

LABVIEW BASED PEAK DETECTION ALGORITHM FOR ELEMENT IDENTIFICATION AND SPECTRAL ANALYSIS

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Abstract--Identification of the unknown (material) is the need of the hour in the world of insecurities. Raman spectroscopy is an important technique for assigning molecular signature for detection and identification of unknown sample. Raman Spectroscopy is based on the inelastic scattering of the incident light by the vibrational test molecule. Raman spectrum is unique for particular molecule or compound and this property is employed for identification. This paper proposes a simpler, cheaper and less complex technique for capturing and analyzing the Raman spectra. A dedicated program has been developed, using Labview software, for analyzing the Raman spectrum and identifying the same. The program has been tested and has proved to detect and identify the element successfully and effectively.

Keywords: Spectroscopy, Rayleigh scattering, Labview, Raman Effect, ICCD.

INTRODUCTION

Raman spectroscopy is a significant tool for studying and analyzing the excited energy levels of an element [1] on interaction with UV or NIR light. For every element, a specific spectrum is build up consisting of the molecular information of the element. As a result, the spectrum generated defines specific identification characteristics of an element and is employed for the detection and identification of the unknown material. In Raman system, a laser is used for stimulating the energy molecules and the dispersed light is assembled with the help of receiving optics and detectors. Various techniques are used for generation of Raman spectra, but due to the existence of background noise in the process of Raman spectroscopy, using visible range technique becomes a restricting factor. Some techniques are used in order to control the fluorescence factor like using UV rays, developing fuzzy models, using artificial neural networks algorithms [5],[6],[7].One of the technique is Ultra violet technique[2],[3].In this technique we use a UV rays for excitation of energy molecules because a large number of transitions take place in UV region resulting in enhancement of the Raman spectra bands. But due to the factors like sample mortification this method works suitable for only a small band of molecules. In this paper, we discuss about the working principle and the Raman experimental setup along with the algorithm employed for Raman analysis and element detection. A program is designed on a virtual interface using Labview software to successfully determine the elements. Testing of the designed program prove that the element matching or identification efficiency is extremely high and the results displayed are reliable.

WORKING PRINCIPLE

When an element is irradiated with a light beam, the photons of the incident light interacts with vibrating molecules of the test element and are either absorbed or scattered away. The reflected light can be elastically or inelastically scattered. The elastically scattered (Rayleigh scattering) beams have the same frequency as that of the incident light. They are insignificant for analysis and hence are filtered out. The inelastically scattered (Raman scattered) beams have a shift in the frequency and energy, depending upon interaction and the vibrational nature of the molecule of the test sample. These variations, also known as Raman Effect [8], are unique for each kind of molecule, and hence act as molecule fingerprint. The inelastically scattered light is given to the spectrometer, which in turn plots the radiation intensity for respective wavelength, known as the Raman spectra. The peaks in the Raman spectra correspond to different molecules or compound in the test element and the amplitude of the peak determines the quantity or the ratio of the particular molecule in that test element.

EXPERIMENTAL SETUP

The experimental setup of Raman Spectra primarily comprises of test sample, laser source, ICCD and a monitoring computer.

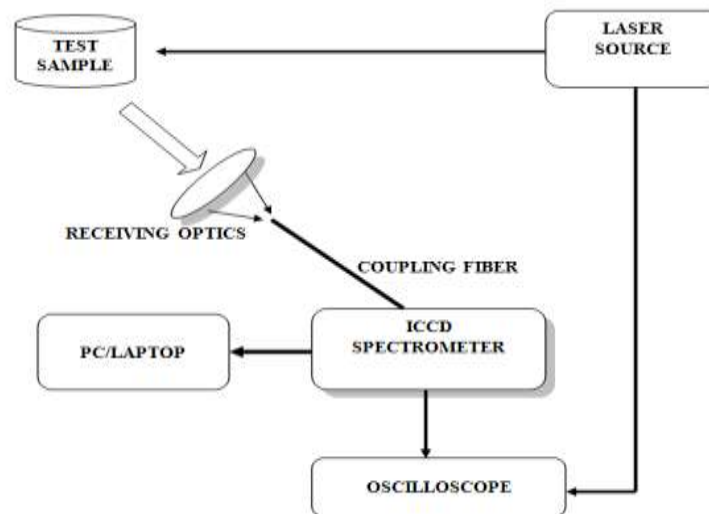


Fig. 1 Block Diagram of Experimental setup for Raman spectrum analysis

The test sample, whose Raman spectrum is to be analyzed, can be any chemical compound or mixture. The sample is irradiated with the monochromatic laser light of known wavelength. The photons of incident light are re-emitted by the sample thereby exhibiting both elastic as well as in-elastic scattering. The in-elastically scattered light shows the Raman Effect i.e. the frequency of the re-emitted light is different from the incident light. The primary purpose of the receiving optics is to filter out the unwanted elastically scattered light and to collimate the in-elastically scattered light into the ICCD coupled spectrometer. The Intensified-CCD boosts the incoming signal and also disintegrates the same into different wavelengths, as per its resolution. The output of the ICCD is coupled to the spectrometer which in turn portrays the intensity of the radiated signal with respect to its respective wavelength. The output of the spectrometer is given to the monitoring computer which analyzes the Raman plot. A dedicated software is designed to parameterize the Raman spectra. The Raman peaks are detected and matched with the library to detect the test sample. A major challenge dealing with Raman Spectroscopy is the inclusion of stray light and fluorescence [12] in the reflected beam, which cannot be completely eliminated but can be reduced significantly [13].

DEVELOPMENT OF VI

A dedicated virtual instrument (VI) program is developed using Labview software for the analysis [8] of spectra obtained from spectrometer. The Raman spectroscopy analysis and detection primarily involves detection of Raman peak location and matching the same with the library to detect the element. The quadratic fit algorithm has been used for peak detection. Since, each element has its own Raman spectroscopic signature, it is an efficient method for detection of chemicals, medicines, explosives, etc.

The whole method involves the following steps

1. The Raman peaks to be analyzed, is acquired from the spectrometer and is split into x and y axis data, where x corresponds to the wavelength (in cm^{-1}) and y corresponds to the radiation intensity.
2. The y axis data i.e. the intensity is passed through filters.
3. The filter function eliminates and smoothens unwanted peaks.
4. The output of the filter is given to peak detection function.
5. The peak detection function gives index value of the location of the peaks as output.
6. Threshold and width of the peak detector function can be set for eliminating unwanted peaks and for regulating noise.
7. From the index value, the exact peak location is derived in terms of wavelength, with the help of x- axis data acquired initially.
8. A program is designed for matching the test sample with data in the library.
9. The peak location data is matched with the data of the known elements, stored in the library.
10. The result of the data matching is then displayed as well as alerted using a text to speech converting sub-VI.

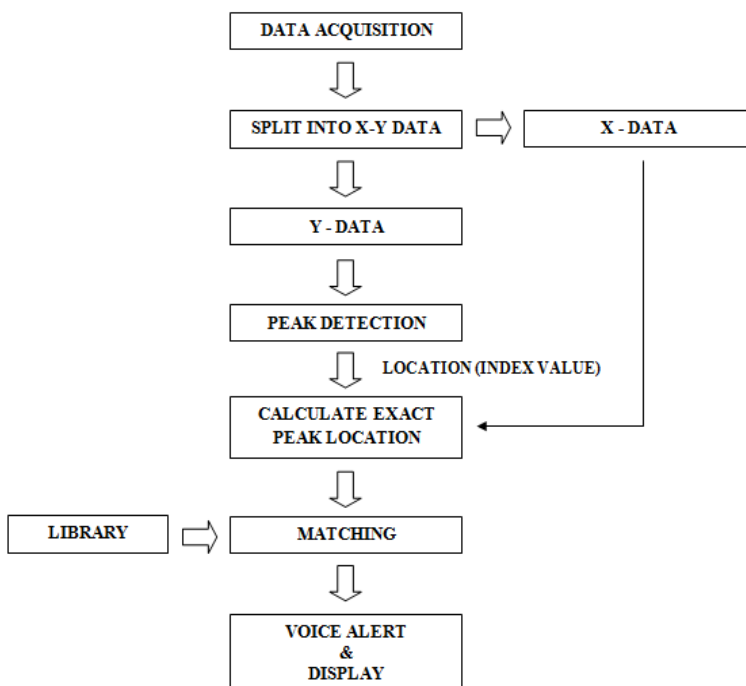


Fig. 2 Block diagram of algorithm employed for peak detection and element identification

RESULT

For our analysis, we took crocine tablet as a test sample, whose Raman spectra is already stored in the library. The test sample is radiated with a monochromatic laser beam of 532nm wavelength. The elastically scattered photons re-emitted by the test sample are filtered out and the inelastically scattered light is focused into ICCD coupled spectrometer. The output of the spectrometer is given to the monitoring computer which in turn analyzes the Raman spectra and parameterizes the same for element detection with the help of the developed VI. The test sample is successfully matched with the library and displays the result as crocine. Fig. 3 GUI developed for Raman spectra analysis and identification

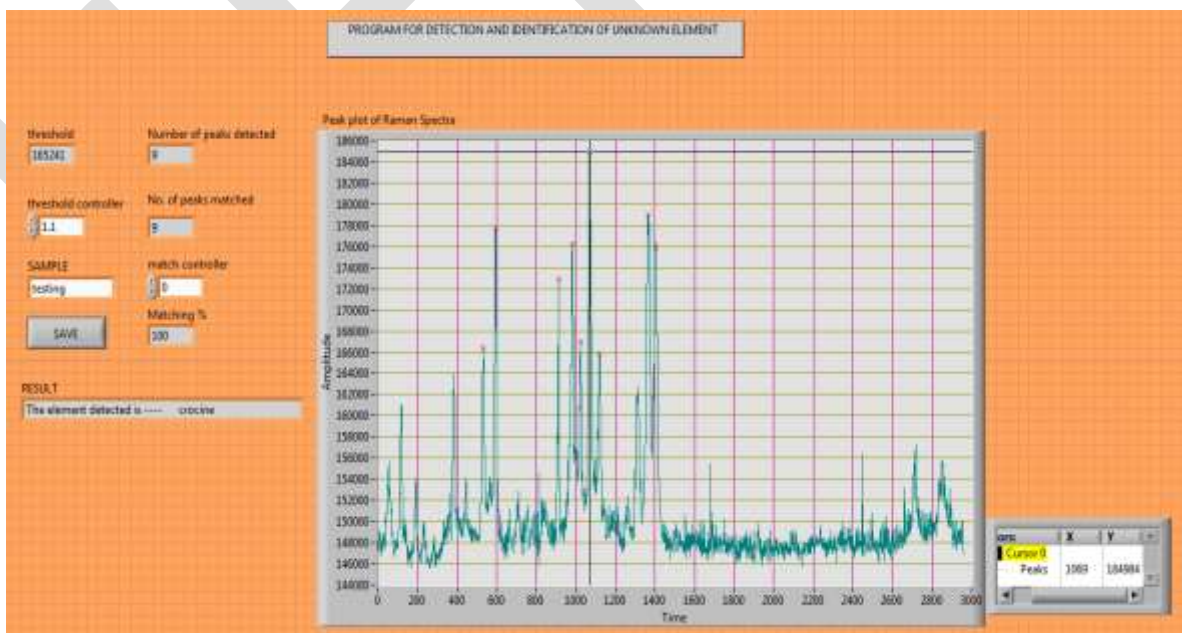


Fig. 3 GUI developed for Raman spectra analysis and identification

CONCLUSION

A simple and efficient method has been discussed for unknown element detection. It employs Raman spectra analysis technique for identifying unknown sample. A Labview based VI has been designed and developed for parameterizing the Raman spectra. Element detection is achieved by matching the Raman peaks of the unknown sample with the peaks of the known sample in the library. Peak detection is done using an inbuilt function, which employs Quadratic fit algorithm, for identifying peak location. It is an efficient method but can be improved by using more parameters like peak amplitude, peak width, peak shape, etc. for increasing matching efficiency. Fluorescence is a primary factor influencing the Raman Spectroscopy which can be dealt with in the pre-processing stage of Raman analysis. This technique can be used for identifying any unknown sample, mixture or compound. With the help of portable Raman setup, it can also be used for security applications for detection of any threatening material.

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