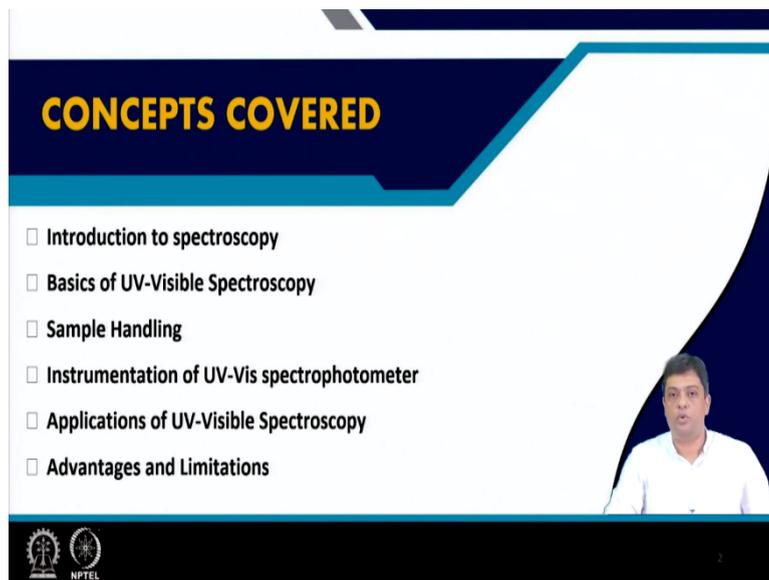


**Physics of Renewable Energy Systems**  
**Professor Amreesh Chandra**  
**Department of Physics**  
**Indian Institute of Technology Kharagpur**  
**Lecture 46**  
**UV – Visible Spectroscopy (UV-Vis)**

Hello, in today's lecture, let us discuss another experimental technique that is called as UV visible spectroscopy and many a times people just call it as UV vis.

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After going today's lecture, you will get an idea about what is UV visible spectroscopy? The importance of preparing the sample carefully before it can undergo characterization using UV visible spectrophotometer. What is UV visible spectrophotometer? What is the principle behind the construction of this spectrophotometer?

How do you collect the data? And how do you analyse the data? We will also give you a brief idea about the way you calculate the energy band gap using the UV visible spectroscopic data and also other advantages, limitations and a wide range of applications for this characterization technique will also be covered in this lecture.

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**KEY POINTS**

- Born-Oppenheimer approximation
- Beer lambert law
- Molar absorption coefficient
- Absorption spectra

The slide features a dark blue header with the title 'KEY POINTS' in yellow. Below the header is a white area with a blue border on the right side. A small video inset of a man in a white shirt is visible in the bottom right corner. At the bottom left, there are logos for IIT Bombay and NPTEL.

You will also understand after going through this lecture what is Born-Oppenheimer approximation, the Beer Lambert law, what is molar absorption coefficient? And finally, how do you plot and analyse an absorption spectrum?

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**Introduction to Spectroscopy**

Definition:

*Spectroscopy is the measurement and interpretation of the interactions between the incident electromagnetic waves and matter characterized by nuclear, molecular, or electronic changes.*

The slide has a white background with a blue header. It contains several icons: gears, a tree-like structure of nodes, an atom, a hard hat, and a flask. A small video inset of a man in a white shirt is in the bottom right corner. Logos for IIT Bombay and NPTEL are at the bottom left.

Till now, we have discussed one characterization technique that is x-ray diffraction and we spent nearly two lectures on that technique. That technique was used for ensuring and collecting data, so that you can extract information regarding phase formation, the type of crystal lattice and various other parameters related to a unit cell formation. Now, we have

extensively used the concept of semiconductors in our earlier modules and we have defined metals, semiconductors and insulators in terms of the difference in their band gaps.

The first question which we need to ask is how do we actually calculate the energy band gap in such materials and one of the most common technique which is used to determine this band gap is the UV visible spectroscopy technique. So, this technique becomes extremely useful for our course. And if you go to laboratory, you will find that this is actually a very simple technique, but again it can give you a lot of information.

Spectroscopy is primarily the measurement and interpretation of the interaction between the incident electromagnetic waves. The moment I mention electromagnetic waves please remember two things should cross your mind that it has an E component and it has a B component. So, in spectroscopy, you are actually analysing the interaction between the electromagnetic waves and matter characterized by changes which can be at the nuclear level, the molecular level or at the electronic states. So, this is what we are going to understand now.

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**Features:**

- (1) ***In NMR spectroscopy, which*** works in the radiofrequency region, the nucleus and electrons are considered to be the tiny charged particles, and their spins is associated with a magnetic dipole. The **interaction with the magnetic field of electromagnetic waves and these magnetic dipoles** at a particular frequency give rise to NMR spectra.
- (2) ***In UV-Vis spectroscopy,*** during the excitation of valence electrons, the movement of electronic charges in the molecules takes place, which subsequently changes in the electric dipole moment. A UV-Vis spectrum is generated when **the interaction of these electric dipoles with the electric field of the electromagnetic waves** occurs.

The slide features a small video inset of a man in a white shirt speaking, and the NPTEL logo is visible in the bottom left corner.

As we say you have E component and B component in the EM wave. So, we have two types of techniques one NMR other UV-Vis. Just a very layman type difference in NMR you are talking about the interaction with the magnetic field of the electromagnetic waves with the magnetic dipoles which are present in a material and in UV-Vis you talk about the interaction

of electric dipoles with the electric field of the electromagnetic waves which are incident on the material where you are seeing these dipoles.

So, NMR interaction is magnetic component UV-Vis interaction with the electric component. NMR works in the radio frequency region. The nucleus and the electrons are considered to be tiny charged particles and their spins is associated with a magnetic dipole. Now, this dipole interacts with the magnetic field of the electromagnetic waves and if you go from one material to the other the magnetic dipole in these materials change and therefore, the signal which you obtain in NMR spectroscopy for different materials would be different.

Similarly, in UV visible spectroscopy what happens? During the excitation of valence electrons, valence electrons means you are exciting the valence electron let us say from valence band to conduction band. Once there is a movement of electron what is associated there is a movement of electronic charge in the molecules, which subsequently changes the electric dipole moment.

So, absorption, excitation, movement, change in the electric dipole moment and a UV-Vis spectrum is generated when there is an interaction of these electric dipoles with the electric field component of the electromagnetic waves. So, this is the way you should understand the two types of techniques which are there to analyse the spectroscopic data.

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The slide is titled "Types of spectroscopy techniques :". It contains the following text:

**Generally, spectroscopy classified into two types:**

- (1) **Atomic Spectroscopy:** In atomic spectroscopy the changes in energy take place at atomic level.  
For instance: **Atomic absorption spectroscopy, etc.**
- (2) **Molecular Spectroscopy:** In molecular spectroscopy, the changes in energy takes place at molecular level.  
For instance: **UV-Vis spectroscopy, IR spectroscopy, etc.**

The slide features a background with various scientific icons like a gear, a lightbulb, a smartphone, a microscope, and a beaker. There are also decorative lines and checkmarks. A small video inset of a man in a white shirt is visible in the bottom right corner. The NPTEL logo is at the bottom left.

Generally, spectroscopy is classified in two categories; one atomic spectroscopy or molecular spectroscopy. The earlier was the technique and now, we are understanding somewhat more in detail whether you are analysing at the atomic scale or the molecular scale. In atomic spectroscopy, the changes in the energy takes place at the atomic level as the name suggests

atomic spectroscopy and you have a technique which is called as atomic absorption spectroscopy and many other.

As the name suggests, molecular spectroscopy would be what? Very simple. In molecular spectroscopy, the changes in the energy takes place at the molecular level. And you have techniques like UV visible spectroscopy, IR spectroscopy, and a few others. We will start with this and in the next lecture, we will start with our discussion on IR spectroscopy.

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**Electronic spectroscopy:**

- (1) Arises due to the **interaction of molecules with UV and Visible** electromagnetic light.
- (2) Absorption of photon results in transition of a molecule/electron between two electronic states.
- (3) Such electronic transitions are accompanied by simultaneous transition between vibrational and rotational energy levels as well.
- (4) According to **Born-Oppenheimer approximation**, the total energy of a molecule in ground state (G.S.) is given by:

$$E_T = E_{el} + E_{vib} + E_{rot} \quad (1)$$

The slide features a blue header, a white background with faint icons, and a small video inset of a man in a white shirt in the bottom right corner. The NPTEL logo is visible in the bottom left corner.

Electronic spectroscopy basically arises due to the interaction of molecules with UV and visible range electromagnetic light. Now, the absorption of photon results in transition of a molecule or electron between two electronic states. So, you absorb energy once you absorb energy, your energy is increased and therefore, there is a transition. Such electronic transitions are accompanied by simultaneous transition between vibrational and rotational energy levels.

And according to the Born-Oppenheimer approximation, the total energy of a molecule in ground state is given as E electronic plus E vibrational plus E rotational, this is the total energy of a molecule in ground state.

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**Electronic spectroscopy:**

The energy change for an electronic transition is given by:

$$\Delta E_T = \Delta E_{el} + \Delta E_{vib} + \Delta E_{rot} \quad (2)$$

The frequency for the electronic transition is given by the **Bohr frequency condition**, viz., lies in UV-Visible region:

$$\nu = \frac{\Delta E_T}{h} \quad (3)$$


And electronic spectroscopy can therefore, be written in terms of the change in the energy when there is an electronic transition and this change  $\Delta T$  is equal to change in electronic level, vibrational level or energy of the rotational level. The frequency of the electronic transition is given by the Bohr frequency condition that is  $\nu$ ;  $\nu$  is equal to  $\Delta E_T$  by  $h$  and this lies in the UV-Vis region.

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**UV-Visible spectroscopy**

**Beer Lambert law**

(1) Measurement of absorbance of the UV-visible spectra is governed by Beer Lambert law.

(2) Beer Lambert Law states that the amount of light absorbed by a solution is proportional to the concentration of the absorbing substance, and to the path length (thickness) of the absorbing material.

(3) Mathematical expression of Beer Lambert law:

$$A = \log(I_0/I_t) = \epsilon Cl \quad (4)$$

A is the Absorbance,  $\epsilon$  is the molar absorptivity coefficient ( $L \text{ mol}^{-1} \text{ cm}^{-1}$ ),  $l$  is the path length of the sample (cm),  $I_0$ ,  $I_t$  are the intensity of the incident light and transmitted light, respectively, and  $C$  is the concentration of the compound ( $\text{mol L}^{-1}$ )



In UV visible spectroscopy there is measurement of absorbance of the UV visible spectra and the whole process is governed by the Beer Lambert law. This law states that the amount of light that is absorbed by a solution, absorbed by a solution is proportional to the concentration

of the absorbing substance and the path length of the absorbing material. I have encircled few terms which are critical what is the Beer Lambert law actually indicating towards?

That light will be absorbed. This is one solution. So, you are talking about the measurement probably when the sample is dispersed or you have formed a solution, is proportional to the concentration. So, if you have high concentration of material in the solution, then the response may be different from the condition when the concentration is much lower.

So, the concentration of the absorbing substance this after the term concentration, concentration of what? Of the absorbing substance the substance which will absorb the energy from the incident UV light. So, you have a substance which will absorb energy. So, concentration is the one thing which will decide, what is the output? And the second is the path length or thickness of the absorbing material.

So, what is the nature of the material? How thick that material is, will also define what would be the output you will obtain. And mathematically the expression is the absorbance  $A$  is given as  $\log$  of  $I_0$  by  $I_t$  where  $I_0$  and  $I_t$  are the intensity of the incident light and transmitted light respectively. And that can be written as  $\epsilon Cl$ , where  $\epsilon$  is the molar absorptivity coefficient in liter per mole per centimeter,  $C$  is the concentration and  $l$  is the path length of the sample in centimeters. So, this is what is mathematical expression of the Beer Lambert law.

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**Importance of Beer Lambert law**

- ❖ According to Beer Lambert's law:  
$$A = \epsilon Cl \quad (5)$$
- If,  $\epsilon$  and  $l$  are constant, then  
**Absorbance  $\propto$  Concentration**  
**Linear relationship**
- ❖ Depending on the above relationship, **quantitative analysis of sample**, i.e. concentration of an unknown sample can be determined.

The slide features a blue header, a white background with faint icons, and a small video inset of a man in a white shirt in the bottom right corner. The NPTEL logo is visible in the bottom left corner.

What is the importance? The basic importance is that the absorbance is proportional to concentration and we have a linear relationship if  $\epsilon$  and  $l$  are considered as constant. Using this relationship, a quantitative analysis of sample that is concentration of an unknown sample can be determined. So, you what will you do? You will have a sample or a solution with zero concentration of the absorbing materials you will get an output corresponding to an incident electro or UV visible electromagnetic ray.

Then you add  $C_1$  concentration the output will change and then you can draw the absorbance as a function of increasing or changing concentration and you will get a curve. And if that is the standard curve which you have obtained after some time if you perform the same measurement for an unknown sample, where the initial solution or the fluid in which the material that is absorbing is dispersed is the same then you can extract the information about the concentration of the absorbing material in an unknown sample. A very simple way of performing the experiment.

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**Importance of Beer Lambert law**

- ❖ This law is successful in describing the absorption behaviour of **dilute solutions only** i.e. of concentration  $> 0.01$  M. If concentration increases, the absorption coefficient and refractive index of the sample changes with increase in concentration.
- ❖ This law is not applicable in case of **suspension**, as scattering of light due to impurities may occur.
- ❖ **Fluorescence or phosphorescence process can occur** as they take place in the same wavelength range of UV-Vis.
- ❖ Strict adherence of an absorbing system to this law is observed **only when radiation used is monochromatic.**

The slide features a background with scientific icons like a beaker, a flask, and a molecular structure. A video inset in the bottom right corner shows a male presenter in a white shirt. The NPTEL logo is visible in the bottom left corner.

The law clearly is able to give us a protocol by which we can perform the experiment to determine the concentration of a particular absorbing substance in an unknown solution. But, there is a limitation, the main limitation is that the absorption behaviour can only be successfully explained in dilute solutions up to let us say concentrations of 0.01 molar and if the concentration increases the absorption coefficient and refractive index of the sample

changes with the increase in concentration and then the analysis becomes a bit more complicated.

The law is not applicable in the case of suspensions, as scattering of light due to impurities may occur and the whole process is much more complex. In addition, fluorescence or phosphorescence processes may occur as they take place in the same wavelength range of UV visible and then the analysis of data becomes more difficult. Strict adherence of an absorbing system to this law is only observed when radiation used is monochromatic.

So, if you use any light, which has let us say components, which can which are not monochromatic. So, if you have a source which is sending out more than one wavelength, then you must use filters to only send one wavelength and if you use radiation which is not, not monochromatic, then using this law, it is difficult to obtain the concentration in solutions for the material which is absorbing the UV visible light.

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The slide contains a list of four steps for quantitative analysis and a calibration curve graph. The graph plots Absorbance (arb. Unit) on the y-axis (0 to 2.5) against Concentration ( $\mu\text{M}$ ) on the x-axis (0 to 30). A linear trendline is shown with data points. A small inset video of a presenter is visible in the bottom right corner of the slide.

**(1) Quantitative analysis of the unknown samples**

- (a) Prepare the 4-5 standards of the unknown concentration analyte to be quantified at known concentrations and measure absorbance at a specified wavelength.
- (b) Prepare calibration curve using absorbance values.
- (c)  $\epsilon$  can be obtained from slope of the calibration curve for a given wavelength.
- (d) Concentration of analyte in the sample can be obtained from the calibration curve using Beer Lambert law.

Calibration curve

This is typically what you do you prepare 4 or 5 standards of unknown concentration analyte and then you have the data which is plotted as a function of absorbance and concentration. After you have prepared the calibration curve, you can then obtain epsilon from the slope of the calibration curve for a given wavelength. And concentration of an analyte in the sample can be obtained from the calibration curve using the Beer Lambert law.

If you now have another solution, where the same material is dispersed or substances dispersed, but the concentration of that substance is not known in the solution. So, that is the way you perform this analysis.

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**Sample Handling**

- ❖ UV-visible spectra are usually recorded either in **very dilute solutions** or in the vapour phase.
- ❖ The sample is dissolved in some **suitable solvent, which does not itself absorb radiation in the region** under investigation.
- ❖ Commonly used solvents are cyclohexane, 1,4 – dioxane, water and 95% ethanol.
- ❖ The chosen solvent should be inert to sample.
- ❖ **Hydrogen bonding, dipole-dipole interactions** between solvent and sample further complicates the **effect of vibrational** and rotational energy levels on electronic transitions, so **non-polar solvents** preferred.

The slide features a blue header with the title 'Sample Handling'. The background is white with faint chemical icons. A video inset in the bottom right shows a man in a white shirt speaking. The NPTEL logo is in the bottom left corner.

Please note that this measurement will give you reliable data only when you are using very dilute solutions or you are performing the measurements when system is in the vapor phase. The sample is dissolved in some suitable solvent. What do you mean by suitable solvent? That is the one which does not itself absorb radiation in the region under investigation.

Otherwise, they will also start giving you signal and obviously, the chosen solvent should be inert to the samples or there should not be the case that you start having reaction between the solvent and the solute. So, once you have set these conditions you will find that this lead to a condition or preferred conditions where non polar solvents are mostly recommended for such kind of measurements.

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### Instrumentation of UV-Vis spectrophotometer

**(1) Light source** ✓

- (a) Deuterium lamp
- (b) Tungsten-Halogen lamp (<350 nm)
- (c) Xenon arc lamp
- (d) Mercury lamp

**(2) Monochromator comprises of**

- (a) Enter slit
- (b) Dispersive device for diffraction grating
- (c) Exit slit

Now, let us start moving towards instrumentation of the whole UV-Vis spectrophotometer and then we will discuss about the data collection and then how that is used to extract information regarding the energy bandgap in semiconductors. So, you have a light source, you can have different types of light source, then you have monochromator as discussed earlier, so as to ensure that one wavelength is incident on the sample.

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### Instrumentation of UV-Vis spectrophotometer

**(3) Reference cuvette and Sample cuvette**

Reference contain pure solvent, it is important to set a reference cell to zero.

- (a) For visible light: Cuvettes made from PMMA, polystyrene or normal glass.
- (b) For UV light : Cuvettes made from quartz glass, or a special type of plastic are used.

**(4) Detectors:**

(a) Photomultiplier tube: consists of

- ✓ A photo-emissive cathode (a cathode which emits electrons when struck by photons of radiation),
- ✓ Many dynodes (which emit several electrons for each electron striking them)
- ✓ An anode.

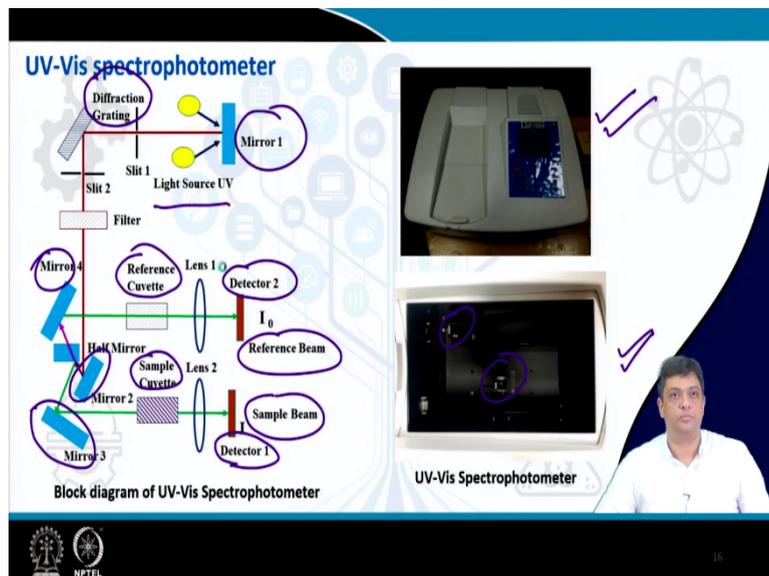
So, in the instrument you have 2 sample rotators. One where you will put the reference cuvette and in the other where you will have the sample cuvette. The reference cuvette has the pure solvent in it, it is important to set the reference cell to zero. So, that the data which you get from the other sample holder is actually coming in only from the absorbing material,

because the signal which can originate from the cuvette or the solvent is collected from the reference cuvette and that is removed from the signal which is obtained from the sample cuvette.

So, there are two types of sample places to put your samples. If you are using visible light cuvettes are made up of PMMA polymethyl methacrylate, polystyrene or normal glass. For UV light the cuvettes are made up of quartz glass or special type of plastics are used. Then, once I have the source, the sample, the light interacts with the sample then you have a signal output this once you have a signal output you must collect this signal and then analyse the signal.

That means, you must have a detector and the detector is a typical photomultiplier tube which you have studied in many courses. What do they include? There is a photo-emissive cathode that absorbs and then you have the emission of electrons and then you have the other components of the photomultiplier tube which you have been studying in earlier classes.

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This is what the UV visible spectrophotometer typically looks like. Sorry I will repeat, no pen not active. This is the instrumentation of the UV visible spectrophotometer. So, this is a typical instrument and this is the picture of the chamber where you have the sample holders and we will see the video in the next slide and things will become very clear. So what happen? You have the light source, the mirror which will reflect the light then you will direct these light using diffraction grating.

These will fall on the half mirror. Half of the intensity will go towards let us say mirror 4 and the remaining will go towards mirror 3 that is 50 percent of the intensity will be falling on mirror 3 and 50 percent will be falling on mirror 4. The light from mirror 4 let us say we will cross the reference cuvette and the light which is reflected from mirror 3 will pass through the sample cuvette and then what you obtain would be the reference beam and the sample beam.

Sample beam detected by detector 1, reference beam detected by detector 2. This is what it is the typical instrumentation. So, you see the optics play a very critical role and therefore, while you are using these instruments, you should be very careful that you should not disturb these instruments. Otherwise, the optics which are very sensitive to vibrations will change and the data will not be the one which is expected or you will get data that needs to be again calibrated with some standards.

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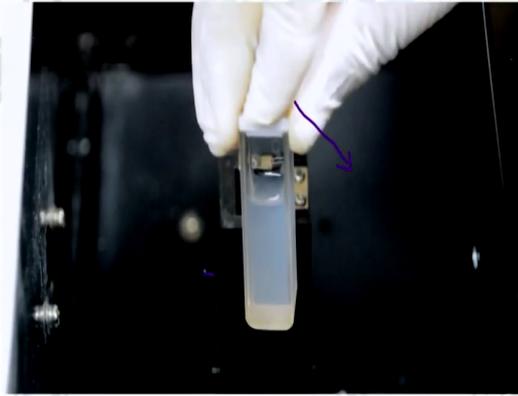
Experimental set up to measure UV-Vis

The slide features a blue header with the title "Experimental set up to measure UV-Vis". Below the title is a large video window showing a dark experimental setup. A person's hand is visible near the setup. To the right of the video window is a smaller window showing a man speaking. The slide also includes a logo of an atom in the top right corner, a logo of an institution and NPTEL in the bottom left corner, and the number "17" in the bottom right corner.

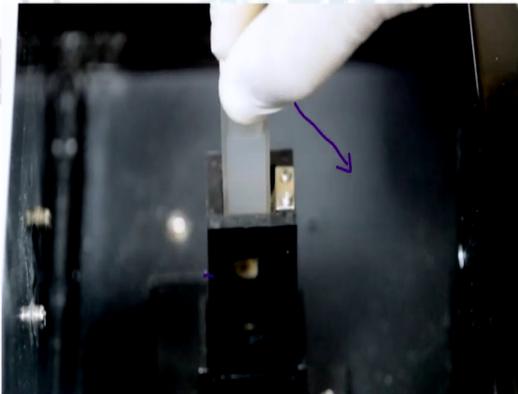
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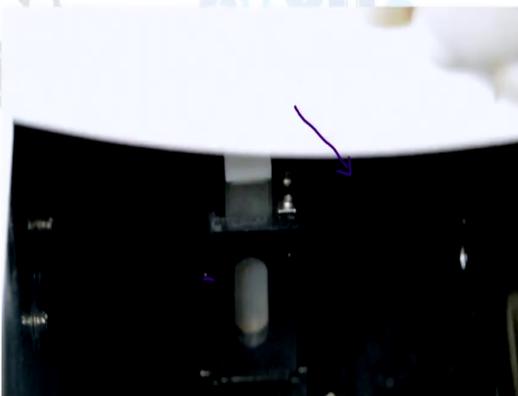
Experimental set up to measure UV-Vis

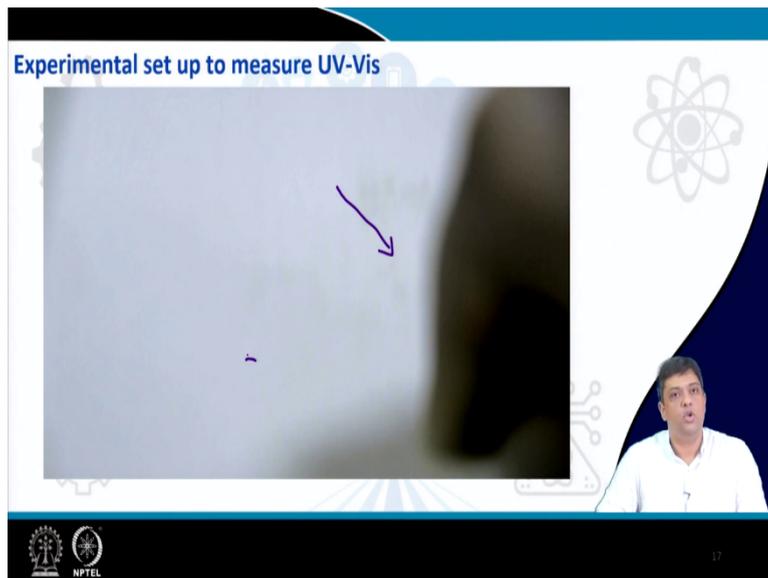


Experimental set up to measure UV-Vis



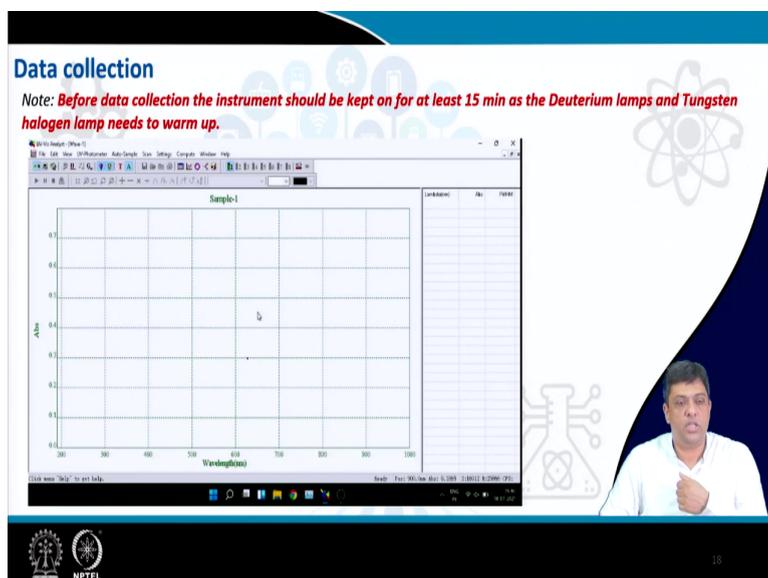
Experimental set up to measure UV-Vis





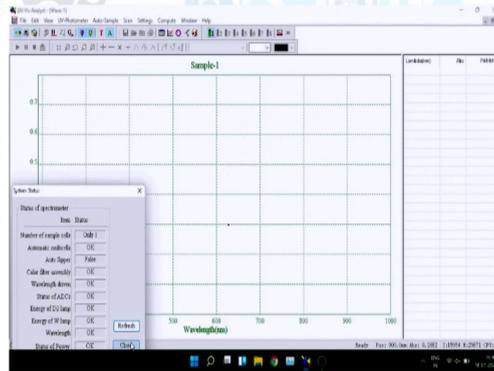
So, let us see the way this is happening you have the source then the optics then the sample holder. This is a typical solution which is prepared and either you can use a standard or you can use the one which is having the reference in it. After you have installed the sample in the sample holder you close the lid and you run the program.

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## Data collection

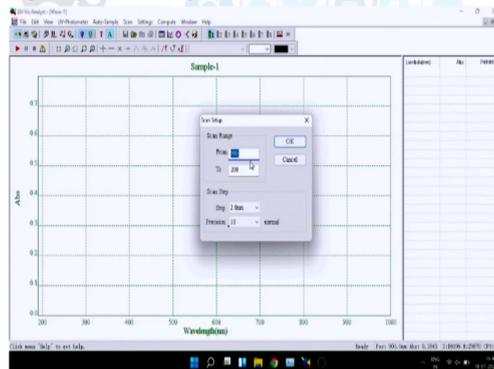
**Note:** Before data collection the instrument should be kept on for at least 15 min as the Deuterium lamps and Tungsten halogen lamp needs to warm up.



18

## Data collection

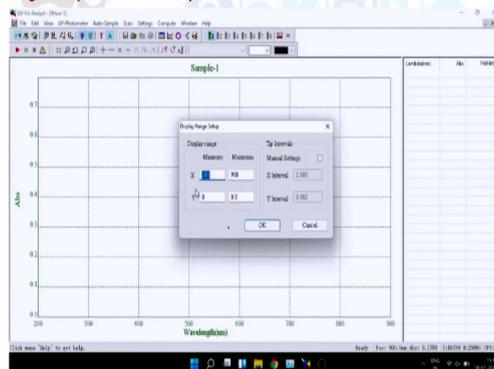
**Note:** Before data collection the instrument should be kept on for at least 15 min as the Deuterium lamps and Tungsten halogen lamp needs to warm up.



18

## Data collection

**Note:** Before data collection the instrument should be kept on for at least 15 min as the Deuterium lamps and Tungsten halogen lamp needs to warm up.



18

### Data collection

Note: Before data collection the instrument should be kept on for at least 15 min as the Deuterium lamps and Tungsten halogen lamp needs to warm up.

The screenshot displays a software window titled 'Sample-2' with a graph of Absorbance (Abs) on the y-axis (ranging from 0.0 to 2.0) versus Wavelength (nm) on the x-axis (ranging from 200 to 900). A red curve shows a sharp peak at approximately 200 nm, followed by a shoulder and then a gradual decline. A dialog box titled 'Wait for Analog' is overlaid on the graph, containing the text 'Wait for analog. Please check the cables, check the power supply.' A purple circle highlights a point on the curve at approximately 400 nm, and a purple arrow points to the x-axis at approximately 800 nm. A small inset image shows a person speaking.

NPTEL

### Data collection

Note: Before data collection the instrument should be kept on for at least 15 min as the Deuterium lamps and Tungsten halogen lamp needs to warm up.

The screenshot displays a software window titled 'Sample-1' with a graph of Absorbance (Abs) on the y-axis (ranging from 0.0 to 2.0) versus Wavelength (nm) on the x-axis (ranging from 200 to 900). A red curve shows a sharp peak at approximately 200 nm, followed by a shoulder and then a gradual decline. A purple circle highlights a point on the curve at approximately 400 nm, and a purple arrow points to the x-axis at approximately 800 nm. A small inset image shows a person speaking.

NPTEL

Once you have closed the lid then you will set the program condition or experimental conditions you will define the range in which you want to have the absorbance and then you will run this scan. But before you run the scan what you need to do, please ensure that the instrument is kept switched on for at least 15 minutes for warming up because the deuterium lamps and the tungsten halogen lamps, they need to warm up before they can be used

And typically it is always advised that you keep the instrument in a switch on mode for 15 minutes before initiating the whole experiment. So, then you set up the software you will decide define all the conditions and then you will tell the let us say the number of cells, what is the number of the solution which you will be using, the kind of solution you are using?

And the various other parameters which you are knowing about the sample. You will give the sample name the wavelength, all the details about the sample you will be defining. For example, in this we are showing the scan setup, we have defined the range from 2. So, what is the wavelength where we are scanning and what is the scan step at which steps you would like to carry out the measurement.

This is just the display range the y axis just so that if you are analysing online, you get an idea of how to you see the spectrum as it is collected. Along with that, you can defy the backgrounds the colours or everything, typically you play with the graphs. Once you have done it, you play the play button and then the data collection starts.

And you will see that you are obtaining the absorbance as a function of changing wavelength and you are getting the data. At the point where the sample is having the excitation you will see some peaks otherwise you will see the typical background, once it has been collected, you can save the data and then you can refine it.

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**Band Gap calculation from UV spectra**

- The Tauc method is based on the assumption that the energy dependent absorption coefficient  $\alpha$  can be express by the following equation :
 
$$(\alpha h\nu)^{1/n} = b(h\nu - E_g)$$
- where  $h$  is the Plank constant,  $\nu$  is the photon's frequency,  $E_g$  is the ban gap energy and  $b$  is the constant.
- The  $n$  factor depends on the nature of the electron transition,  $n$  is equal to  $\frac{1}{2}$  for direct band gap and  $n$  is equal to 2 for indirect band gap.
- For example: a typical experiment could be like:-  
Collect UV-visible spectra in the range 200 nm to 800 nm.  
For direct band gap materials, plo  $(\alpha h\nu)^2$  vs Energy ( $h\nu$ ). Fit a linear line. The intercept will give the band gap.
- For indirect band gap, plot  $(\alpha h\nu)^{1/2}$  vs Energy ( $h\nu$ ). Repeat the process.

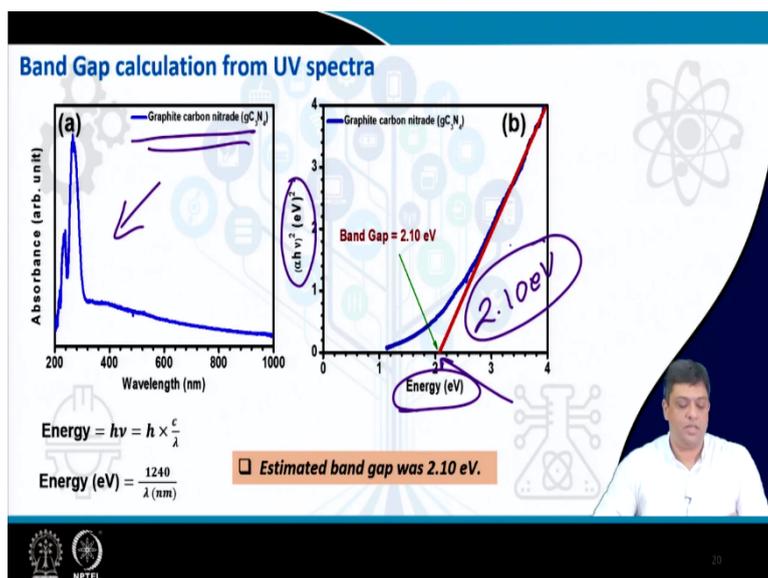
This will become clear in next slide.

Once you have obtained the absorbance data you can use the Tauc relation to calculate the bandgap. So, for example, you have two types of semiconductors the direct bandgap semiconductor and the indirect type. The Tauc relation is based on the assumption that the energy dependent absorption coefficient alpha can be expressed as alpha h nu raised to the power of 1 by n is equal to b into h nu minus Eg, where Eg is the bandgap, h is the Planck's constant, nu is the photon frequency and you have the absorption coefficient as alpha.

The factor  $n$  is half for direct bandgap and equals to 2 for indirect bandgap. So, if you are measuring a material where you are seeing direct bandgap then you will plot  $\alpha h \nu$  as a function of  $h \nu$ . So, you will plot  $\alpha h \nu$  squared as a function of  $h \nu$ . And you will get a curve and, in the region, where you can fit a linear line, you will fit a linear line.

And then extrapolate it the intercept on the x axis will give you the band gap and in case of indirect type material, you will get plot  $\alpha h \nu$  raised to the power of half as a function of energy that is  $h \nu$  and you will get a similar curve and then you will fit a linear line.

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This is what you actually perform. This is the data you have obtained for let us say graphite carbon nitride. Then you plot  $\alpha h \nu$  whole square as a function of  $h \nu$  energy you get a plot and then this is the linear region which is shown in the red solid line. You plot the red solid line and extrapolate and the point it intersects with the x axis is the value for bandgap and this is for example 2.10 electron volts for graphite carbon nitride. And this is the way the bandgap in semiconductors are estimated.

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**Applications of UV-Vis spectroscopy**

**(2) Structure elucidation of samples**

UV-Vis spectroscopy helps in prediction of presence or absence of saturation, unsaturation, various functional groups and hetero atoms in various organic compounds viz. different electronic transitions such as  $\pi$  to  $\pi^*$  to n to  $\pi^*$  transitions.

**(3) In Nanotechnology**

UV-Vis can be used to determine the color absorption properties of metallic nanoparticles.

**(4) As Detector**

UV spectrometer used as a detector in HPLC (High-Performance liquid Chromatography)

Other applications of UV-Vis range from the field of nanotechnology to high performance liquid chromatography that can be used in polymers, rubbers, biophysics, nanofluids and a

large number of applications are there. You can also talk about understanding the electronic transitions in organic compounds.

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**Applications of UV-Vis spectroscopy**

**(5) Chemical kinetics**

Kinetics of chemical reaction can also be studied using UV spectroscopy. The UV radiation is passed through sample and absorbance variation with respect to time observed.

**(6) DNA/Protein Measurement**

UV-Vis absorbance spectroscopy is the preferred method to estimate nucleic acid concentration such as DNA or RNA.

NPTEL

Or there are other applications which are very common and used extensively like understanding the kinetics of chemical reactions. So, what you do you pass the UV radiation through the sample and as the chemical reaction takes place, there is a change in the absorbance and from there you can extract information about the kinetics also. You can use this technique to talk about the concentration of nucleic acid such as DNA or RNA in any biological samples.

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**CONCLUSION**

(1) Most fundamental spectroscopic technique for qualitative and quantitative analysis of samples.

(2) Determination of band gap in semiconductors is quite easy.

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So, let us end this lecture by clearly indicating that UV visible spectroscopy is one of the most fundamental spectroscopic techniques for qualitative and quantitative analysis of samples which have been discussed during this course. And this technique actually makes the determination of bandgap in semiconductors a very easy concept and is also routinely used.

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These are the references which were followed while preparing this lecture or for obtaining the data. And in the next lecture, we will talk about another technique which is the FTIR technique for sample characterization. And I thank you for attending today's lecture.