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Review Paper

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A Review on Portable Spectrometry

Jewel Merry Jijo[1*], Jose George[2], K.J. John[3], Parvathy R.[4], Safi Sulaiman[5], Sandra John[6], Godwin D.[7]

[1,2,3,4,5,6,7]Department of Electronics and Communication Engineering, Amal Jyothi College of Engineering, APJ Abdul Kalam Technological University, Kottayam, India

[*]Corresponding Author: jewelmej@gmail.com, Tel.: +91 9447615575

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***Abstract*—**Spectrometers are one of the most important optical analytical tools used to separate the spectral components of a physical occurrence and they are used in different fields of research as well as for educational purposes. Various spectrometers have been developed after extensive research and improvement however conventional spectrometers are very pricey paving way to the development of portable spectrometers which are affordable for research and educational purposes in individual university labs. This review covers various types of spectroscopy and their corresponding portable spectrometers.

Keywords—Spectrometer, Portable Spectrometer, Spectroscopy

I. INTRODUCTION

Spectroscopy is the study of interaction between the electromagnetic radiation and the matter, where the matter can be atoms, molecules or ions. The nature of the interaction can be absorption, emission or scattering. Spectroscopy helps in the study of matter with respect to qualitative and quantitative study. The effect of electromagnetic radiation on interaction with the matter depends on the energy associated with the radiation, like very energetic radiations such as UV and x-ray may cause an electron to be emitted from the molecule causing electronic transitions whereas the infrared radiation has lower energy and they cause molecular vibrations [1]. Microwave radiation is not as energetic as the infrared radiation and it can neither induce electronic transitions nor can cause molecular vibrations but only results in molecular rotation. Depending on the interaction between the electromagnetic radiation and the matter, spectroscopy can be classified into absorption spectroscopy, emission spectroscopy, scattering spectroscopy and luminescence spectroscopy.

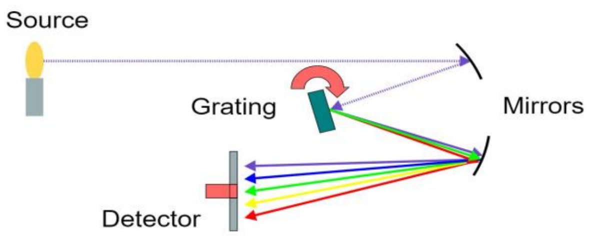

Figure 1. Basic Spectrometer

In absorption spectroscopy, the electromagnetic radiation is absorbed by an atom or a molecule, which makes the atom or the molecule undergo transformation from the lower energy state to the higher energy state [2]. When a monochromatic light falls on a substance, the light may be reflected, absorbed or scattered by the substance which helps in measuring certain physical properties by examining the amount of light scattered by the substance at certain wavelengths. Raman spectroscopy is light scattering spectroscopy. Emission spectroscopy measures the wavelength of the photons emitted by the atom or the molecule during their transformation from the higher energy state to the lower energy state where the emission can be induced by the energy sources like flame or electromagnetic radiation. Luminescence spectroscopy is one of the most selective and sensitive methods for analysing inorganic and organic compounds [3]. Fluorescence spectroscopy is used to analyse fluorescence from a substance, where a light beam, usually an UV radiation, excites electrons in molecules of a compound that causes them to emit light not always in the visible spectrum.

II. RELATED WORK

TYPES OF SPECTROSCOPY

2.1 UV - VISIBLE SPECTROSCOPY

Ultraviolet region in the electromagnetic spectrum ranges from 10nm to 400nm whereas the visible region from 400nm to 800nm. UV - visible spectroscopy is an absorption spectroscopy, which is used for attenuation of the light beam passing through a substance or that got reflected from the substance [4]. The basic principle behind the UV - visible spectroscopy is the transformation of the electron from the lower energy to the higher energy state, when a molecule absorbs ultraviolet light.

2. 2 FLUORESCENCE SPECTROSCOPY

Fluorescence spectroscopy occurs when a light beam, usually a UV light, excites the electrons in the molecule of the substance causing the emission of light, typically at a lower energy level [5]. The devices that measure fluorescence are called the fluorometer or the fluorimeter.

2. 3 RAMAN SPECTROSCOPY

Raman spectroscopy is a non-destructive analysis technique which is in accordance with the study of vibrational modes of a molecule, which helps to distinguish different components. When a monochromatic light falls on a molecule, most part of the radiation will be transmitted while some part of the radiation will be scattered at an angle 90° from that of the incident radiation by the molecule [6]. Scattering can be elastic or inelastic. In elastic scattering, the frequency of the scattered radiation is the same as that of the incident radiation, that is, there is no change in the radiation after scattering. This is also known as the Rayleigh scattering. Most of the light is scattered without any change in the frequency, it undergoes elastic scattering. In inelastic scattering, there is a change in the frequency of the radiation after scattering. It is also known as the Raman scattering. Only one percent of the radiation undergoes inelastic scattering, that is, the incident light frequency is not the same as the scattered light frequency. In accordance with the difference between the incident light frequency and the scattered light frequency, Raman spectroscopy can be classified into two types. When the scattered light frequency is lower than the incident light frequency, it is called as the stokes scattering and the lines visible are known as the Stokes lines whereas if the scattered light frequency is higher than the incident light frequency, it is called as the anti-stokes scattering and the lines visible are termed as the anti-Stokes lines [7].

In the Rayleigh scattering, the molecule in the ground state will absorb the incident light and will be excited to the virtual state and when it emits the radiation it goes back to the ground state and there will not be any net change in the incident energy and the scattered energy whereas in the stokes scattering, the molecule at the ground state will absorb the incident light and will be excited to the virtual state and when it emits the radiation it goes back to another state above the ground state called as the first excited state and as a result, the intensity of the scattered radiation is lower than that of the incident radiation [8]. When the molecule at the first excited state absorbs the incident light, it will be excited to the higher level state and it will fall back to the ground state when it emits the radiation. Thus, the scattered light frequency will be higher than the incident light frequency resulting in the anti-stokes scattering. There are many disadvantages with Raman spectroscopy. One among them is the weak nature of the Raman effect, leading to its low sensitivity, making it difficult to measure the substances at low concentration. Another major disadvantage is it's low scattering cross-section which is only about one in 10^2 or 10^6. SERS is the surface enhanced Raman spectroscopy, introduced in the year of 1973 has attracted a lot of attention because of its simple Operation, fast detection speed, high sensitivity and also it's remarkable ability to provide the fingerprint molecular information about the analytes.

2. 4 X-RAY SPECTROSCOPY

X-ray spectroscopy is the technique in which the chemical and the elemental properties of an object are found using x-ray excitation. The x-ray emission analysis provides the qualitative results of composition of elements of the specimen. The principle is that the electrons will be transformed from the lower energy state to the higher energy state, when an atom is bombarded with high energy particles [9]. When this electron returns to the lower energy state, the previously absorbed energy is released in the form of a photon, which is the characteristic for element [10]. The two main techniques for this analysis are energy-dispersive X-ray spectroscopy(EDS) and wavelength dispersive X-ray spectroscopy(WDS). EDS will measure the energy of incoming photons while WDS will measure the wavelength diffracted by the crystal. An x-ray spectrometer consists of an x-ray tube, collimator, monochromators and detectors [11].

2. 5 IR SPECTROSCOPY

Infrared Spectroscopy is associated with the infrared region of the electromagnetic spectrum. In the IR region, the wavelength of the light is longer and has lower frequency. The infrared region consists of three regions namely near, mid and far infrared regions. The near infrared region is a higher energy region which can excite the harmonic vibrations. The mid infrared region is used for the study of fundamental vibrations and the associated rotational-vibrational structure whereas the far infrared region has reduced energy level and is used for the rotational spectroscopy [12]. These absorptions are resonant frequencies i.e., frequency of absorbed light matches with frequency of bond of the compound. A molecule can vibrate in many ways called vibrational modes. The band is in the Raman spectrum, if the molecule is symmetrical in nature and not in the IR spectrum whereas the band is in the IR spectrum, if they are unsymmetrical diatomic molecules. More complex molecules are found to have many bonds and their vibrational spectra are more complex thus have many peaks in their IR spectra. The instruments used in spectroscopy are dispersive infrared spectrometer and Fourier transform infrared spectrometer. Dispersive infrared spectrometer is mainly composed of radiation source, monochromator and detector. Dispersive infrared spectrometer examines component frequencies individually. This slows down the speed and also reduces the sensitivity. Fourier transform infrared (FTIR) is capable of handling all frequencies simultaneously with high throughput The radiation sources of the dispersive infrared spectrometer can be used in FTIR spectrometers too but instead of the monochromator in the dispersive spectrometer, FTIR spectrometer uses interferometer.

Table 1. TYPES OF SPECTROSCOPY

METHOD	QUANTITY MEASURED	EXAMPLES
Absorption	Absorbance	Atomic absorption, UV-Visible molecular absorption, IR absorption.
Emission	Radiant Emission Power	ICP & DCP emission , Spark emission , Laser induced breakdown emission , Flame emission , DRC ARC emission
Luminescence	Radiant Luminescence Power	Molecular fluorescence and Phosphorescence, Chemi- and Bioluminescence, Atomic fluorescence.
Scattering	Radiant Power of Scattering	Raman Scattering, Mie Scattering, Turbidity

III. RESULTS AND DISSCUSSIONS

PORTABLE SPECTROMETER AND TYPES

Nowadays, Portable spectrometers are more preferred by the individual university laboratories as well as for the research purposes, because of its numerous advantages compared to the conventional spectrometers such as the simple maintenance, less cost, high data quality, on-site applications and so much more. There have been numerous developments after extensive study and improvements, for the design of portable spectrometers. [13].

3. 1 ULTRAVIOLET - VISIBLE SPECTROMETER

In terms of miniaturization, UV-vis range is the most advanced and it is also notable that the possibility of spectral sensor products with small laboratory instruments were available since a long time. Colorimetric analyzers, a traditional instrument, use a classical method of chemical analysis and their portable versions are still in use in areas like water analysis. Portable instruments are available ranging from low cost versions using four to six discrete LEDs to more sophisticated versions using simple spectrograph. Here, the bands being measured may be in the half-width range of 50–100 nm. Therefore, the optical resolution is not considered as a critical parameter. This principle is used by the clinical analyzers in some analyses along with the luminescence and fluorescence-based assays. Color matching and illumination analysis also comes under the applications of portable UV-vis spectroscopy [14]. A variety of handheld and portable spectrometers, some incorporating integrating spheres, are commercially available in markets.

Figure 2. Portable UV-VIS Spectrometer

3. 2. INFRARED SPECTROMETER

3. 2.1 Visible Infrared Portable Spectrometer

Visible - Near IR region is considered as the extended visible region and is in the range of 400nm to 1050 nm and this region is found handy with the silicon - based detectors. Absorption in the region ranging from 700nm to 1050nm occurs mainly through the third and the fourth overtones of molecular transitions and is restricted to the C-H, O-H, and N-H groups as a result of which the spectroscopic information bounded as the structure of bands collapses. This region has applications such as the handheld instrument for alcohol in beverages and also in the field geology and also paved the way to development of commercial fruit sorters [15]. The remarkable ability for the visible infrared portable spectrometer is to evaluate the ripeness of fruits and the tissue oxygenation and hydration [16].

Figure 3. Portable Vis-NIR Spectrometer

3. 2.2 Near Infrared Portable Spectrometer

A portable Near - IR spectrometer assures reliability as well as speed of analyses as it is compact, sensitive and non-destructive analyses. This has wide applications in food as well as pharmaceutical industries. The latest version is only palm sized and is controlled through smartphones or even wrist watches.

Figure 4. Portable NIR Spectrometer

3. 2.3 Mid - IR portable Spectrometer
Handheld FT - mid - IR spectrometers are built based on the small versions of standard interferometer type and have a wide range of applications in military, chemical pharmaceutical industries [17].

Figure 5. Portable FTIR Spectrometer

3. 3 XRF SPECTROMETER
The X-ray Fluorescence Spectroscopy(XRF) uses energy dispersive techniques. The incoming X-rays in XRF produce a pulse of electrons in the detector. This pulse of electrons is found proportional to energy of X-rays. In handheld form, it is hard to focus the X-rays therefore, the source, sample and detector is kept in close proximity to improve the efficiency [18]. Near to the exit of the X-ray source there are metallic filters and apertures which are closely assembled. Also the radiation safety regulations reduce the voltage and power of X-ray sources which are unshielded as they are open beam instruments [19]. The main applications of portable XRF are metal alloy analysis, lead detection and quantitation, refining and manufacturing processes of metals [20]. XRF needs minimum training and little sample preparation nevertheless of the sample size. The key components of XRF like, X-ray tubes and detectors, also silicon drift detectors used for X-ray detection are expensive [21]. They are also used by combining with other analytical techniques like XRF diffraction and XRF Raman. They have large applications in metal markets.

Figure 6. Portable XRF Spectrometer

3. 4 PORTABLE RAMAN SPECTROMETER
In a portable Raman spectrometer, even though the size is reduced it does not affect the performance [22]. The portable setup consists of a laser source, a CCD sensor for image capturing and a control unit which carries out the detection and display process. Usually the portable Raman instruments use 785 nm laser as the excitation source. This wavelength is used because it is convenient and cost-effective compared to laser sources of longer wavelength excitation, and also this laser is capable of using a silicon CCD or CMOS linear. Laser sources of 830 nm, 1030 nm, or 1064 nm excitation are sometimes used to reduce fluorescence. But their spectral range is very limited, this reduces the efficiency of the spectrometer in detecting the compounds [23]. Two techniques used in the laboratory for portable Raman Spectroscopy are the use of surface-enhanced Raman spectroscopy (SERS) substrates and offset techniques which are used to see through containers. In this technique semi-transparent containers are used to keep the samples and the Raman spectra of this is collected by separating optical excitation and collection points. The development of these instruments is beneficial to military and space research missions. These are vehicle-portable and human-portable. Other applications include military safety and security, and field geology.

Figure 7. Portable Raman Spectrometer

IV. CONCLUSION AND FUTURE SCOPE

The table shows the applications of portable spectrometer in various fields. Spectroscopy is a technique which has many useful applications. It is not considered as a common due to its large cost. Since this technique is a non-destructive method of analysis, it is very helpful in many industries.

Table 2. APPLICATIONS OF PORTABLE SPECTROMETERS

PORTABLE SPECTROMETER	**APPLICATION**
X-ray Fluorescence (XRF) Spectrometer	Alloy analysis Lead and heavy metal detection Precious metal detection Mining and mineral detection
Raman Spectrometer	Biological agent detection Drug detection and analysis Explosive detection
Ultra Violet-Visible(UV-VIS) Spectrometer	Clinical analysis Medical research field
Near Infrared(NIR) Spectrometer	Quantitative, qualitative analysis in the agriculture sector Soil analysis
FT-Mid Infrared(FT-IR) Spectrometer	Military application Chemical and pharmaceutical industries Narcotics detection
Hyperspectral Imaging Spectrometer	Earth remote sensing Agriculture sector Geology and mineral sector Global change detection and meteorology Food contamination and adulteration

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