

Using Raman Spectroscopy to Identify Unknown Materials

Siham M. Hassen^{#1}, Manahil E.E.Mofdal^{*2}

Collage of education, department of physics Peace University, Alfula , Sudan
Collage of education, department of physics, West- Kordofan University, anhood, Sudan

Abstract

Raman Spectroscopy is one of the most essential laser spectroscopic methods based on elastic scattering when monochromatic light interact with molecule and energy of photon shifts to lower or higher frequencies are known as Raman shift . In this work Raman Spectroscopy was used to identification unknown Materials, the sample was irradiated using 2mW double frequency Nd-YAG laser with 532 nm at room temperature , the spectra database was used for the spectral analysis of the Raman shift of these sample , the result obtained show the spectra are appeared of unknown sample it's the spectra of zinc oxide (ZnO).

Keywords - Unknown Materials, identification, Raman Spectroscopy

I. INTRODUCTION

Raman spectroscopy is a spectroscopic technique used to study vibrational, rotational, and other low-frequency modes in a system. It is widely used to provide information on chemical structures and physical forms, to identify substances from the characteristic spectral patterns (fingerprinting), and to determine quantitatively or semi-quantitatively the amount of a substance in a sample. So, thinking in

Raman spectra like a fingerprint it is possible identify materials through the study of their Raman spectra [1]. The it's based on inelastic scattering of light t by matter. When a photon of light, too low in energy to excite an electronic transition from one state to another, strikes a molecule, it can be scattered in one of three different ways. Firstly the incident photon can be scattered elastically, i.e. the incident photon energy is the same as the scattered photon energy. This is also known as Rayleigh scattering. The incident photon can also be in elastically scattered by either losing energy to, or removing energy from the molecule. The photon that loses energy to the molecule under goes what is known as Stokes scattering and this excess energy within the molecule appears as vibrational energy in the form of a phonon, whereas the photon which gains energy from the molecule experiences anti-Stokes scattering, and the molecule loses vibrational energy in the form of a phonon as all indicated in figure 1.1 [2]. At room temperatures, most molecular vibrations are in the ground state and thus the anti-Stokes transitions are less likely to occur than the Stokes transitions, resulting in the Stokes Raman scattering being more intense. For this reason, it is usually the Stokes Raman spectrum that is usually studied [3].

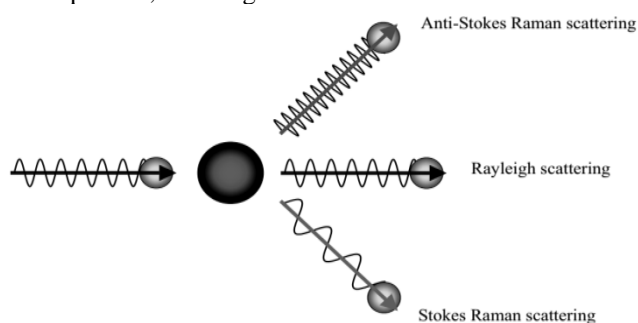


Figure (1-1): diagram showing of Raman scattering and Rayleigh scattering

A. Page layout

page layout of this paper include introduction of laser Raman spectroscopy, basic principles of Raman spectroscopy , experimental part which includes the experimental setup, and experimental procedure , results, analysis, discussion and conclusions .

III. THEORY OF RAMAN SCATTERING

As discussed above the incident electromagnetic radiation was induced dipole moment during the light interaction with material the strength of the induced dipole moment, P , is given by

$$P = \alpha E \quad (1)$$

where α is the polarizability and E is the strength of electric field of the incident EM wave. For light of frequency w_0 , the magnitude of the electric field may be written:

$$E = E_0 \cos 2\pi w_0 t \quad (2)$$

Thus, the induced dipole moment oscillates in phase with the applied field:

$$P = \alpha E_0 \cos 2\pi w_0 t \quad (3)$$

Because the ability to perturb the local electron cloud of a molecular structure depends on the relative location of the individual atoms, it follows that the polarizability is a function of the instantaneous position of constituent atoms. For any molecular bond, the individual atoms are confined to specific vibrational modes, in which the vibrational energy levels are quantized in a manner similar to electronic energies. The vibrational energy of a particular mode is given by

$$E_{\text{vib}} = (n + \frac{1}{2}) h w_{\text{vib}} \quad (4)$$

Where h is Planck's constant, w_{vib} is the vibrational ground frequency, and n is the vibrational quantum number controlling the energy of that particular vibration and it has values of 0, 1, 2, 3, etc. The physical displacement dQ of the atoms about their equilibrium position due to the particular vibrational mode may be expressed as

$$dQ = Q_0 \cos 2\pi w_0 t \quad (5)$$

where Q_0 is the maximum displacement about the equilibrium position. For a typical diatomic molecule, the maximum displacement is about 10% of the bond length. [4]. For such small displacements, the polarizability may be approximated by a Taylor series expansion, namely

$$\alpha = \alpha_0 + (d\alpha/dq)_0 (r-r_0) + \dots \quad (6)$$

where α_0 is the polarizability of the molecular mode at equilibrium position. Based on the vibrational displacement of Eq. (5), the polarizability may be given as

$$\alpha = \alpha_0 + (d\alpha/dq) \cos(2\pi w_i) \quad (7)$$

Finally, Eq. (7) may be substituted into Eq. (3), which yields

$$P = \alpha_0 E_0 \cos 2\pi w_0 t + (d\alpha/dq) q_0 E_0 \cos 2\pi [(w_0 + w_i) t + (w_0 - w_i) t] \quad (8)$$

Equation (8) reveals that the induced dipole moment is created at three distinct frequencies, namely w_0 , $(w_0 + w_i)$, and $(w_0 - w_i)$, which results in scattered radiation at these same three frequencies. The first scattered frequency is responsible for Rayleigh scattering at w_0 while the second and third terms describe inelastic Raman scattering shifted by the frequency of the vibration, w_0 , to frequencies which are higher (anti-Stokes, $w_0 - w_i$) and lower (Stokes, $w_0 + w_i$), respectively than the incident light frequency. In addition, equation (2.6) shows that for Raman scattering to occur the condition is:

$$d\alpha/dQ \neq 0 \quad (9)$$

That is, the polarizability of the molecule must change during a vibration if that vibration is to be Raman active. If the polarizability does not change during a vibration, this coefficient is zero, and the vibration is not Raman-active [5].

IV. INSTRUMENT

Microscope Raman spectrometer model burker sentra incorporates many features that make it the ideal choice for the analytical laboratory as multiples wavelength (532nm, 785nm,...), High wavenumber accuracy, All-in-one compact, confocal design and Removal of fluorescence background. burker sentra micro Raman spectrometer was used to identify unknown chemical specie at room temperature at wave length 532nm and out power 2Mw shown in figure (1-2)

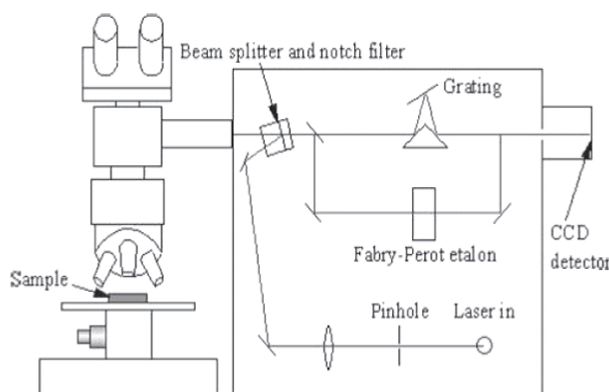


Figure (1-2): shows the structure diagram of burker sentra micro Raman spectrometer

V. THE EXPERIMENTAL PROCEDURE

the spectra properties of the sample was investigated in order to know what is material. Laser Raman spectra was collected at room temperature using burker sentra micro Raman spectrometer. Frequency doubled Nd-YAG laser was used to excite the samples. The laser power was set at 2mW (is recommended; high power settings can burn samples). The recording time was set at between 20 and 30 s. The powder sample employed was placed on the microscope stage of the Olympus confocal Raman microscope attached to the spectrograph. The radiation passes through pin holes and lens. The beam is directed to the microscope (Olympus 100X objective) via mirrors and then directed into the microscope via one beam splitter and holographic

notch filter, which rejects any Rayleigh scattering. The backscattered Raman radiation is filtered through the spectrograph entrance and then onto the CCD detector and computer.

VI. RESULT AND DISSECTION

Figure (1-3) show Raman spectrum of sample after irradiation with Nd-YAG laser with wavelength of 532 nm and 2mW output power. The spectrum shows clear peaks and by comparison with the vibrations recorded in some references we found that these vibrations are attributed to components of zinc oxide that are listed in table 1

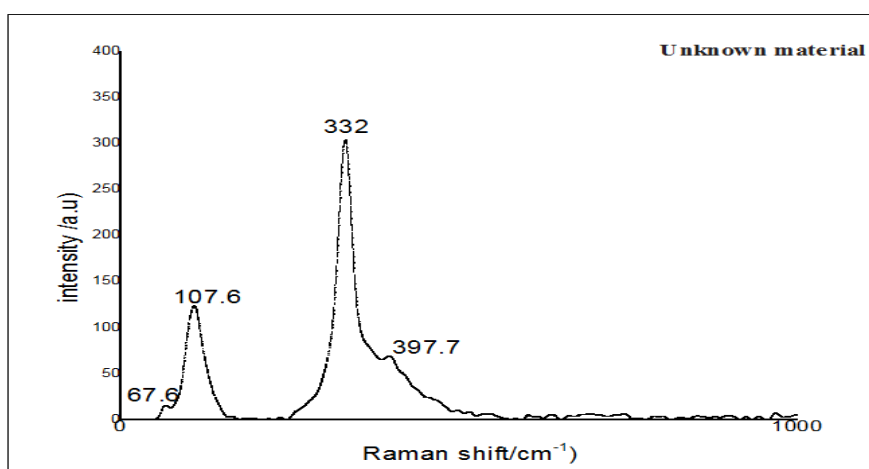


Fig 1-3 :Raman spectrum of unknown material in the range from 0 to 1000 cm^{-1}

Table 1.Raman spectrum data analysis of unknown materials

Raman shift (cm^{-1})	Intensity (a.u)	Assignment	References
67.6	33.44	Zn-O	(Kafka, K.R., 2017)
107.5	136.1	Zn-O	(Damen, et al. 1966)
397.7	90.27	Zn-O	(Damen, et al. 1966, Arguello , C.A.,et al.1969)
332	323.07	Zn-O	(Arguello, C.A.,et al.1969)

in addition must of Raman shift for vibration modes of unknown chemical material are appeared between 0- 1000 cm^{-1} . Low intensity band appeared at 67.6 was assigned to zinc oxide according to (Kafka, K.R., 2017)[6]. Another band appeared at 107.5 cm^{-1} was attributed to zinc oxide and mentioned in the literatures (Damen, et al. 1966)[7]. And high intensity band appeared at 332 cm^{-1} was assigned to zinc oxide according to (Arguello, C.A.,et al.1969)[8]. at last band at 397.7 cm^{-1} is noticed was assigned to zinc oxide and this agreed with the results of other research (Damen, et al. 1966, Arguello , C.A.,et al.1969) [7,8].

VII.CONCULIONS

The result presented in this work show that Raman spectroscopy is technical fast and efficient method to indentify unknown materials and Raman microscope for imaging and comparing the images with the spectra.

ACKNOWLEDGEMENTS

First and foremost I thank Allah, for guiding and give me strength to bring forth to light this thesis , I wish to thank the ministry of high

educational and research of Sudan for supporting this research, All thanks, respect and sincere gratitude and appreciation are directed to my supervisor Professor Nafie Abd Allattief Almuslet, for guiding and support.

REFERENCES

- [1] Isaac Hermosilla Rodríguez,. "Automatic Identification of Raman Spectra." (2012).
- [2] Ian ,Robertson,. Applications of Raman spectroscopy and chemometrics to semiconductor process control. Diss. Dublin City University, 2000.
- [3] Siegfried ,Wartewig .IR and Raman spectroscopy: fundamental processing. John Wiley & Sons, 2006.
- [4] Hahn, D. W, Hahn . (2007). Raman scattering theory. Department of Mechanical and Aerospace Engineering, University of Florida.
- [5] Gardiner, Derek J, Gardiner .. "Introduction to Raman scattering." Practical Raman Spectroscopy. Springer, Berlin, Heidelberg, 1989. 1-12.
- [6] Kyle RP, Kafka. Laser-Induced Damage with Femtosecond Pulses. Diss. The Ohio State University, 2017.
- [7] B. Tell Co, S. P. S. Porto and Damen, T.,,. "Raman effect in zinc oxide." Physical Review 142.2 (1966): 570.
- [8] Sérgio Pereira da Silva Porto, Denis L. Rousseau ,and Arguello, C. A.,. "First-order Raman effect in wurtzite-type crystals." Physical Review 181.3 (1969): 1351.