

Detection of Raman Peaks for Identification of Chemicals using Labview

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Abstract: - Peak Detection is one of the most important parameter of Signal processing. LabVIEW (Laboratory Virtual Instrumentation Engineering Workbench) is a graphical programming language where flow of data determines the execution. A number of applications have been built using the LabVIEW like: Robotics, Instrumentation and Control, Signal processing etc. In this paper for determining the peaks of Chemical we are using LabVIEW 2012 SP1 environment, upon which we are implementing the logic of peak detection after acquisition of Chemical spectra using Raman Spectroscopy. Here we are going to analyze some raw spectra of Chemicals like PNBA, Benzene, and Chalk powder and find out the Raman peaks of the input spectra. A complete database is maintained for Chemicals. If a Chemical is examined for the first time its peaks are detected and a new database is created for it and if existing Chemical is examined then it will just match it from database and generates the sound of Chemical detected.

Index Terms— Raman Spectroscopy, Peak Detection, Raman peaks, Signal processing, LabVIEW

I. INTRODUCTION

Raman Spectroscopy is used to find out the vibrational information of molecules like chemical bonds. Each molecule has its own Raman peaks which act as a fingerprint for that molecule that makes its spectra different from others. Raman spectroscopy is based on the fact that molecules absorb and emit light at certain wavelength which acts as their Raman Peaks. While taking spectra of molecules using spectrometer some environmental factors are also present like light, dust particles due to which noise enter and we get Noisy spectra. To eliminate noise, we have to use filters and make the spectra noise free so that accurate peaks can be identified.

In LABVIEW we design code for peak detection, comparison & identification of any chemicals by building database for chemical spectra.

The software is concentrated on the Raman spectroscopy of different chemicals. Raman setup is used to perform the experiments on different chemicals. Raman spectra give a unique fingerprint of the

molecules under study which makes it a very useful technique for many application areas. Once a signal is acquired, it's processed and matched with the existing ones in the database library and subsequently identified. The matching and identification is done by matching the first to peaks of the chemical in question with every peaks of rest of ones in the database library. If a match is found its value is set as TRUE else FALSE and set as an operand. The Boolean AND of the two operands is TRUE if we have achieved an identification.

II. DETECTION OF RAMAN PEAKS

Peak Detection Problem:

Peak detection is a general problem in a wide range of applications. As peak detection is a pre-processing step for many advanced signal processing systems its accuracy for validation of the output is crucial.

Material & Method:

For detection of Raman peaks of the molecule taken by the spectrometer we need a complete experimental setup of Spectrometer, Laser, Light Source, Computer system for controlling and simulating the software.

A. Steps for Data Acquisition:

- 1) Conversion of Photo signal to Electro signal by Photo detector.
- 2) Transfer of Pixel output in terms of Intensity Vs Wavelength in Labview window.

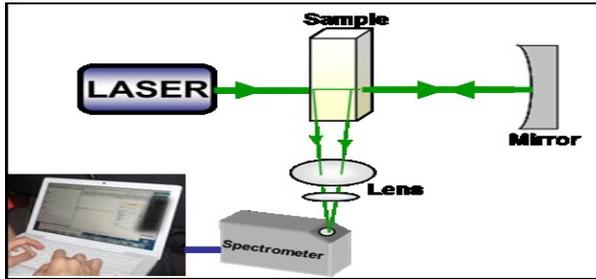
Acquisition in LabVIEW can be done by two ways:

- a) Using Read from Spreadsheet file: In this option we have an inbuilt option for taking spectra values directly in a spreadsheet file from the already performed experiment and then using index array make all values to be acquired in a 2-d array form.
- b) Using Hardware devices incorporated with Laser, Spectrometer, and Detector: In this option in real time we setup the experiment and proceed step by step.

B. Steps for Analysis:

- 1) Finding the peaks from the acquired spectra.
- 2) Matching of those peaks with library data to identify the material.

Experimental Setup for Raman Spectra



Signal Processing:

Signal Processing is the process to analysis the spectra such as filter the input spectra, detect peaks to know the chemical. For this purpose we had built a VI in LABVIEW which filter out the Raman spectra, detect peaks and find the name of chemical from an inbuilt database. The first step is to acquire the captured Raman spectra in LabVIEW. For this purpose we take raw spectra and convert the spectra into text file and then import that file in LabVIEW using “read from spreadsheet” control as shown in Figure 1.

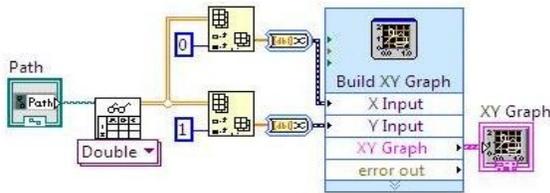


Fig. 1 Spectral Acquisition and Display
After Spectra Acquisition, filtering has to be done using filter as shown in Fig. 2.

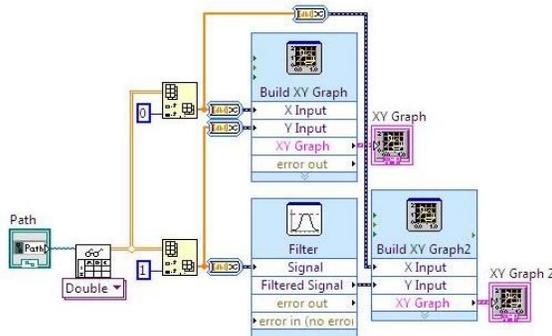


Fig. 2 Spectral Filtering and Display

Steps for Approaching the Problem:

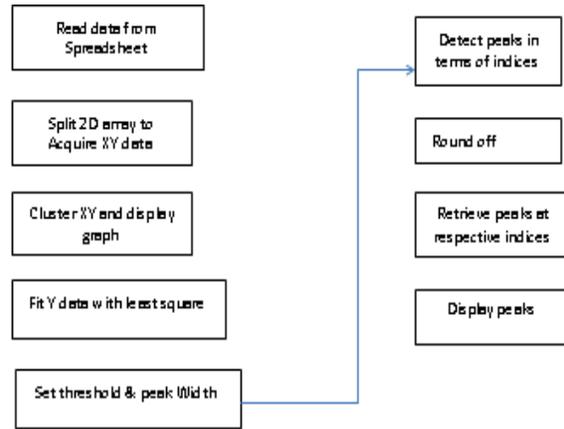


Fig. 3 Flowchart: Data Acquisition and Display

After filtering peaks are detected using peak detection tool in Lab VIEW. The detected peaks in terms of wavelengths and their corresponding amplitude are displayed in form of arrays. Hence, two arrays are used; one for wavelength and another for amplitude.

Once we have acquired spectra of a molecule it is matched with that of existing ones in the library for its unique identification.

Algorithm for comparing a peak with an existing one in the database

1. The first two peaks of the acquired spectra are considered for its matching and identification.
2. A tolerance value is assigned for the match by algebraic subtraction.
3. If a match is successful then its Boolean value is set as TRUE else FAILSE.
4. Both values are set as operands for the Boolean AND.
5. If the output of the AND operation is TRUE, an identification has been achieved.

Both peaks under consideration are matched with every peaks of the first molecule in the database library.

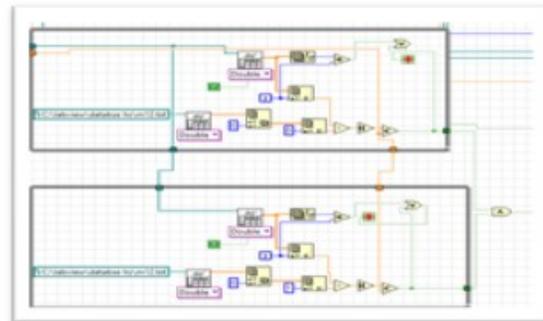


Fig 4 Peaks Detection

III. RESULTS

Initially we are taking the peak values of 20 chemicals of the database. Parameters like threshold, tolerance power and width are set before running the executable file in offline mode. After processing the spectra in question we get its peaks in terms of its wavelength and amplitude. We match the peak wavelengths with that of all 20 chemicals. Two plots shown in the Fig.4 are the raw and processed representation of the spectra i.e. first one is unfiltered and the other one is filtered. The textual display "BENZENE" is the identified chemical. Here X-axis represents the Wavelength and Y-axis represents the Amplitude.

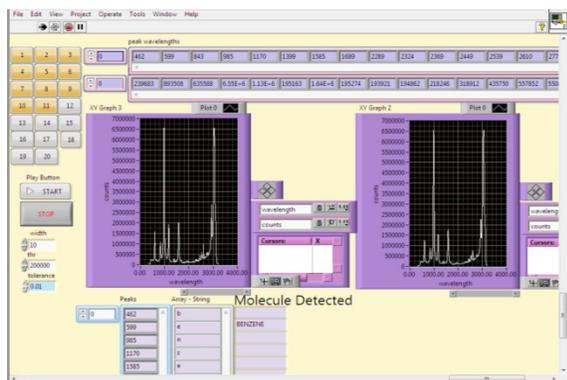


Fig. 5 Spectral Peak Identification

A number of recorded audio are saved in database for the various chemicals. After chemical detection the corresponding audio is played by the software confirming detection.

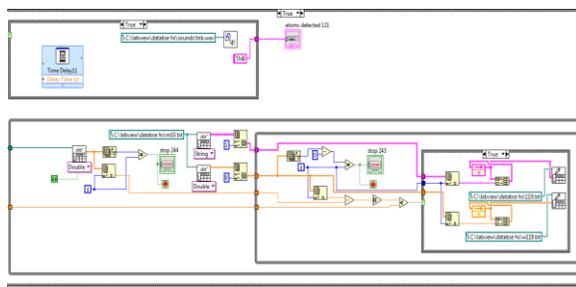


Fig. 6 Audio Notification

IV. CONCLUSION & FUTURE WORK

Raman spectroscopy is a versatile tool. Raman Spectroscopy is a molecular spectroscopy. Virtual instrumentation has been designed for acquiring the spectra of laser ablated samples and performing the spectral analysis of the same. The experiments have been performed in normal laboratory conditions. The

VIs developed in LabVIEW has been created for acquiring the offline spectra, detecting of the peaks. The database is created for peak detection. The virtual instrument developed has been cross checked by various number of experiments performed and the results obtained are accurate for the sample detection.

Our present work focuses on offline spectral analysis through Lab VIEW. Better results would be achieved by constantly updating the database as per the requirement. Moreover, online spectral analysis through Lab VIEW has to be done. The current work focuses mainly on qualitative estimation from the generated data. Various algorithms for quantitative estimation can be developed in future. These include CWT and various other analytical procedures. This work could be used anywhere the unknown detection of the substance is to be carried out. The GUI could be improved further so that more number of people could operate it easily.

Also we can apply this software application for detecting Explosives Material in Secure places like in Defense , Airport , Metro Stations.

V. REFERENCES

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