & tempering :	Yes to some extent
Structure :	-
Toughness :	Tougher than mild steel

### Applications:

- \* Hydraulic fittings (like cylinders, rams, shafts, etc.)
- \* Agricultural tools and implements.
- \* Heavily stressed parts in general engineering casting for automobile engine components.
- \* Rifle barrels, gun parts, wheel gears, clutch plate, etc.

### High-carbon steel:

Composition: 0.8 - 1.5 % of carbon

#### Properties:

Strength : 65 kg/mm<sup>2</sup>

Weldability by forging : Difficult

Ability to withstand shock & impact : Better

Possibility of hardening and tempering : Yes easily

Structure : Granulate

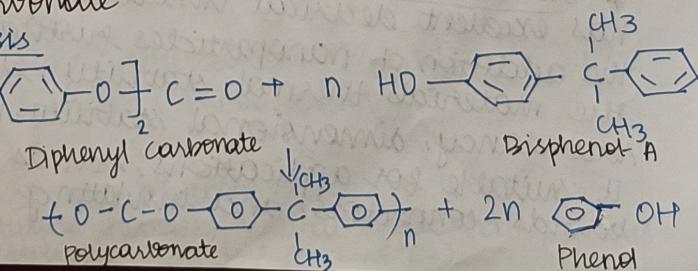
Toughness : -

### Applications:

- \* Metal cutting tools (lather planers and slotters)
- \* Smith's cutlery knives, wear resistant forging, boring & engraving tools, wood working tools like saw drills, tiles, hammer, etc.

7) Describe the applications of nano incorporated polycarbonate

#### Synthesis



### Properties

Has high impact and tensile strength over a wide range of temperature.

### Uses:

- Used in making moulded domestic wares, electrical insulators and electronic gadgets.
- Also used to make composite materials as a replacement of metallic structures.

### Applications of nano-reinforced polycarbonate:

\* Lightweight and impact-resistant eyewear: Provides both durability and lightweight properties. Adding nanoparticles enhances the material's strength and impact resistance, making it suitable.

\* Protective coatings: The nanoparticles dispersed within the polycarbonate matrix can enhance the material's scratch resistance, UV resistance and chemical resistance. This makes it useful for applications such as automotive, electronic device and corrosion-resistant coatings.

\* Electronics and electrical components: It has excellent electrical insulation properties. The addition of nanoparticles further improves the material's thermal stability, flame retardancy, dimensional stability, making it suitable for applications such as circuit boards, connectors, and insulating components.

\* Transparent armor: For military and security applications. The addition of nanoparticles enhances the material's strength and impact resistance, providing protection against ballistic threats while maintaining transparency. It is commonly used in bulletproof windows, shields and protective visors.

\* Drug delivery systems: By incorporating nanoparticles into the polycarbonate matrix, it becomes possible to control the release of drugs, improve their stability, and enhance their targeted delivery. This enables the development of more efficient and precise drug delivery systems for medical applications.

Q) What is meant by lacquer? Describe its various constituents and their functions with example.

It is a colloidal dispersion of cellulose derivative, resin and plasticizer in solvent and drier. On contact with air, solvent evaporates leaving behind a transparent, protective layer. It is mainly used to protect wooden furniture.

### Constituents:

i) cellulose derivatives: provide

- a) water proofness
- b) hardness
- c) durability

Eg: (Cellulose nitrate, cellulose acetate, ethyl cellulose, aceto-butyrate, etc.)

(ii) Resins: Their function is to increase the solid contents so as to enhance

- a) thickness of the film
- b) retention of original gloss
- c) adhesion

d) water resistance.

Eg: phenol-aldehyde, alkyd, copal, dammar, etc.

(iii) Plasticizers: They are added to reduce brittleness.

Eg: castor oil (raw or blown), blown soyabean oil, triethyl phosphate, etc.

(iv) Solvents are used to dissolve film forming constituents (e.g. cellulose derivatives and resins).

Eg: Ethyl acetate, ethyl lactate, etc.

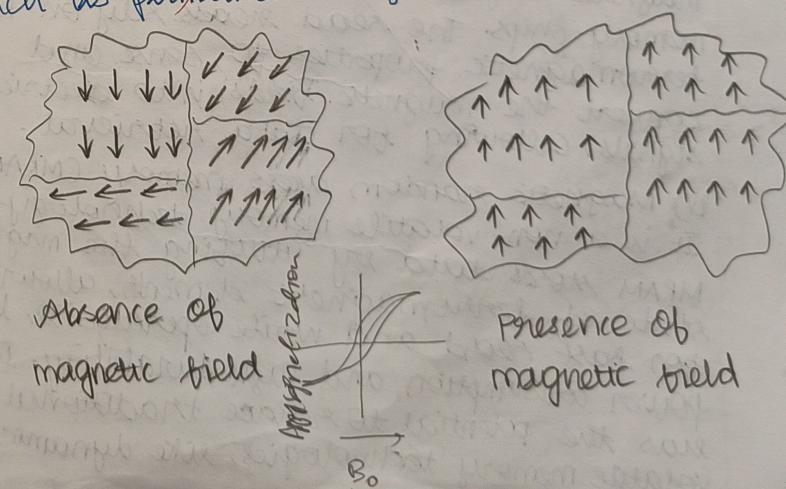
(v) Diluents are used to reduce the viscosity of lacquer.

Eg: Toluene, benzol, etc.

Q) What is meant by ferromagnetism? Describe its applications in data storage.

Ferromagnetism is a phenomenon exhibited by certain materials that possess strong permanent magnetic properties. These materials are called ferromagnetic materials, and they include substances such as iron, nickel and cobalt, as well as their alloys. The key characteristic of ferromagnetic materials is the presence of magnetic

domains. Magnetic domains are regions within the material where the magnetic moments of atoms or atomic clusters are aligned in the same direction. When these domains are randomly oriented, the material does not exhibit a net magnetic field. However, when an external magnetic field is applied to the material, the domains align themselves in the field, resulting in a strong magnetic response. One important aspect of ferromagnetism is hysteresis. It refers to the property of a ferromagnetic material to retain its magnetization even after the external magnetic field is removed. This means that once a ferromagnetic material is magnetized, it will remain magnetized until acted upon by another magnetic field in the opposite direction. The property is utilized in applications such as permanent magnets.



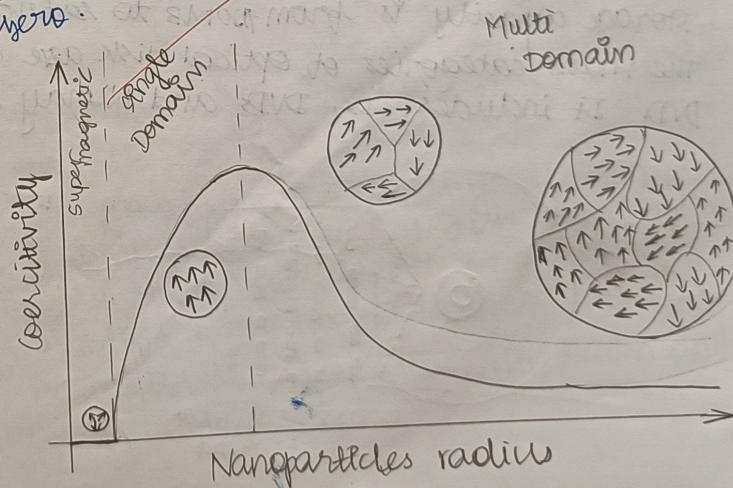
### Applications

- (i) Hard disk drives (HDDs): The magnetic properties of these materials allow data to be stored and retrieved using read/write heads. The ability to magnetize and demagnetize the material quickly and reliably enables the storage of vast amounts of digital information on spinning disks.
- (ii) Magnetic tapes: They are coated with ferromagnetic particles and can store large amounts of data in a sequential manner. This technology is commonly used for archival purposes, backup storage, and in industries that require long-term data retention.
- (iii) Magnetic read heads in solid-state drives (SSDs): Ferromagnetic materials are used in the read heads to detect and interpret the magnetic signals stored on the NAND flash memory chips. The read heads rely on the ferromagnetic properties to sense and convert the magnetic fields into electrical signals, allowing for data retrieval.
- (iv) Magnetic random access memory (MRAM): It is a non-volatile memory technology. MRAM stores data by utilizing the magnetic state of ferromagnetic elements, allowing for fast read and write operations, low power consumption, and high durability. It has the potential to replace traditional volatile memory technologies, like dynamic

random-access memory (DRAM) and flash memory.

(v) Magnetic sensors: These sensors utilize the changes in magnetic fields to detect and measure position, motion and other parameters. They find applications in diverse areas, including automotive systems, robotics, navigation devices and medical equipment.

- 10) What is meant by super-paramagnetism?
- Advances in nanotechnology have provided a way of obtaining superparamagnetic properties of nanomaterials by reducing the size of the ferro- or ferrimagnetic material to few nanometers (below the so-called superparamagnetic diameter). When they are below the diameter, the nanoparticles are able to return quickly to a non-magnetized state after an external magnet is removed. Larger ferro- and ferrimagnetic materials have remnant magnetism after the applied magnetic field returns to zero.

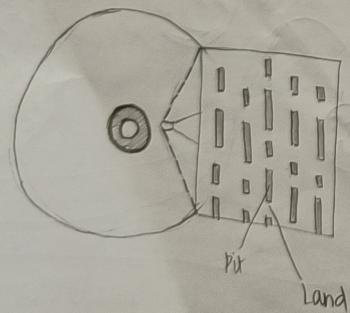


### Magnetic properties of nanoparticles

- Used for drug delivery, therapeutic treatment, contrast agents for MRI imaging, bioseparation and in-vitro diagnostics.
- They are not magnetic when located in a zero magnetic field, but they quickly become magnetized when an external magnetic field is applied.
- When returned to a zero magnetic field they quickly revert to a non-magnetized state.
- Used for biomagnetic separation.

ii) What is meant by optical disk? Give any two examples.

It is a form of removable storage. Optical drives use a laser to read and write data on optical disks. Laser beam writes on the surface by creating a small pit (hole) on the disc. They commonly store data in single track. Storage capacity is from 700MB to several GB. The main categories of optical disk are CD & DVD. It includes CDs, DVDs and Blu-ray discs.



### CD (Compact Disk)

It is mainly used to store photos, audio and computer software.

(i) CD-ROM (Compact Disc Read-Only Memory): The data stored on CD-ROM can be only read. It cannot be deleted or changed. It can store up to 700MB of data.

(ii) CD-R (CD-Recordable): The user can write data on CD-R only once but can read it many times. The data written on CD-R cannot be erased. CD-R drives are known as CD burners. The process of recording data on CD-R is called burning. CD-R is known as WORM (Write Once Read Many).

(iii) CD-RW (CD-Rewritable): It is also known as erasable optical disc. The most common type erasable and rewritable optical disc is magneto-optical disc.

### DVD (Digital Video Disk)

The storage of DVD is much greater than CD. It can store up to 17 GB of data.

(i) DVD-ROM (DVD-Read Only Memory): It is high capacity optical disk that the users can only read but not write or erase.

(ii) DVD-R (DVD-Recordable):

It is similar to CD-R disc, the written data cannot be erased.

(iii) DVD-RW (DVD - Rewritable):

The user can write data on CD-RW many times by erasing the existing contents.

Blu-ray disc:

It is a new and more expensive DVD format. It provides higher capacity and better quality than standard DVDs especially for high-definition videos. It can store upto to 100GB of data.

Q2) What is meant by flash memory storage? Give any two examples.

Flash memory is a solid-state chip that maintains stored data without any external power source. It is commonly used in portable electronics and removable storage devices, and to replace computer hard drive.

It is widely used in smartphones, digital camera, portable media player.

Types of flash memory:

→ Solid State Drives (SSDs): It can replace a computer's hard drive. They have no moving parts, so mechanical failure is never zero. SSDs are quieter and smaller than hard drives, and they provide faster response, access and boot up times but consume much less power and run cooler.

→ USB Flash Drive: A small, portable flash memory card that plugs into a computer USB port and functions as a portable hard

drive. They are touted as being into any computer with a USB drive. They have less storage capacity than an external hard, but they are smaller and more durable because they do not contain any internal moving parts.

→ Memory cards: It is an electronic flash memory data storage used for storing digital information. These are commonly used in portable electronic devices, such as digital cameras, mobile phones, laptops, tablets, MP3 players and video game consoles. It can be inserted into a slot on computer or mobile device. However a card reader can be attached to a computer if it does not have a slot.

Q3) Expand the following terms

SEM - Scanning Electron Microscope

TEM - Transmission Electron Microscope

AFM - Atomic Force Microscope

XRD - X-Ray Diffraction

FT-IR - Fourier Transform Infrared

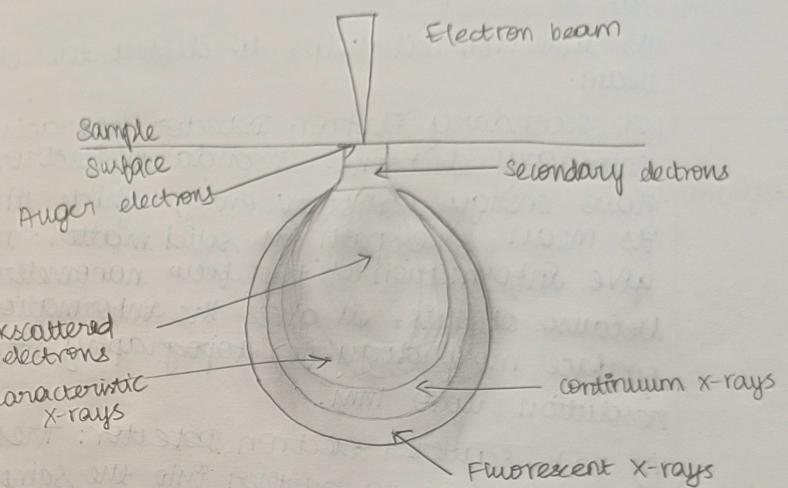
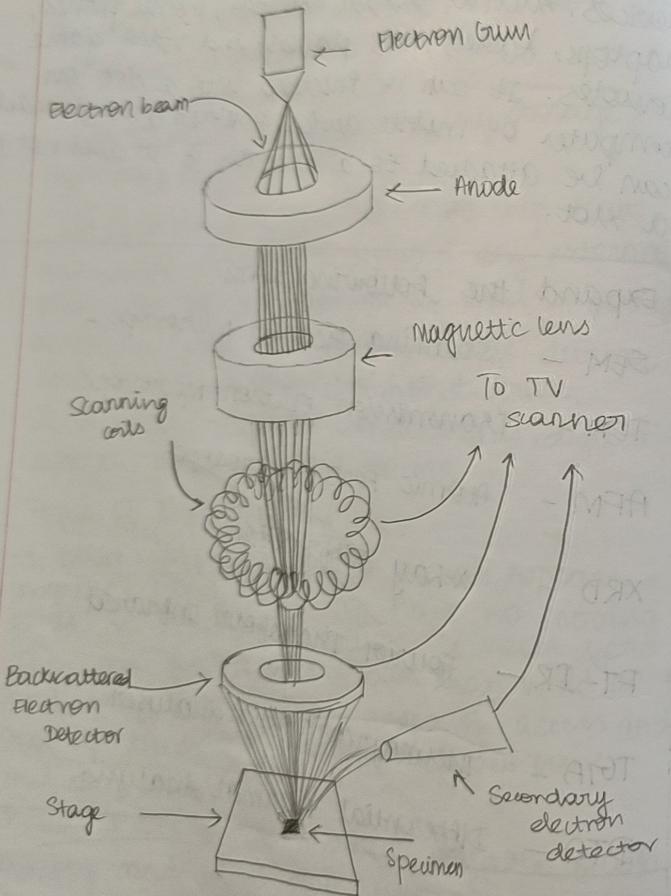
TGIA - Thermogravimetric analyser

DTA - Differential Thermal Analysis

c) 14)

With a neat diagram explain the principle, working and applications of scanning electron microscope. Mention its advantages and disadvantages.

SEM is used to inspect topography, composition and electrical conductivity of a specimen at a resolution of upto 30000x.



#### Principle:

- The basic principle is that a beam of electrons is generated by suitable source, typically a tungsten filament or a field emission gun.
- The electron beam is accelerated through a high voltage and pass through a system of apertures and electromagnetic lenses to produce a thin beam of electrons.
- When the beam scans the surface of the specimen, electrons are emitted from the specimen by the action of the scanning beam and collected by a suitably positioned detector.

#### Components involved:

- i) Electron Gun consists of
  - catode - to release  $e^-$
  - Anode - to accelerate  $e^-$
- ii) condenser Lens controls the amount of  $e^-$  travelling down the column.
- iii) objective lens focuses the beam onto a spot

on the sample.

(iv) Deflection coil helps to deflect the electron beam.

(v) Secondary Electron Detector attracts the secondary electrons. Secondary electrons have energy of 50eV only, which limits its mean free path in solid matter. It can give information at top few nanometers, because of this, it gives the information of surface morphology (e) topography with resolution upto 1nm.

(vi) Back-scattered electron detector: These electron beams go further into the sample to give the information about the distribution of different elements in sample.

(vii) characteristic X-rays are measured by energy dispersive X-ray spectroscopy. It is used to identify the elements present in the sample.

#### Advantages:

→ It gives detailed 3D and topographical imaging and the versatile information.

→ This works very fast.

→ Modern SEMs allow for the generation of data in digital form.

→ Most SEM samples require minimal preparation actions.

#### Disadvantages:

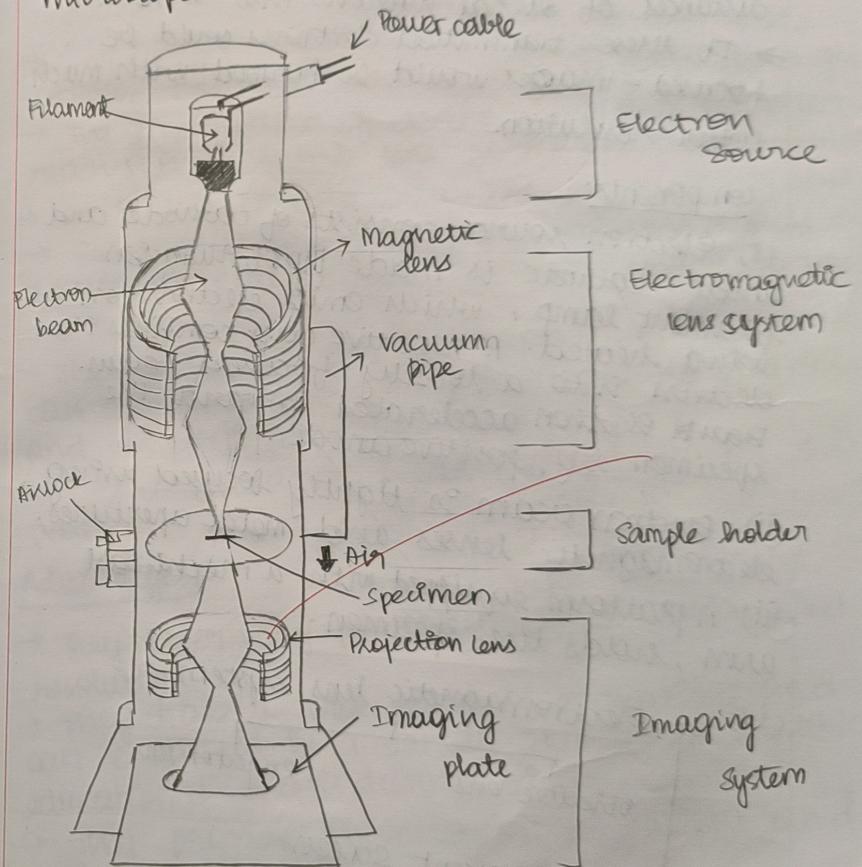
→ Expensive and large

→ Special training is required to operate.

→ Limited to solid samples

→ Small risk of radiation exposure associated with the electrons that scatter from beneath the sample surface.

15) With a neat diagram explain the principle, working and applications of transmission electron microscope. Mention its advantages and disadvantages

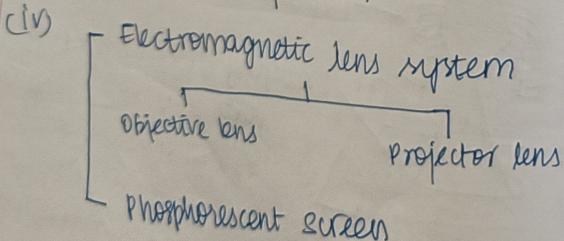


### Principle:

- Electrons possess a wave-like character.
- Electrons emitted into vacuum from a heated filament with increased accelerating potential will have small wavelength.
- Such higher-energy electrons can penetrate distances of several microns into a solid.
- If these transmitted electrons could be focused - images would be formed with much better resolution.

### Components:

- (i) Electron source consists of cathode and anode. Cathode is made up of tungsten filament lamp, which emits electrons on being heated. A negative cap confines the electron into a loosely focused beam. Beam is then accelerated towards the specimen by positive anode.
- (ii) Electron beam is tightly focused using electromagnetic lenses and metal apertures.
- (iii) A platform equipped with a mechanical arm, holds the specimen.



### Working:

- Specimen is bombarded by a beam of electrons, the primary electrons. The bombarding electrons are focused to a bundle onto the object.
- In areas on the object where these electrons encounter atoms with a heavy atomic nucleus, they rebound.
- In regions where the material consists of lighter atoms, the electrons are able to pass through.
- The fine pattern of electrons leaving the object, reaches the objective lens forms the image.
- It is then greatly enlarged by projector lens.
- Eventually, the traversing electrons reach the scintillator plate at the base of the column of the microscope.
- The scintillator contains phosphor compounds that can absorb the energy of the striking electrons and convert it to light flashes.
- Thus a contrasted image is formed on this plate.

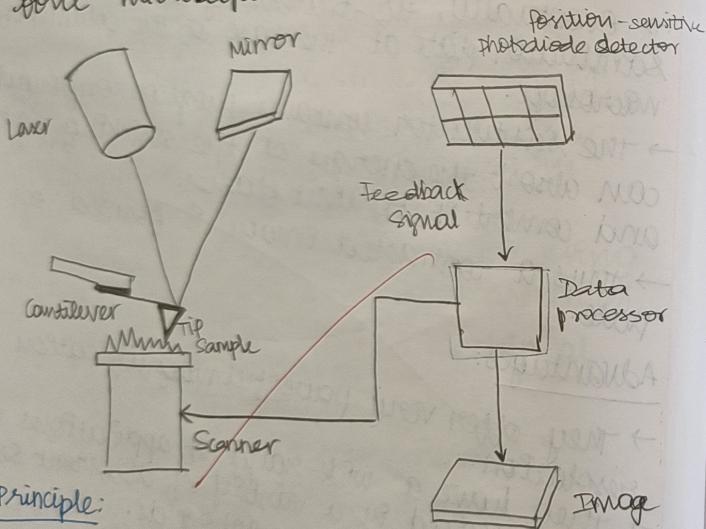
### Advantages:

- They offer very powerful magnification and resolution.
- They have a wide-range of applications and can be utilized in a variety of different scientific, educational and industrial fields.
- They provide information on element and compound structure.
- Images are high-quality and detailed.

### Disadvantages:

- they are large and very expensive.
- laborious sample preparation.
- operation and analysis requires special training.
- samples are limited to those that are electron transparent.
- Images are black and white.

1b) with a neat diagram explain the principle, working mode and applications of atomic force microscope.



### Principle:

- working principle of AFM nanolithography is based on the interaction between the probe and substrate.
- A tiny cantilever which has a sharp tip is scanned across a surface.

→ The interaction between the surface and the tip cause the cantilever to bend and the bending is monitored using a laser beam.

→ In this way, nanometer changes in height can be measured and used to generate a 3D image of the surface.

### Components & Working:

i) Probe and Cantilever: A sharp probe tip mounted on a flexible cantilever. The probe interacts with the sample's surface, and the cantilever measures the forces between the tip and the surface.

ii) Sample Preparation: It is prepared by fixing it to a sample stage. The surface of the surface should be relatively flat to ensure accurate scanning.

iii) Scanning Process: The probe is brought into close proximity of the sample's surface without making contact. As it scans across the surface, it moves up and down based on the forces between the tip and the sample.

iv) Force Detection: The deflection of the cantilever is detected using various methods, that measure the changes in the position of the cantilever as it interacts with the sample surface.

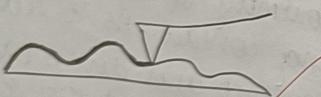
v) Feedback System: A feedback mechanism adjusts the position of the probe tip to

maintain a constant force between the tip and the sample, resulting in accurate topographical measurements.

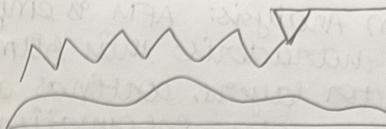
(i) Data collection and Image Formation: The deflection data collected from the cantilever is processed and used to create an image of the sample's surface that represents the topography and properties at an atomic scale. Done using the data acquisition and control system.

#### Working modes:

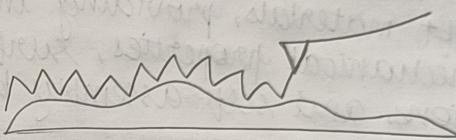
(i) Contact mode (static mode): AFM tip makes soft physical contact with the sample. The tip is attached to the end of a cantilever with a low spring constant. The constant force causes the cantilever to bend to accommodate changes in topography.



(ii) Non-contact mode (dynamic mode): The cantilever is vibrated near but not in contact to the sample surface at a frequency slightly above its resonance frequency (100 - 400 kHz) where its amplitude is typically a few nm.



(iii). Intermittent contact mode (Tapping mode): The cantilever is driven to oscillate up and down. The amplitude of this oscillation is greater than 10nm, typically 100 to 200 nm.



#### Applications:

(i) Nanoscale Imaging: AFM provides high-resolution imaging of surfaces at the atomic or nanoscale. It is used to study the topography, morphology, and surface properties of various materials.

(ii) Material Characterization: AFM is used to investigate the mechanical, electrical and chemical properties of materials-like surface roughness, adhesion forces, elasticity and friction at the nanoscale.

(iii) Biological Research: AFM plays a significant role in biological research by imaging biomolecules, cells, tissues. It helps in studying protein structures, cell membranes, DNA and interactions between biomolecules.

(iv) Thin film analysis: AFM is employed to analyse and characterise thin films, such as semiconductor layers, coatings and polymers. It provides information about film thickness, surface roughness, grain boundaries and defects.

(v) Polymer science and soft materials: AFM is valuable for studying polymers and soft materials, providing insights into their mechanical properties, surface interactions, and self-assembly behaviour.

- Q) Describe the principle and working of UV-visible spectrophotometer with a diagram. Mention its application for the analysis of solid and liquid samples.

Principle:

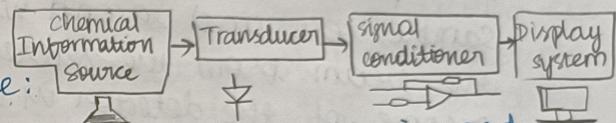
- Basically spectroscopy is related to the interaction of light with matter.
- As light is absorbed by matter, the result is an increase in the energy content of the atoms or molecules.
- When UV radiations are absorbed, this results in the excitation of the electrons from the ground state towards a higher energy state.
- Molecules containing  $\pi$ -electrons or non-bonding electrons ( $n$ -electrons) can absorb energy in the form of ultraviolet light to excite these electrons to higher anti-bonding molecular orbitals.

→ The more easily excited the electrons, the longer the wavelength of light they can absorb. There are four possible types of transitions ( $\pi-\pi^*$ ,  $\pi-\pi^*$ ,  $\sigma-\sigma^*$ , and  $n-\sigma^*$ ) and they can be ordered as follows:  $\sigma-\sigma^* > n-\sigma^* > \pi-\pi^* > \pi-\pi^*$

→ the absorption of UV light by a chemical compound will produce a distinct spectrum that aids in the identification of the compound.

Working:

- i) Light source:



Jungsten filament lamps are rich in red radiations; more specifically they emit the radiations at 375 nm, while the intensity of Hydrogen-Deuterium lamps falls below 375 nm.

- ii) Monochromator:

Composed of prisms and slits. Radiation emitted from the primary source is dispersed with the help of rotating prisms. Various wavelengths of the light source which are separated by the prism results in a series of continuously increasing wavelengths to pass through the slit for recording purposes. The beam selected by the slit is monochromatic and further divided into two beams with the help of another prism.

- iii) Sample and reference cells:

One of the two divided beams is passed through the sample solution and the second beam is passed through the reference solution. Both

sample and reference solution is contained in the cells. These cells are made of either silica or quartz. Glass cannot be used for the cells as it also absorbs light in the UV region.

(iv) Detector:

Two photocells, one which receives the sample cell and second which receives the beam from the reference, serve the purpose of the detector in UV spectroscopy. Intensity of the radiation from the reference cell is stronger than the beam of the sample cell. This results in the generation of pulsating or alternating currents in the photocells.

(v) Amplifier:

The AC current generated in the photocells is transferred to the amplifier, which is coupled to a small servometer. Generally, the current generated in the photocells is of very low intensity. The main purpose of the amplifier is to amplify the signals many times so we can get clear and recordable signals.

(vi) Recording devices:

Most of the times, amplifier is coupled to a pen recorder which is connected to the computer which stores all the data generated and produces the spectrum of the

desired compound.

UV-visible spectrophotometer plays a crucial role in the analysis of both solid and liquid samples.

Analysis of Solid Samples:

(i) Quantitative analysis: solid samples can be analysed by preparing solutions or suspensions.

The UV-visible spectrophotometer measures the absorbance or transmittance of light through these solutions to determine the concentration of a particular compound in the solid sample.

(ii) Characterization of materials: UV-visible spectrophotometry helps in studying the optical properties of solid materials. It provides information about the absorption and reflectance characteristics, allowing researchers to identify specific compounds or functional groups present in the material.

(iii) Material identification: solid samples can be analysed by comparing their UV-visible absorption spectra with reference spectra or databases. This allows for the identification of unknown materials based on their unique spectral patterns.

(iv) Quality control: It is employed for quality control of solid materials. By measuring the absorbance or transmittance of light, it ensures that materials meet specific standards or specifications.

### analysis of liquid sample

(i) Quantitative analysis: UV-visible spectrophotometry is widely used for quantitative analyses of liquid samples. It determines the concentration of a specific compound by measuring its absorbance or transmittance at characteristic wavelengths.

(ii) Chemical analysis: Liquid samples, such as solutions or extracts, can be analyzed to determine the presence and concentration of various chemical components. This includes analyzing the concentration of drugs, pollutants, nutrients or other substances of interest.

(iii) Environmental monitoring: It plays a vital role in maintaining water quality and environmental samples. It can measure the presence of contaminants such as heavy metals or organic pollutants and assess their concentration levels.

(iv) Biological and biochemical analysis: Liquid samples, such as biological fluids or biochemical solutions, can be analyzed using UV-visible spectrophotometry. It helps in determining enzyme activity, protein concentration, DNA concentration and other biomolecular analyses.

Broad features makes it not ideal for sample identification. However, one can determine the analyte concentration from absorbance at one wavelength and using Beer-Lambert law:

$$A = -\log \left( \frac{I}{I_0} \right) = \alpha b c$$

18) Describe the principle and working of FT-IR spectrometer with a diagram. Mention its applications for the analysis of solid and liquid samples.

#### Principle:

→ Molecules and crystals can be thought of as systems of balls (atoms or ions) connected by springs (chemical bonds).

→ These systems can be set into vibration and vibrate with frequencies determined by the mass of the balls (atomic weight) and by the stiffness of the springs (bond strength).

→ With these oscillations of the system, a impinging beam of infrared EMR could couple with it and be absorbed.

→ These absorption frequencies represent excitations of vibrations of the chemical bonds and, thus, are specific to the type of bond and the group of atoms involved in the vibration.

→ In an IR experiment, the intensity of a beam of IR is measured before and after it interacts with the sample as a function of light frequency.

### Working:

A beam source of various IR wavelength light is sent through a beam splitter, where half reaches a fixed mirror and half a mirror that moves with a constant velocity. These two split beams are then reflected and recombined (now with a path difference between the beams) to construct an interference pattern reflecting the constructive and destructive interference pattern of the recombination. After, this interference pattern (or interferogram) is sent to the sample, and the transmitted portion of the interferogram is sent to a detector. After comparison with a reference sample beam spectrum in the detector, a Fourier transform is performed to obtain the full spectrum as a function of wavenumber.

### Analysis of solid samples:

(i) Identification: It is used to identify unknown solid substances by comparing their infrared spectra with a spectral library.

(ii) Chemical characterization: It provides information about the chemical composition and functional groups present in the solid sample.

(iii) Quality control: It helps verify the composition, purity and consistency of solid materials.

(iv) Polymer analysis: It is used for studying the structure, additives and properties of polymers.

(v) Forensic analysis: It aids in identifying and comparing solid evidence, such as fibers, paints, drugs and explosives.

### Analysis of liquid samples:

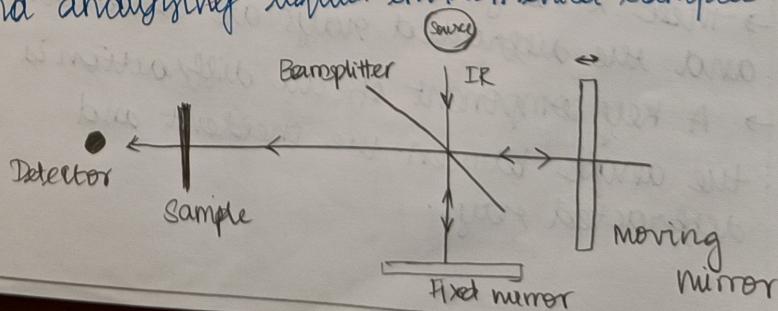
(i) Identification: It is used to identify unknown liquids comparing their infrared spectra with a reference database.

(ii) Quantitative analysis: It allows for the measurement of concentration of specific compounds or functional groups in liquid samples.

(iii) Chemical characterization: It provides information about the molecular structure and functional groups present in liquids.

(iv) Quality control: It helps verify the composition, purity and consistency of liquid materials such as raw materials and products.

(v) Environmental analysis: It assists in studying air-pollutants, water contaminants and analysing liquid environmental samples.



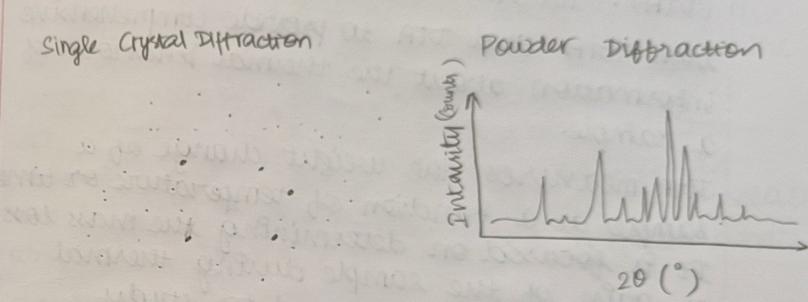
Q) Describe the fundamental principles, working and applications of X-ray powder diffraction.

### Principle and Working:

- This law relates the wavelength of electromagnetic radiation to the diffraction angle and the lattice spacing in a crystalline sample.
- The diffracted X-rays are then detected, processed and counted.
- By scanning the sample through a range of  $2\theta$  angles, all possible diffraction directions of the lattice should be attained due to the random orientation of the powdered material.
- Conversion of the diffraction peaks to  $d$ -spacings allows identification of the mineral because each mineral has a set of unique  $d$ -spacing.
- Typically, this is achieved by comparison of  $d$ -spacings with standard reference patterns.
- All diffraction methods are based on generation of X-rays in an X-ray tube.
- These X-rays are directed at the sample, and the diffracted rays are collected.
- A key component of all diffraction is the angle between the incident and diffracted rays.

→ Single crystals vs Powder Crystal XRD:  
The patterns essentially contain the same information but in the former case, the information is distributed in three-dimensional space whereas in the latter case the 3D data are compressed into one-dimension.

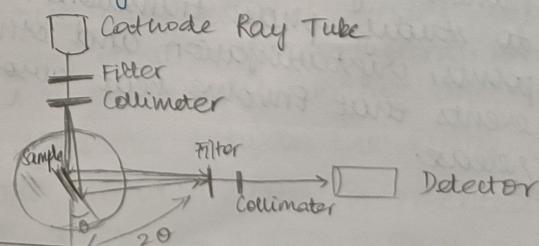
Single Crystal Diffraction



Powder Diffraction

### Applications:

- \* Characterization of crystalline materials.
- \* Identification of fine-grained minerals such as clays and mixed layer clays that are difficult to determine optically.
- \* Determination of unit cell dimensions
- \* Measurement of sample purity
- \* Determining modal amounts of minerals (Quantitative analysis)



20)

With a neat diagram, explain the principle, working and applications of TGA-DTA.

TGA-DTA is indeed the combination of two individual techniques: Thermogravimetric Analysis (TGA) and Differential Thermal Analysis (DTA). TGA-DTA combines the capabilities of both TGA and DTA to provide comprehensive information about the thermal behaviour of a sample.

TGA measures the weight change of a sample as a function of temperature or time. It is focused on determining the mass loss or gain of the sample during thermal treatment. It is often used to study thermal deposition, oxidation, desorption and other chemical reactions that result in weight changes.

DTA measures the temperature difference between a sample and a reference material as they are subjected to the same thermal conditions. It detects exothermic and endothermic reactions in the sample by monitoring the heat flow. DTA is used to study phase transitions, melting points, crystallization and other thermal events that involve heat absorption or release.

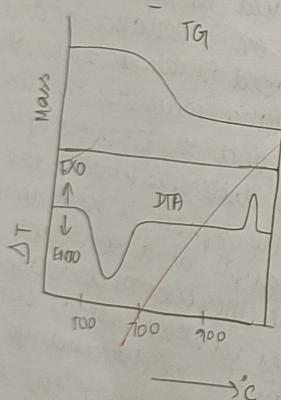
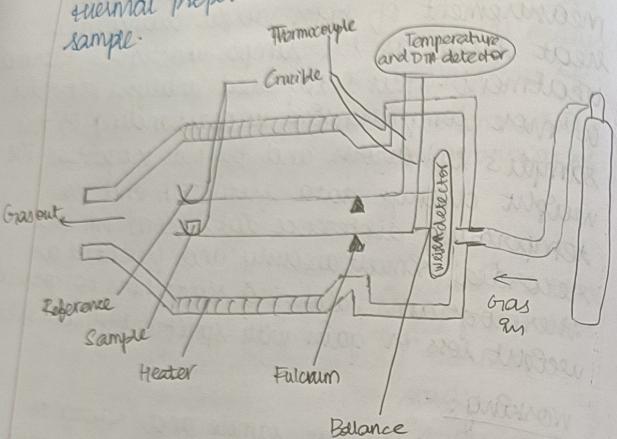
### Principle:

By combining TGA and DTA in a single instrument, TGA-DTA allows simultaneous measurement of both weight change and heat flow as the sample undergoes thermal treatment. This integrated analysis provides a more comprehensive understanding of the sample's behaviour and thermal properties. The weight change data from TGA and the temperature difference data from DTA are recorded simultaneously and presented as thermograms, allowing researchers to correlate weight loss or gain with specific thermal events.

### Working:

In the setup, the sample and reference material are placed in separate pans, which are then positioned on a balance and a thermocouple. The pans are placed inside a temperature-controlled furnace. The balance measures the weight change of the sample, and the thermocouple measures the temperature difference between the sample and reference. The system is programmed to heat or cool the sample at a constant rate. As the temperature increases or decreases, the sample undergoes various thermal events, which are reflected in the weight change and the temperature difference between the sample and reference. The recorded data is presented as thermograms, where the weight change and

temperature difference are plotted against time or temperature. By analysing these thermograms, scientists can determine the thermal properties and behaviour of the sample.



### Applications:

- Characterisation of materials: thermal stability, decomposition kinetics, phase transitions, and thermal behaviour of materials.
- Determination of purity: It can be employed to determine the purity of substances by analysing the melting points and thermal behaviour of samples.
- Quality control: Used in industries to monitor the thermal properties and behaviour of materials during production process, ensuring consistent quality and performance.
- Environmental analysis: It is used to analyse the thermal degradation and emissions of materials, such as plastics, during incineration or waste treatment process.
- Pharmaceutical process: Valuable in drug development and formulation, providing insights into the thermal stability and behaviour of active pharmaceutical ingredients and excipients.

- 2) write a note on the following software tools - ChemOffice, ImageJ, Origin, molecular docking.

ChemOffice: Software suite for chemists and researchers, offering tools for molecular modelling, drug discovery and data analysis. It includes modules like Chem3D for drawing chemical structures and Chem3D Pro for 3D visualisation. ChemOffice is widely used in academia and pharmaceutical companies.

ImageJ: It is an open-source image processing and analysis tool used in biology, medicine and materials science. It allows users to perform tasks such as filtering, segmentation and measurement. It is popular due to its versatility, extensibility and user-friendly interface.

Origin: It is a data analysis and graphing software tool for scientific and engineering research. It offers tools for data visualization, statistical analysis, curve fitting and signal processing. Origin is commonly used in academia and industry for data analysis and visualisation purposes.

Molecular Docking: It is a computational technique for predicting ligand-protein interactions. It helps in drug discovery by predicting the binding affinity for small molecules to target proteins. Molecular docking software uses algorithms and scoring functions to predict optimal binding poses and energies. AutoDock, Vina and GOLD are widely used docking tools in drug design and research.

Q2) What is meant by backscattered electrons? Backscattered electrons refer to the  $e^-$  that are deflected or scattered back when a beam of electrons interacts with a solid sample. In electron microscopy,

a beam of highly-energetic  $e^-$  is directed towards the specimen and as the  $e^-$  interact with the atoms in the sample, they undergo various interactions including scattering. They are used to provide information about the sample's composition, density and surface characteristics.

Q3) What is meant by secondary electrons? Secondary electrons, in the context of electron microscopy, are low-energy  $e^-$  that are emitted from the surface of a specimen as a result of  $e^-$  interactions. When a high-energy  $e^-$  beam interacts with a solid sample, it can cause various interactions, including elastic and inelastic scattering. They are utilised in techniques like SEM to generate detailed images of a sample's surface features and properties.

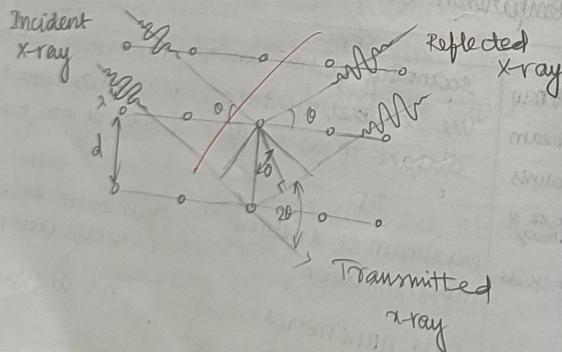
Q4) Comparison between SEM and TEM.

	SEM	TEM
Tool/beam	Scanning electron microscope	Transmission electron microscope
$e^-$ beam	Use scattered/reflected $e^-$	Use transmitted $e^-$
Analysis	Surface of the sample	Internal structure of sample
Nature of image	3D	2D
Magnification	Maximum of 2 million magnification	Maximum of 50 million magnification
Resolution	0.4 nanometres	0.5 angstroms

25) Difference between optical and electron microscope.

Light Microscope	Electron Microscope
→ Illuminating source is light.	→ Illuminating source is electron beams.
→ Specimen preparation takes hours.	→ Specimen preparation takes days.
→ Live or dead specimen can be seen.	→ Dead or dried specimen can be seen.
→ Magnification 500X - 1500X	→ Magnification 100000X - 300000X
→ Image is coloured	→ Image is black and white.
→ Vacuum is not required	→ Vacuum is required
→ No need of high voltage electricity.	→ Need of high voltage electricity.

26) What is Bragg's law?



Cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence ( $\theta$ )

→  $d$  is the distance between atomic layers in a crystal.

→  $\lambda$  is the wavelength of the incident X-ray beam.

→  $n$  is an integer.

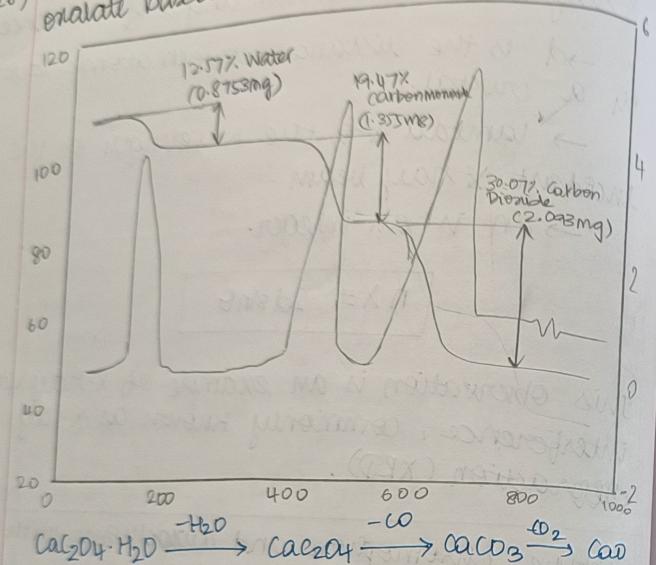
$$n\lambda = 2d \sin\theta$$

This observation is an example of X-ray wave interference, commonly known as X-ray diffraction (XRD).

27) Define chromophore and auxochrome with an example.

	Auxochrome	Chromophore
Definition	Group of atoms that can get attached to a chromophore, thereby increasing the colorfulness of the chromophore.	Chromophore is the part of a molecule that is responsible for the colour of that molecule.
Intensity of colour	Increases the colour intensity of chromophore.	Responsible for the colour of a colourless compound.
Example	Pale yellow coloured nitrobenzene becomes dark yellow colored when an hydroxyl group is attached to the molecule.	Colourless benzene gets a pale yellow colour when a nitro group is added to the benzene molecule.

28) Illustrate the thermal decomposition of calcium oxalate based on the graph.



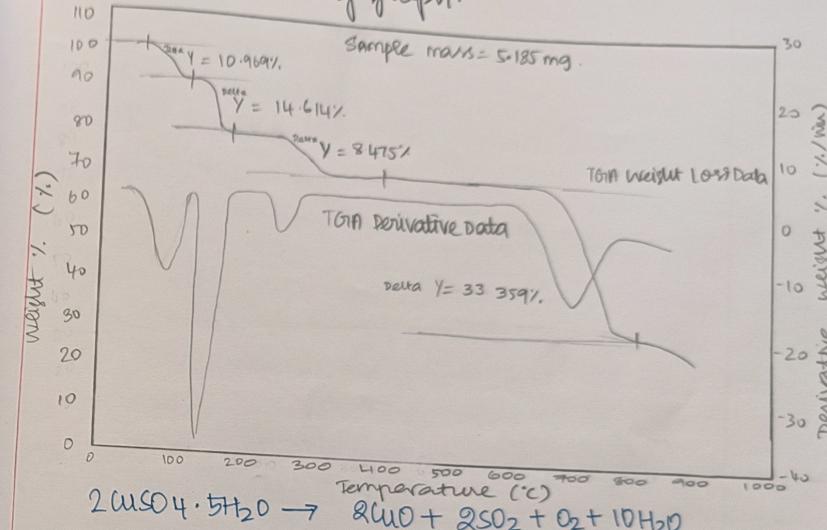
Step 1: Involves loss of water of crystallisation to form anhydrous calcium oxalate.

Step 2: calcium oxalate then thermally decomposes to calcium carbonate with the loss of carbon monoxide.

Step 3: Involves thermal decomposition of calcium carbonate to calcium oxide with the loss of carbon dioxide.

29)

Illustrate the thermal decomposition of CuSO<sub>4</sub>·5H<sub>2</sub>O based on following graph.



→ 50°C - 330°C ⇒ Loss of five waters of crystallisation

→ 550°C - 870°C ⇒ Loss of SO<sub>2</sub> and O<sub>2</sub>.

→ the shape of first derivative curve which almost duplicates the shapes of the total evolved gas profile seen at the mass spectrometer. This is an important feature as it demonstrates that all the gases evolved have reached the mass spectrometer although with the linked gas evolved species here is less useful.