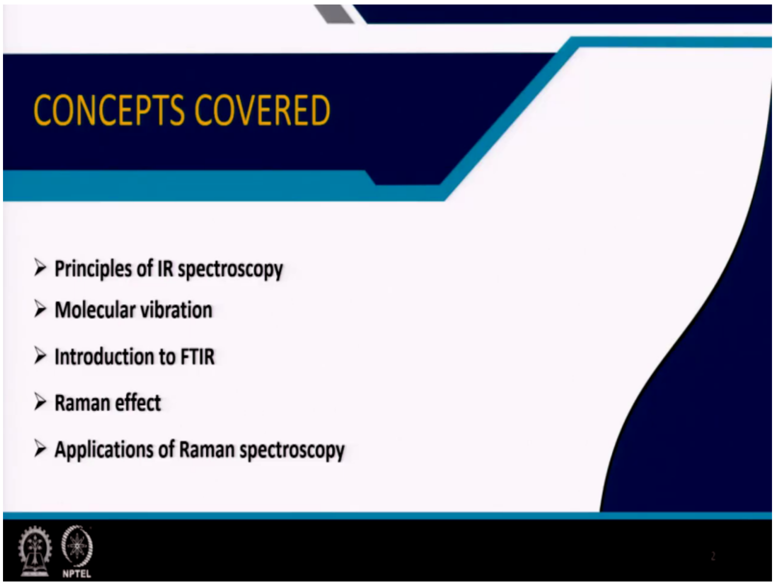
Non - Metallic Materials
Prof. Subhasish Basu Majumder
Department of Materials Science Centre
Indian Institute of Technology, Kharagpur

Module - 09
Characterization of structure, composition, and microstructure of non - metallic materials
Lecture - 47
Infra-red and Raman spectroscopy

Welcome to my course Non-Metallic Materials and we are in module number 9, Characterization of structure, composition, and microstructure of non-metallic materials. This is lecture 47, where I will be describing the Infra-red and Raman spectroscopy that is used as tool for material characterization.

(Refer Slide Time: 00:51)

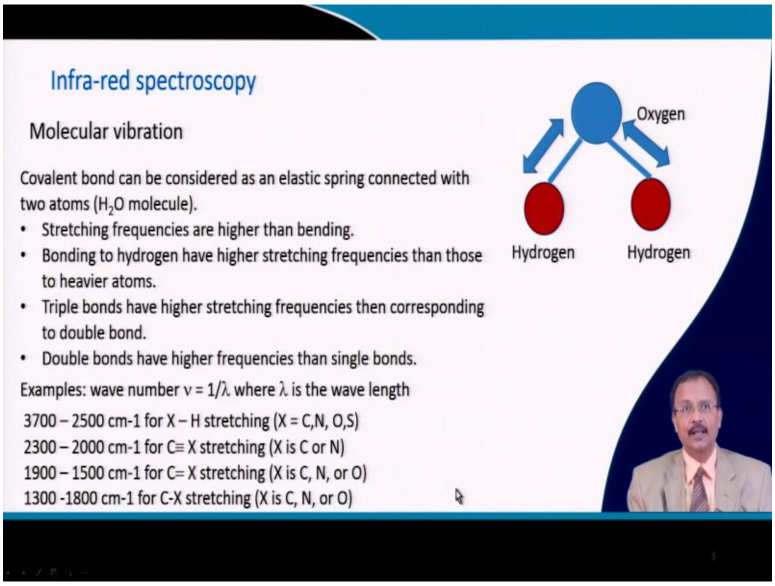


CONCEPTS COVERED

- Principles of IR spectroscopy
- Molecular vibration
- Introduction to FTIR
- Raman effect
- Applications of Raman spectroscopy

So, first principle of IR spectroscopy that will be described in terms of molecular vibrations and then we will introduced the Fourier transform IR spectroscopy. Then Raman effect and Raman spectroscopy will be introduced and the applications of Raman spectroscopy some examples will be cited.

(Refer Slide Time: 01:16)



Infra-red spectroscopy

Molecular vibration

Covalent bond can be considered as an elastic spring connected with two atoms (H_2O molecule).

- Stretching frequencies are higher than bending.
- Bonding to hydrogen have higher stretching frequencies than those to heavier atoms.
- Triple bonds have higher stretching frequencies then corresponding to double bond.
- Double bonds have higher frequencies than single bonds.

Examples: wave number $\nu = 1/\lambda$ where λ is the wave length

3700 – 2500 cm-1 for X – H stretching (X = C,N, O,S)
2300 – 2000 cm-1 for C≡X stretching (X is C or N)
1900 – 1500 cm-1 for C=X stretching (X is C, N, or O)
1300 -1800 cm-1 for C-X stretching (X is C, N, or O)

So, infrared spectroscopy that is basically based on molecular vibration. Covalent bond that can be considered as elastic spring that is connected with two atoms here I have shown a typical water molecule, you can see this hydrogen and oxygen they are forming this types of bonds and this bonds can have various types of movement usually the stretching the frequency the stretching frequency that is usually higher if you bend it corresponding to bending frequency it is usually higher.

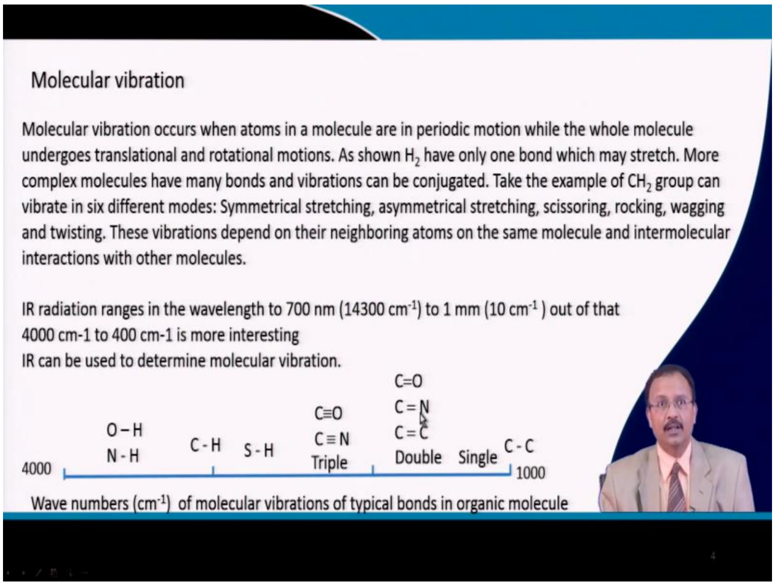
So, bonding to this hydrogen ion they have higher stretching frequencies, then if you compare it with usually heavier atoms triple bond if you consider, they have higher stretching frequency as compared to the double bonds of a polymeric material or organic base material.

And double bonds again have higher frequency than single bonds. So, triple bond they have higher frequencies than corresponding double bond and double bond is having higher frequencies as compared to the single bond.

So, some examples can be cited where one can also use the wave number which is inverse of the lambda value. So, that lambda is the wavelength of the IR radiation. So, if this molecules they are in the range of 3700 to 2500 wave number, that usually corresponds to the stretching bond of this X and H, X could be carbon, nitrogen, oxygen or sulphur.

Similarly, in the range of 2300 to 2000 it is a triple bond C X stretching, again X could be carbon and nitrogen in the range 1900 to 1500 wave number, this is C double bond X stretching and 13 to 1800 it is single bond C X stretching, it is 1300 to 1800. So, that is a general kind of picture and for analysing the IR spectra one can use it.

(Refer Slide Time: 04:07)



Molecular vibration

Molecular vibration occurs when atoms in a molecule are in periodic motion while the whole molecule undergoes translational and rotational motions. As shown H_2 have only one bond which may stretch. More complex molecules have many bonds and vibrations can be conjugated. Take the example of CH_2 group can vibrate in six different modes: Symmetrical stretching, asymmetrical stretching, scissoring, rocking, wagging and twisting. These vibrations depend on their neighboring atoms on the same molecule and intermolecular interactions with other molecules.

IR radiation ranges in the wavelength to 700 nm (14300 cm^{-1}) to 1 mm (10 cm^{-1}) out of that 4000 cm-1 to 400 cm-1 is more interesting
IR can be used to determine molecular vibration.

Wave numbers (cm^{-1}) of molecular vibrations of typical bonds in organic molecule

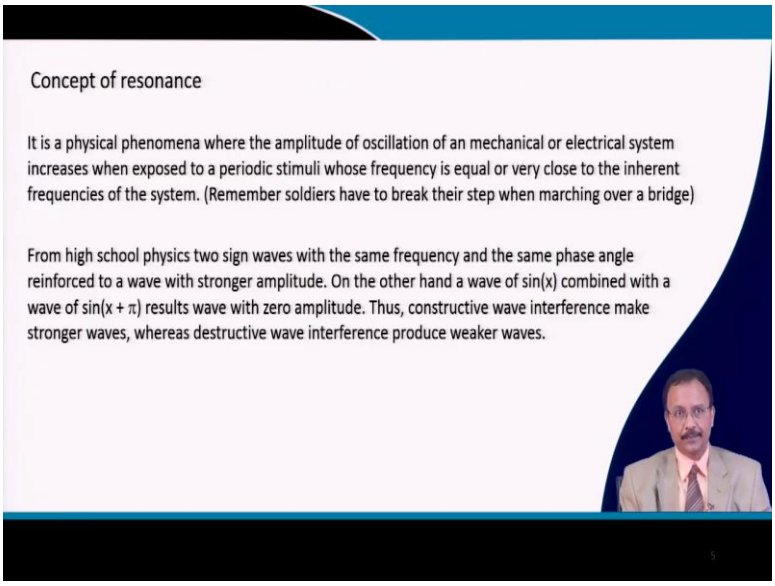
So, the molecular vibration they occurs when the atoms and molecules they are in periodic motion. The whole molecules they undergo a translation or rotational motions. So, in the last slide we have seen that hydrogen have only one bond in case of pure hydrogen which can only be stretched. So, if you consider a complex molecule, they have many bonds and vibration can be actually conjugated.

So, if you take the example of CH 2 group that vibration could be six different modes symmetrical stretching can be there, asymmetric stretching can be there or scissoring effect, rocking effect, wagging and twisting. So, this many vibrations are possible. So, it is due to the fact that the neighbouring atoms of the same molecule and the interact intermolecular reaction they can have different types of vibration mode.

So, IR radiation range that interact with this type of vibration mode and basically the IR radiation is absorbed and we will discuss a resonant effect in the next slide. So, usually the wavelength, if you consider the wavelength the 700 nanometres that is in terms of wave number it is 14300 to 1 millimetre, which is 10 wave number. So, that is important and usually the working range is 4000 wave number to 400 wave number for most of the material characterization.

So, this IR they can be used to determine the type of molecular vibration. So, this is one example if you take from 1000 to 4000. So, various types of single bond carbon carbon bond or double bond, triple bond, sulphur hydrogen. So, specific type of vibration that is defined here.

(Refer Slide Time: 06:50)



Concept of resonance

It is a physical phenomena where the amplitude of oscillation of an mechanical or electrical system increases when exposed to a periodic stimuli whose frequency is equal or very close to the inherent frequencies of the system. (Remember soldiers have to break their step when marching over a bridge)

From high school physics two sign waves with the same frequency and the same phase angle reinforced to a wave with stronger amplitude. On the other hand a wave of sin(x) combined with a wave of sin(x + π) results wave with zero amplitude. Thus, constructive wave interference make stronger waves, whereas destructive wave interference produce weaker waves.

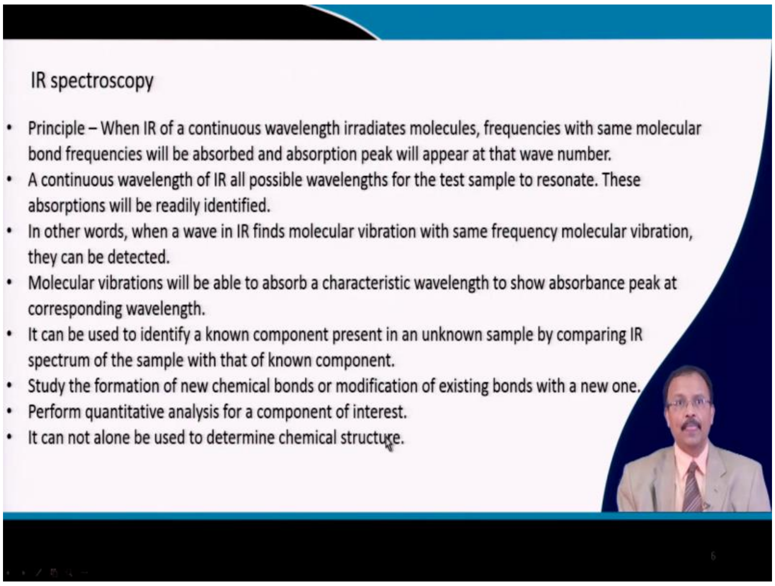
So, the physical phenomena of resonance is important in this case. So, the amplitude of oscillation of a mechanical or electrical system that they increases when they are exposed to a periodic stimuli, whose frequency is equal or very close to the natural frequency of vibration of that particular system.

So, this is a very well-known example one might have heard that soldiers they are not allowed to march on a bridge because bridge is having its natural frequency. So, if it matches with the frequency, then they start to vibrate and that can be catastrophic for the destruction of the bridge.

In fact, it happened. So, that is the concept of resonance and from the high school physics you know that two sine waves with the same frequency and the same phase angle they reinforced to a wave with stronger amplitude.

Again, if you consider a wave sin x combined with a wave of sin x plus some phase angle pi they result a wave with zero amplitude because they are out of phase. So, constructive wave interference make a stronger wave with stronger amplitude and destructive wave produces a weaker wave.

(Refer Slide Time: 08:34)



IR spectroscopy

- Principle – When IR of a continuous wavelength irradiates molecules, frequencies with same molecular bond frequencies will be absorbed and absorption peak will appear at that wave number.
- A continuous wavelength of IR all possible wavelengths for the test sample to resonate. These absorptions will be readily identified.
- In other words, when a wave in IR finds molecular vibration with same frequency molecular vibration, they can be detected.
- Molecular vibrations will be able to absorb a characteristic wavelength to show absorbance peak at corresponding wavelength.
- It can be used to identify a known component present in an unknown sample by comparing IR spectrum of the sample with that of known component.
- Study the formation of new chemical bonds or modification of existing bonds with a new one.
- Perform quantitative analysis for a component of interest.
- It can not alone be used to determine chemical structure.

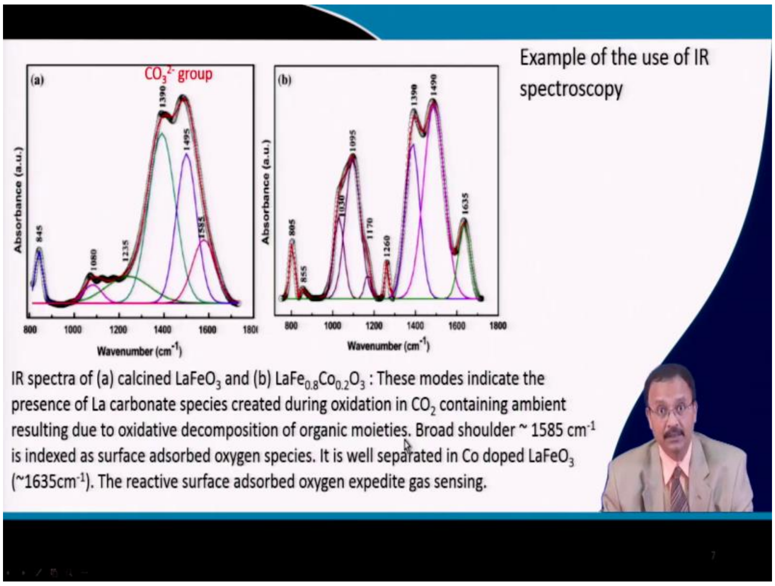
So, this resonance effect is taken in into consideration while we understand the IR spectroscopy. So, when IR a continuous wavelength irradiates a molecule, which is having a frequency with the same molecular bond frequency they will be absorbed and absorption peak will appear at that particular wave number. So, a continuous wavelength of IR all possible wavelengths for the test samples to resonate. So, this absorption will be readily identified.

So, when a IR wave they find a molecular vibration inside the material which is having the same type of frequency, they will show a absorbance peak at and that molecular vibration can be detected. So, it can be used to identify an unknown component present in the sample, once you compare the IR spectrum of the sample with a with the known component.

So, if it matches with a known component, then you can identify that that particular constituent is there in the test sample. So, study of a new chemical bond formation that is also possible along with the existing bond in the material and one can also do a quantitative analysis of this various modes of molecular vibration that is present in the crystal.

But this alone cannot be used to characterize the sample fully. So, IR spectroscopy must be used something else maybe that would be X-ray diffraction that could be some other spectroscopic technique in order to completely characterize the materials.

(Refer Slide Time: 10:45)



Example of the use of IR spectroscopy

IR spectra of (a) calcined $LaFeO_3$ and (b) $LaFe_{0.8}Co_{0.2}O_3$: These modes indicate the presence of La carbonate species created during oxidation in CO_2 containing ambient resulting due to oxidative decomposition of organic moieties. Broad shoulder ~ 1585 cm^{-1} is indexed as surface adsorbed oxygen species. It is well separated in Co doped $LaFeO_3$ (~1635cm^{-1}). The reactive surface adsorbed oxygen expedite gas sensing.

So, one example that is cited here it is a IR spectra of a lanthanum iron oxide which is perovskite oxide and this has been compared with a cobalt doped lanthanum iron oxide. So, here you can see the presence of this CO 3 kind of group. So, this is identified in fact, if this is not fully resolved, then one will have to do the deconvolution of the peak to identify this peak position.

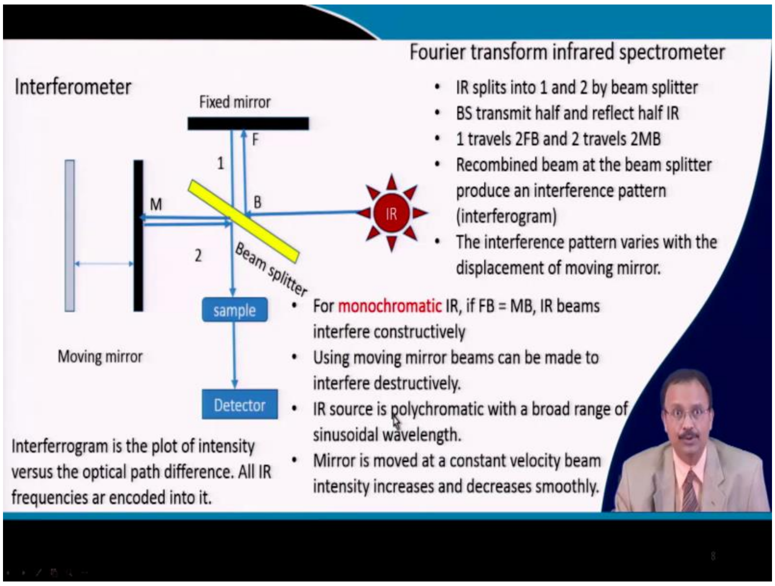
So, actually this carbonate group comes from the carbon dioxide containing ambient. So, you will have to analyse that the origination originate where from its originates. So, solely it cannot be used as a characterizing tool, but it indicates something. So, this samples were prepared in a from a wet chemical synthesis.

So, due to the decomposition of organic moieties, the ambient was rich in carbon dioxide. So, that carbonate groups form along with that you can see here a shoulder which is basically denotes a surface adsorbed oxygen species which is quite active.

So, once this doped with cobalt, then you see that this species that is more prominent here. So, the surface active oxygen species that is more prominent in cobalt doped lanthanum iron oxide sample and in fact, it was tested that compared to this and this when used as a gas sensing material, this exhibit say higher gas sensing response because of the presence of this surface active oxygen.

So, for characterizing the material and correlate it with the properties to understand the so, called structure property relationship IR spectroscopy is used.

(Refer Slide Time: 13:24)



Fourier transform infrared spectrometer

- IR splits into 1 and 2 by beam splitter
- BS transmit half and reflect half IR
- 1 travels 2FB and 2 travels 2MB
- Recombined beam at the beam splitter produce an interference pattern (interferogram)
- The interference pattern varies with the displacement of moving mirror.

Interferometer

- For monochromatic IR, if FB = MB, IR beams interfere constructively
- Using moving mirror beams can be made to interfere destructively.
- IR source is polychromatic with a broad range of sinusoidal wavelength.
- Mirror is moved at a constant velocity beam intensity increases and decreases smoothly.

Interferrogram is the plot of intensity versus the optical path difference. All IR frequencies ar encoded into it.

So, usually a Fourier transform IR spectra is used and in order to understand this Fourier transform infrared spectrometer, this inter the construction of the interferometer is important. So, here you can see that this is a IR source its having all possible kind of radiation. So, this is splitted into beam number 1 and 2 by this beam splitter.

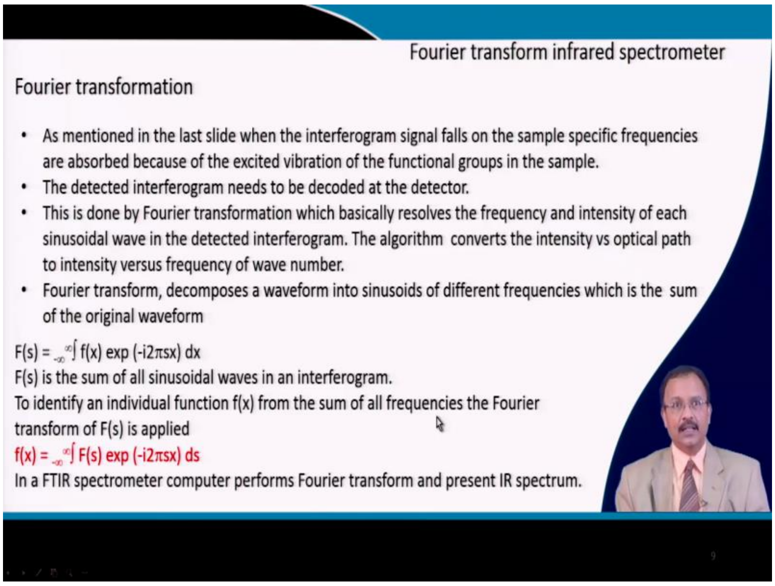
So, half is transmitted and half of the beam is reflected. So, there is one mirror here and another mirror here. So, one of the mirror is fixed and another one it is translated. So, once it is in this particular position, then this the beam splitter that half it is reflected and half part it is transmitted as I said. So, beam 1 travel this 2FB distance and beam 2 travel this 2MB this distance.

So, they are recombined in the beam splitters and since they are in phase, they are in phase to each other they produce a interference pattern. So, this interference pattern this can be changed if you change the mirror position here. So, if you start changing this mirror position. So, this can be varied, this varied and accordingly this interference pattern can be changed.

So, for a monochromatic IR beam if FB and MB they are equal, x then IR beams interfere constructively. So, once you use this moving mirror they can be made to interfere destructively. So, IR source it is polychromatic. So, they have a broad range of sinusoidal waveform. So, mirror is continuously moved as a constant velocity. So, the beam intensity you can expect increase and decrease very smoothly.

So, we can get a interferrogram that is basically a plot of intensity versus optical path difference and all IR frequencies are encoded into it.

(Refer Slide Time: 16:17)



Fourier transform infrared spectrometer

Fourier transformation

- As mentioned in the last slide when the interferogram signal falls on the sample specific frequencies are absorbed because of the excited vibration of the functional groups in the sample.
- The detected interferogram needs to be decoded at the detector.
- This is done by Fourier transformation which basically resolves the frequency and intensity of each sinusoidal wave in the detected interferogram. The algorithm converts the intensity vs optical path to intensity versus frequency of wave number.
- Fourier transform, decomposes a waveform into sinusoids of different frequencies which is the sum of the original waveform

$F(s) = {}_{-\infty}^{\infty}\int f(x) \exp(-i2\pi sx)\, dx$

F(s) is the sum of all sinusoidal waves in an interferogram.

To identify an individual function f(x) from the sum of all frequencies the Fourier transform of F(s) is applied

$f(x) = {}_{-\infty}^{\infty}\int F(s) \exp(-i2\pi sx)\, ds$

In a FTIR spectrometer computer performs Fourier transform and present IR spectrum.

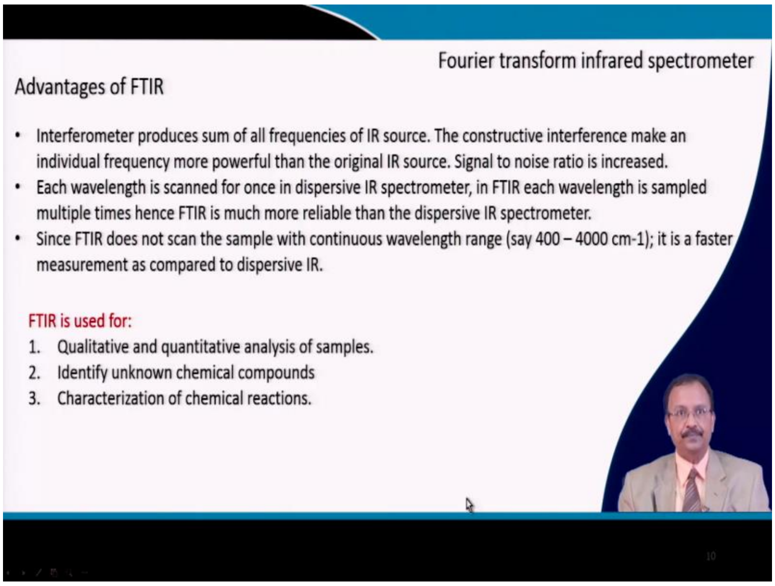
So, interferrogram is nothing but a signal I mean intensity versus path difference plot. So, when this signal falls to a sample a specific frequencies are absorbed because they are excited the vibration of the functional group present in the sample.

So, this detected interferrogram needs to be decoded at the detector shown in the last slide. This is basically done by Fourier transform which basically resolves the frequency and intensity of each sinusoidal wave in the detected interferrogram. So, the algorithm that converts the intensity versus optical path that plot to intensity versus frequency or wave number plot.

So, the Fourier transform they basically decomposes a wavelength into sinusoidal of different frequencies which are basically the sum of the original wave front. So, this Fourier transform can be defined by this formula. So, where this F s is the sum of all sinusoidal wave in the interferrogram. So, if you want to identify a individual function from the sum of all frequencies the Fourier transform is applied.

So, in a Fourier transform once you do it this is given by this relation and in an actual FTIR spectrometer computer that performs the Fourier transform present in the IR spectrum.

(Refer Slide Time: 18:12)



Fourier transform infrared spectrometer

Advantages of FTIR

- Interferometer produces sum of all frequencies of IR source. The constructive interference make an individual frequency more powerful than the original IR source. Signal to noise ratio is increased.
- Each wavelength is scanned for once in dispersive IR spectrometer, in FTIR each wavelength is sampled multiple times hence FTIR is much more reliable than the dispersive IR spectrometer.
- Since FTIR does not scan the sample with continuous wavelength range (say 400 – 4000 cm-1); it is a faster measurement as compared to dispersive IR.

FTIR is used for:

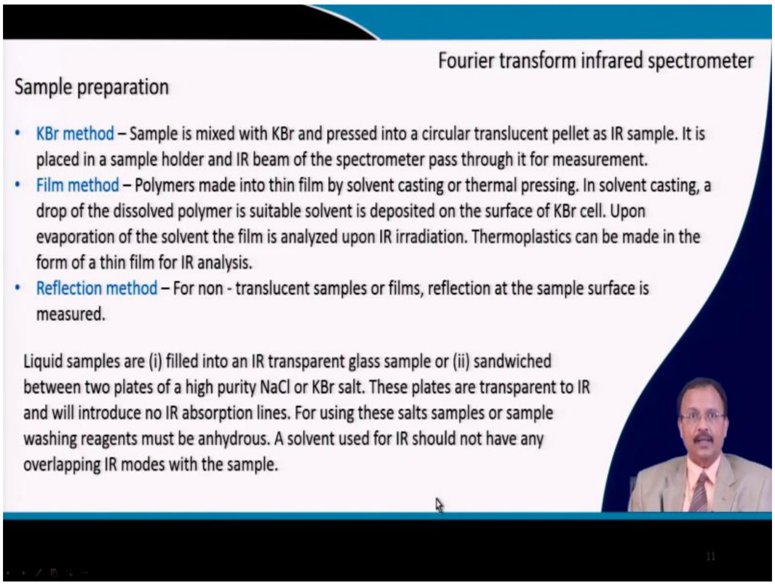
1. Qualitative and quantitative analysis of samples.
2. Identify unknown chemical compounds
3. Characterization of chemical reactions.

So, there are certain advantages of using the FTIR. So, the first one is the interferometer they produces some of all frequencies in a IR source. So, the constructive interference make an individual frequency more powerful than the original IR source because the interference is taking place.

So, as a result the signal to noise ratio is grossly increased as compared to ordinary IR spectrometer and each of this wavelength usually scanned only once for a dispersive IR spectrometer which scans from say 700 nanometre onwards in a normal IR scan. So, FTIR each wavelength is scanned multiple times and hence this one the later FTIR they are more reliable as compared to the dispersive IR spectrometer and FTIR they does not scan the sample continuous in the wavelength range say typically 400 to 4000.

So, suddenly it is much faster as compared to the dispersive IR. So, FTIR is used for qualitative as well as quantitative analysis of the sample, it is also used to identify unknown chemical compounds and characterization of chemical reaction that is also possible by using the FTIR spectrum.

(Refer Slide Time: 19:57)



Fourier transform infrared spectrometer

Sample preparation

- **KBr method** – Sample is mixed with KBr and pressed into a circular translucent pellet as IR sample. It is placed in a sample holder and IR beam of the spectrometer pass through it for measurement.
- **Film method** – Polymers made into thin film by solvent casting or thermal pressing. In solvent casting, a drop of the dissolved polymer is suitable solvent is deposited on the surface of KBr cell. Upon evaporation of the solvent the film is analyzed upon IR irradiation. Thermoplastics can be made in the form of a thin film for IR analysis.
- **Reflection method** – For non - translucent samples or films, reflection at the sample surface is measured.

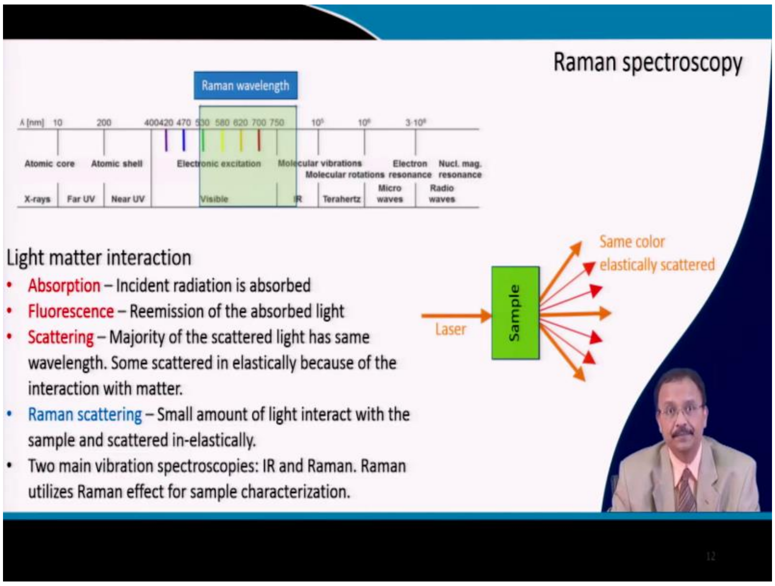
Liquid samples are (i) filled into an IR transparent glass sample or (ii) sandwiched between two plates of a high purity NaCl or KBr salt. These plates are transparent to IR and will introduce no IR absorption lines. For using these salts samples or sample washing reagents must be anhydrous. A solvent used for IR should not have any overlapping IR modes with the sample.

Sample preparation usually is done either by KBr method when this KBr which does not absorb IR that is mixed with the sample, it is pressed in the form of a pellet and then IR spectra is recorded. For polymers a film can be prepared and that can be directly analysed or you can put a drop of this polymer solution onto the KBr thing KBr pellet and the resulting film can be analyzed.

If the sample is non translucent then the reflection mode also can be used. Liquid sample usually they are placed into a higher transparent glass sample, holder or it can be sandwiched between two plus two plates of highly pure sodium chloride or KBr and this plate this salts are transparent to IR.

So, using the salt sample one should be cautious that the sample should be anhydrous otherwise the water will start react with it and also if you are using a particular solvent, that solvent also should not give you any IR band otherwise many spurious line will come and it will be difficult for you to analyse the IR spectrum.

(Refer Slide Time: 21:36)



Raman spectroscopy

Light matter interaction

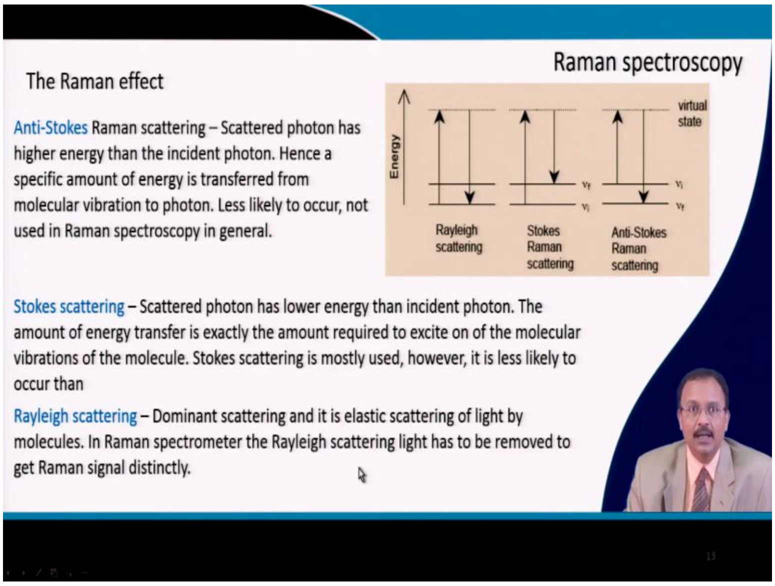
- Absorption – Incident radiation is absorbed
- Fluorescence – Reemission of the absorbed light
- Scattering – Majority of the scattered light has same wavelength. Some scattered in elastically because of the interaction with matter.
- Raman scattering – Small amount of light interact with the sample and scattered in-elastically.
- Two main vibration spectroscopies: IR and Raman. Raman utilizes Raman effect for sample characterization.

So, another spectroscopy which is something similar to IR spectroscopy, but this is a bit different that is Raman spectra where the scattering of light it is important. We have already talked about absorption incident radiation is absorbed we talked about fluorescence where the reemission occur in the absorbed light. So, here in this case scattering is important. So, majority of the scattered light has the same wavelength. So, it is an elastic type of scattering.

So, some scattered in elastically because of its interaction with the matter. So, Raman scattering is a small amount of light interact with the sample and scattered in elastically. So, two different types of vibration mode is important and usually the wavelength in the visible range that is chosen for a Raman spectrum spectroscopy, although UV Raman is nowadays also playing a major role in material characterization, but usually the monochromatic laser light in this visible wavelength is used.

So, two main types of Raman spectroscopy is there, we will be talking about it and as far as the IR and Raman they are complementary to each other.

(Refer Slide Time: 23:10)



Raman spectroscopy

The Raman effect

Anti-Stokes Raman scattering – Scattered photon has higher energy than the incident photon. Hence a specific amount of energy is transferred from molecular vibration to photon. Less likely to occur, not used in Raman spectroscopy in general.

Stokes scattering – Scattered photon has lower energy than incident photon. The amount of energy transfer is exactly the amount required to excite on of the molecular vibrations of the molecule. Stokes scattering is mostly used, however, it is less likely to occur than

Rayleigh scattering – Dominant scattering and it is elastic scattering of light by molecules. In Raman spectrometer the Rayleigh scattering light has to be removed to get Raman signal distinctly.

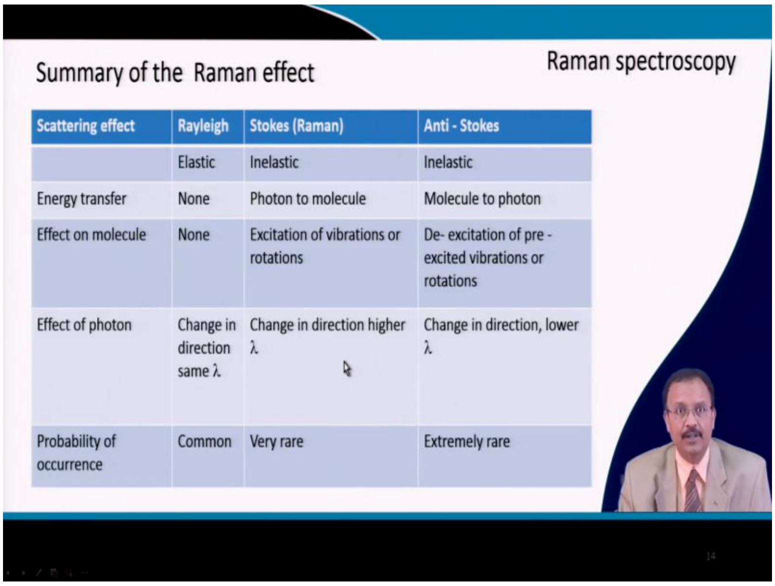
So, in the Raman effect as I said that the Rayleigh scattering you have an elastic type of scattering. So, the energy of the incident radiation they do not change, but in case of anti-stoke Raman scattering scattered photon they have usually has higher energy as compared to the incident photon. So, they have the higher energy than the incident photon and in a specific amount of energy is transferred from the molecular vibration to the photon.

So, this is not a very common phenomena to occur. So, it is a bit uncommon, but most common part is the stokes scattering. So, this scattered photon has lower energy as compared to the incident form.

So, the amount of energy transfer is exactly the amount required to excite on the molecular vibration of the molecules. So, the stokes scattering is mostly used; however, it is less likely to occur then the so, called Rayleigh scattering it is a dominant scattering mechanism and this elastic scattering of light by the molecules in the test sample.

So, in Raman spectrometer the Rayleigh scattering light has to be removed to get the Raman signal which is very weak. So, distinct identification of the Raman signal requires the removal of these Rayleigh scattering one.

(Refer Slide Time: 24:59)



Summary of the Raman effect

Raman spectroscopy

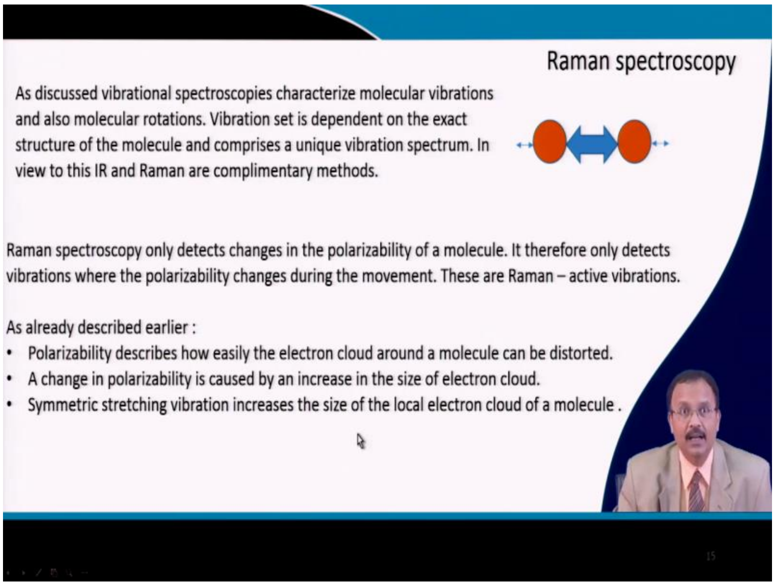
Scattering effect	Rayleigh	Stokes (Raman)	Anti - Stokes
	Elastic	Inelastic	Inelastic
Energy transfer	None	Photon to molecule	Molecule to photon
Effect on molecule	None	Excitation of vibrations or rotations	De- excitation of pre - excited vibrations or rotations
Effect of photon	Change in direction same λ	Change in direction higher λ	Change in direction, lower λ
Probability of occurrence	Common	Very rare	Extremely rare

So, if you consider the scattering effect then energy transfer for Rayleigh scattering this is elastic in nature for stokes and anti-stokes both are inelastic. So, there is no energy transfer here, but in case of strokes scattering the energy is transferred from photon to the molecules in the sample and in case of anti-stokes from molecule to photon it transfers. So, it gains energy which is not very common.

So, it does not have any effect in case of Rayleigh scattering here, but in case of stokes it excitation of the vibration or rotation that takes place and in case of anti-stokes the de-excitation of the pre-existed vibrations or rotation that takes place if you consider in the effect of photon.

So, it only changes the direction in case of Rayleigh scattering and it changes the direction to higher lambda because the energy is lost and changes the direction and lambda is lowered because of the gain in energy. Probability of occurrence is very common in case of Rayleigh scattering and stokes is relatively rare and anti-stokes are extremely rare to occur.

(Refer Slide Time: 26:43)



Raman spectroscopy

As discussed vibrational spectroscopies characterize molecular vibrations and also molecular rotations. Vibration set is dependent on the exact structure of the molecule and comprises a unique vibration spectrum. In view to this IR and Raman are complimentary methods.

Raman spectroscopy only detects changes in the polarizability of a molecule. It therefore only detects vibrations where the polarizability changes during the movement. These are Raman – active vibrations.

As already described earlier :

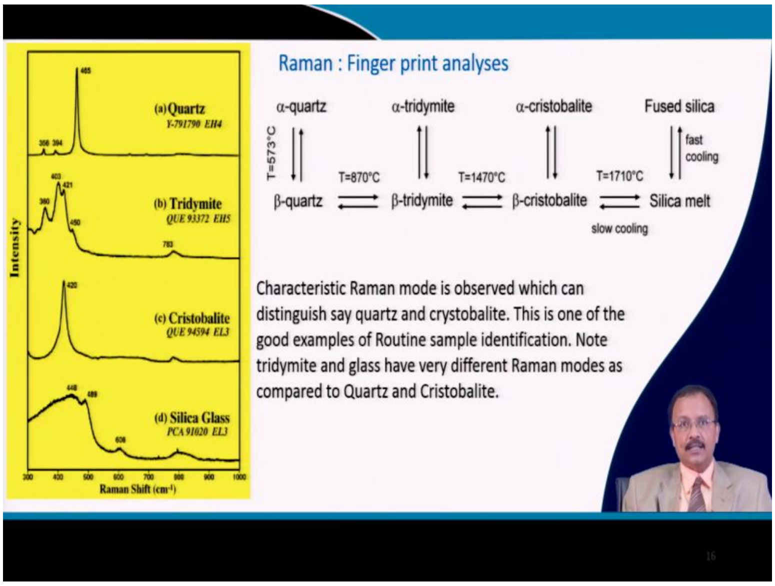
- Polarizability describes how easily the electron cloud around a molecule can be distorted.
- A change in polarizability is caused by an increase in the size of electron cloud.
- Symmetric stretching vibration increases the size of the local electron cloud of a molecule .

So, as we have discussed vibrational spectroscopy characterize the molecular vibration and also the molecular rotation. So, vibration sets depends on the exact structure of the molecule and comprises a unique vibrational spectrum in view to this IR and Raman are complementary in nature.

Raman spectroscopy only detects changes in the polarizability you know what is polarizability. So, it only detects the vibrations were the polarizability changes during its movement. So, these are called Raman active vibrations. So, polarizability described how easily because we are talking about the optical range of vibration, the electron cloud along the molecule can be distorted that already I have talked about in my earlier lectures.

So, a change in polarizability is caused by an increase in the size of the electron cloud and symmetric stretching vibration increases the size of this local electron cloud of the molecule and that can be easily detected by the Raman spectroscopy.

(Refer Slide Time: 28:13)



Raman : Finger print analyses

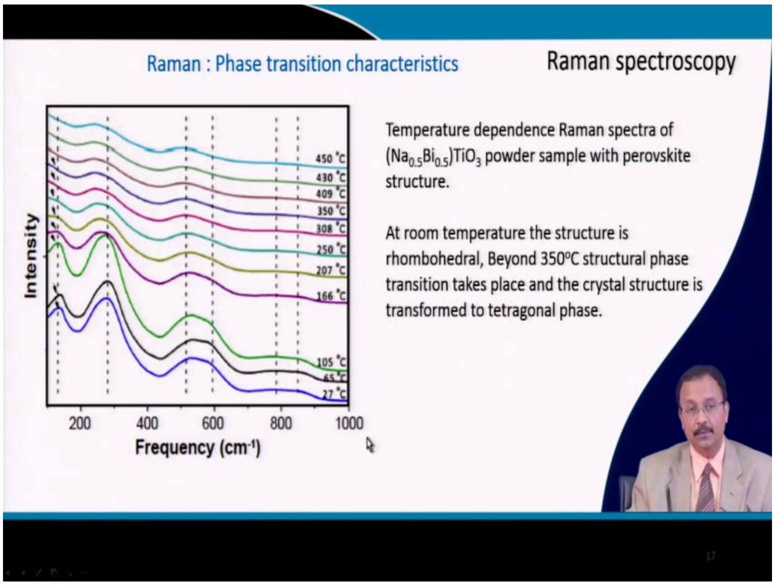
$$\begin{tikzcd}
\alpha\text{-quartz} \arrow[d, shift left] & & \alpha\text{-tridymite} \arrow[d, shift left] & & \alpha\text{-cristobalite} \arrow[d, shift left] & & \text{Fused silica} \arrow[d, shift left] \\
\beta\text{-quartz} \arrow[u, shift left, "T=573^{\circ}C"] \arrow[rr, shift left, "T=870^{\circ}C"] & & \beta\text{-tridymite} \arrow[u, shift left] \arrow[ll, shift left] \arrow[rr, shift left, "T=1470^{\circ}C"] & & \beta\text{-cristobalite} \arrow[u, shift left] \arrow[ll, shift left] \arrow[rr, shift left, "T=1710^{\circ}C"] & & \text{Silica melt} \arrow[u, shift left, "\text{fast cooling}"'] \arrow[ll, shift left, "\text{slow cooling}"]
\end{tikzcd}$$

Characteristic Raman mode is observed which can distinguish say quartz and crystobalite. This is one of the good examples of Routine sample identification. Note tridymite and glass have very different Raman modes as compared to Quartz and Cristobalite.

I will cite certain example. So, first Raman can be used as a fingerprint analysis. You know polymorphic phase transformation of quartz, from quartz to tridymite, to tridymite to cristobalite and finally, the melt. If you compare the Raman spectra so, the characteristics modes are observed for each of this phase.

So, you can distinguish from quartz to the other polymorphic form for example, cristobalite and molten silica is having very different Raman spectra. So, that is routinely done and also for certain pharmaceutical use it is a very common technique it is used as a fingerprint. So, that is Raman is used.

(Refer Slide Time: 28:59)



Raman : Phase transition characteristics

Raman spectroscopy

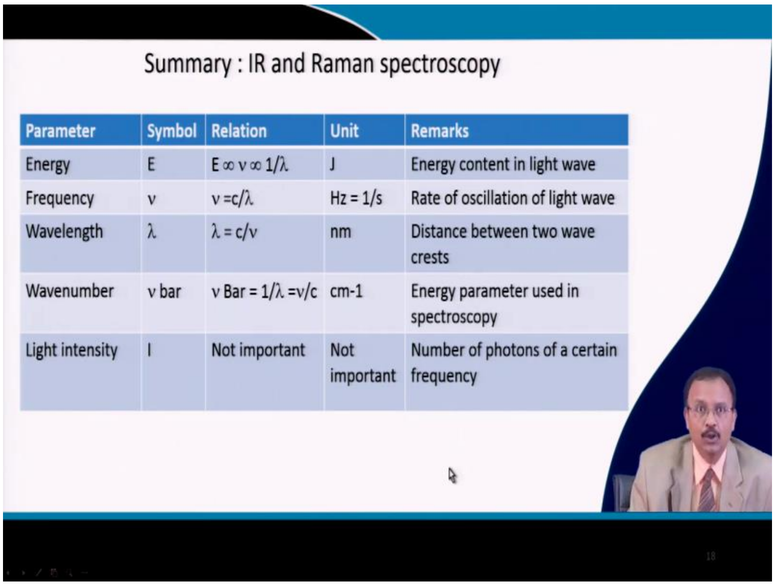
Temperature dependence Raman spectra of $(Na_{0.5}Bi_{0.5})TiO_3$ powder sample with perovskite structure.

At room temperature the structure is rhombohedral, Beyond 350ºC structural phase transition takes place and the crystal structure is transformed to tetragonal phase.

Another example one can cite that from the temperature dependence of the Raman spectra one can easily identify the phase transformation. One example I have cited for sodium bismuth titanium oxide. They are having perovskite structure at room temperature if you see the structure is a rhombohedral crystal structure and the roman mode changes and beyond 350 this structural phase transformation takes place in the crystal structure transform to a tetragonal phase.

By analysing the Raman mode one can identify the phase transition this is one of the good method to characterize the phase transformation in non-metallic materials.

(Refer Slide Time: 29:52)



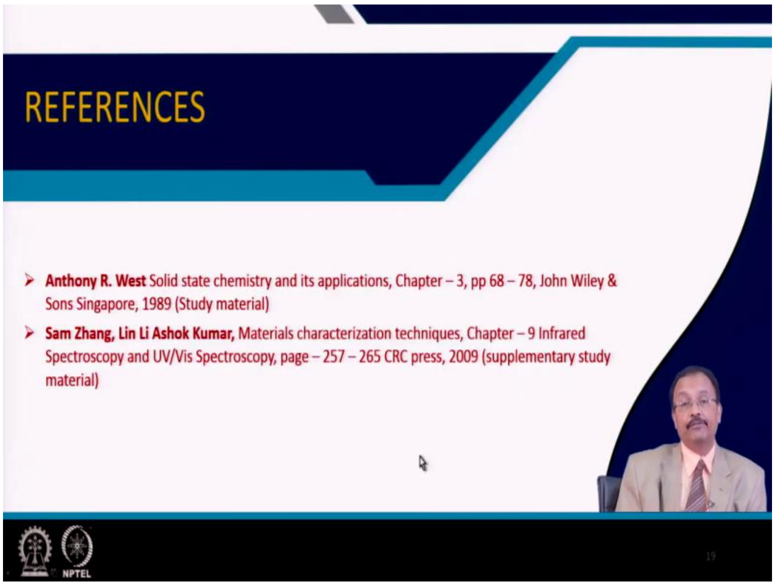
Summary : IR and Raman spectroscopy

Parameter	Symbol	Relation	Unit	Remarks
Energy	E	E ∞ ν ∞ 1/λ	J	Energy content in light wave
Frequency	ν	ν =c/λ	Hz = 1/s	Rate of oscillation of light wave
Wavelength	λ	λ = c/ν	nm	Distance between two wave crests
Wavenumber	ν bar	ν Bar = 1/λ =ν/c	cm-1	Energy parameter used in spectroscopy
Light intensity	I	Not important	Not important	Number of photons of a certain frequency

So, if I now summarize the IR and Raman spectra, the parameters which are important are energy, frequency, wavelength, wave number and light intensity. Light intensity they are not important for any of these two techniques, but energy content in the life light wave that is important for Raman frequency.

That is the rate of oscillation of the incident radiation, wavelength it can also be characterized. So, that is basically the distance between two crest or two trough of a sinusoidal kind of wave and wave number that is used as a energy parameter that is used for both these two types of spectroscopy and they are complementary in nature and very useful for characterizing the vibration mode of the non-metallic materials in particular.

(Refer Slide Time: 31:00)



REFERENCES

- **Anthony R. West** Solid state chemistry and its applications, Chapter – 3, pp 68 – 78, John Wiley & Sons Singapore, 1989 (Study material)
- **Sam Zhang, Lin Li Ashok Kumar,** Materials characterization techniques, Chapter – 9 Infrared Spectroscopy and UV/Vis Spectroscopy, page – 257 – 265 CRC press, 2009 (supplementary study material)

So, the reference is the book by Anthony R West and chapter number 3 and the book by Zhang Lin and Ashok Kumar Material characterization chapter 9, where the IR spectroscopy is described.

(Refer Slide Time: 31:22)

CONCLUSION

- Principles of Raman spectroscopy
- Fourier transform infra-red spectroscopy
- Applications of IR spectroscopy
- Raman effect and principles of Raman spectroscopy
- Applications of Raman spectroscopy

So, in this particular lecture we talked about principles of Raman spectroscopy, then Fourier transform infrared spectroscopy, application of IR spectroscopy, then Raman effect and the details of the Raman spectroscopy used for various types of material characterizations.

Thank you for your attention.