**Design and Integration of Portable Optical Spectrometer**

Submitted by

Aung Myin Kyaw

Department of Electrical & Computer Engineering

In partial fulfilment of the

requirements for the Degree of

Bachelor of Engineering

National University of Singapore

Table of Contents

[LIST OF FIGURES 3](#_Toc527993723)

[ABSTRACT 4](#_Toc527993724)

[INTRODUCTION 5](#_Toc527993725)

[Background Raman spectroscopy 5](#_Toc527993726)

[REFERENCES 9](#_Toc527993727)

[Appendix A 10](#_Toc527993728)

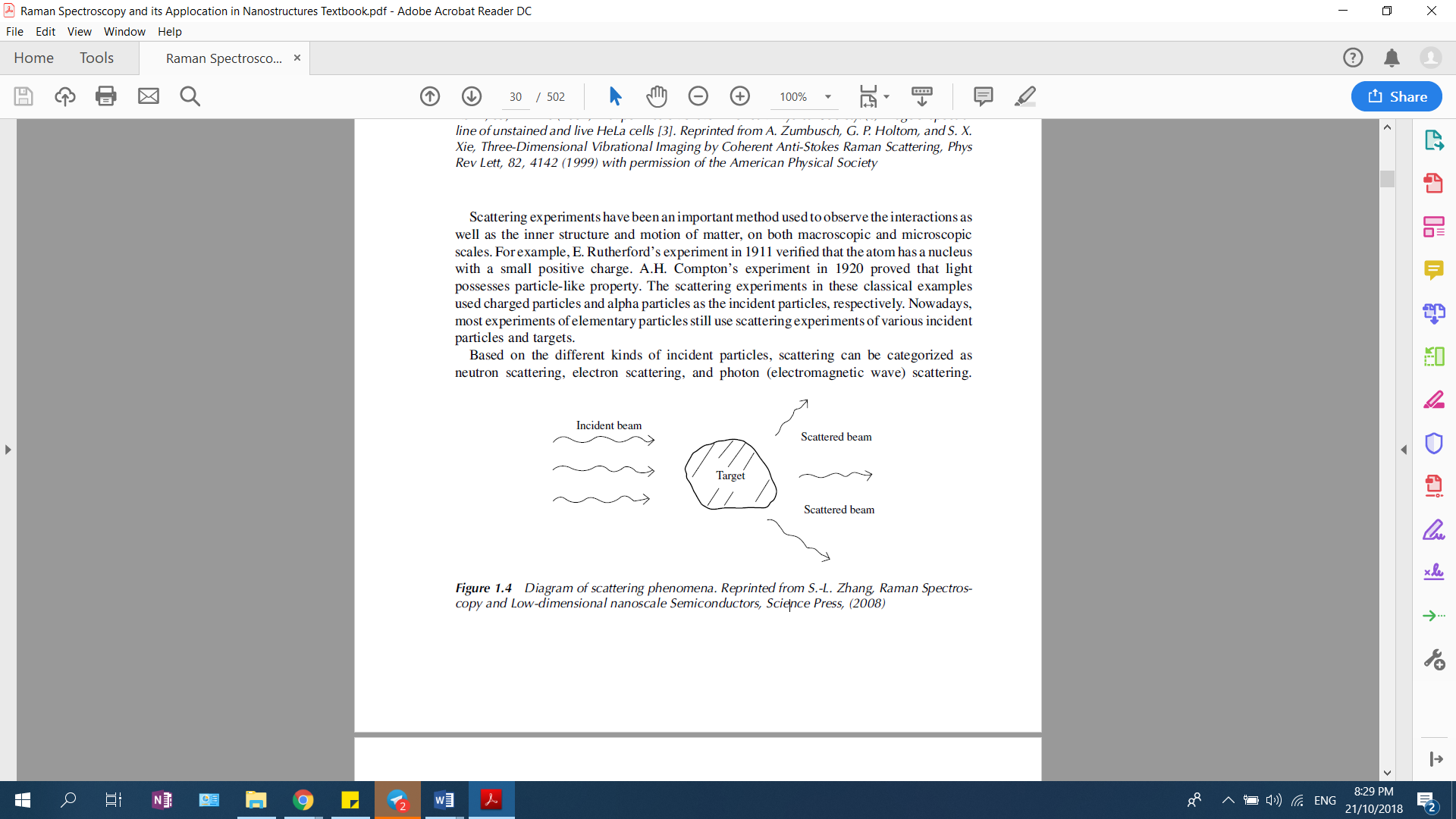
LIST OF FIGURES

Figure 1.1 Diagram of scattering phenomena. Reprinted from S.-L. Zhang, Raman Spectroscopy and Low-dimensional nanoscale Semiconductors, Science Press, (2008)

ABSTRACT

Spectrometers are commonly used for spectroscopic analysis of sample materials. However, the sizes of the conventional spectrometers are large, and it is restricted only in the laboratory. This project is to design and integrate portable optical spectrometer.

This part of the project is the development and implementation of a user interface component of the portable optical spectrometer. Though there are some existing user interfaces, it has limitations such us customisation, controlling and communicating with different components of the portable spectrometer. Thus, the report will discuss the implementation using C# programming language to integrate the user interface.

INTRODUCTION

Optical spectrometer is a tool used to measure the intensity of light over a specific portion of electromagnetic wave spectrum. Raman spectroscope are widely used to observe different materials, chemical substances and many more as it has many advantages depending on the purposes of the analysis. However, size of conventional Raman spectroscope is rather large, and it is inconvenient for measurements outside the laboratories. This project is to develop a multifunctional portable Raman spectroscope for point-of-care diagnostics. This report will be discussing the implementation and integration of the user interface using C# programming language. Firstly, for the background information this report will provide the overview and properties of Raman scattering. After which, it will discuss the different programming languages available for the implementation and the reason behind choosing C# for the implementation. Next, will be the documentation the implementation methods and difficulties that encountered during the process. Lastly, the report will present the outline of what the end-product will look like.

BACKGROUND OF RAMAN SCATTERING

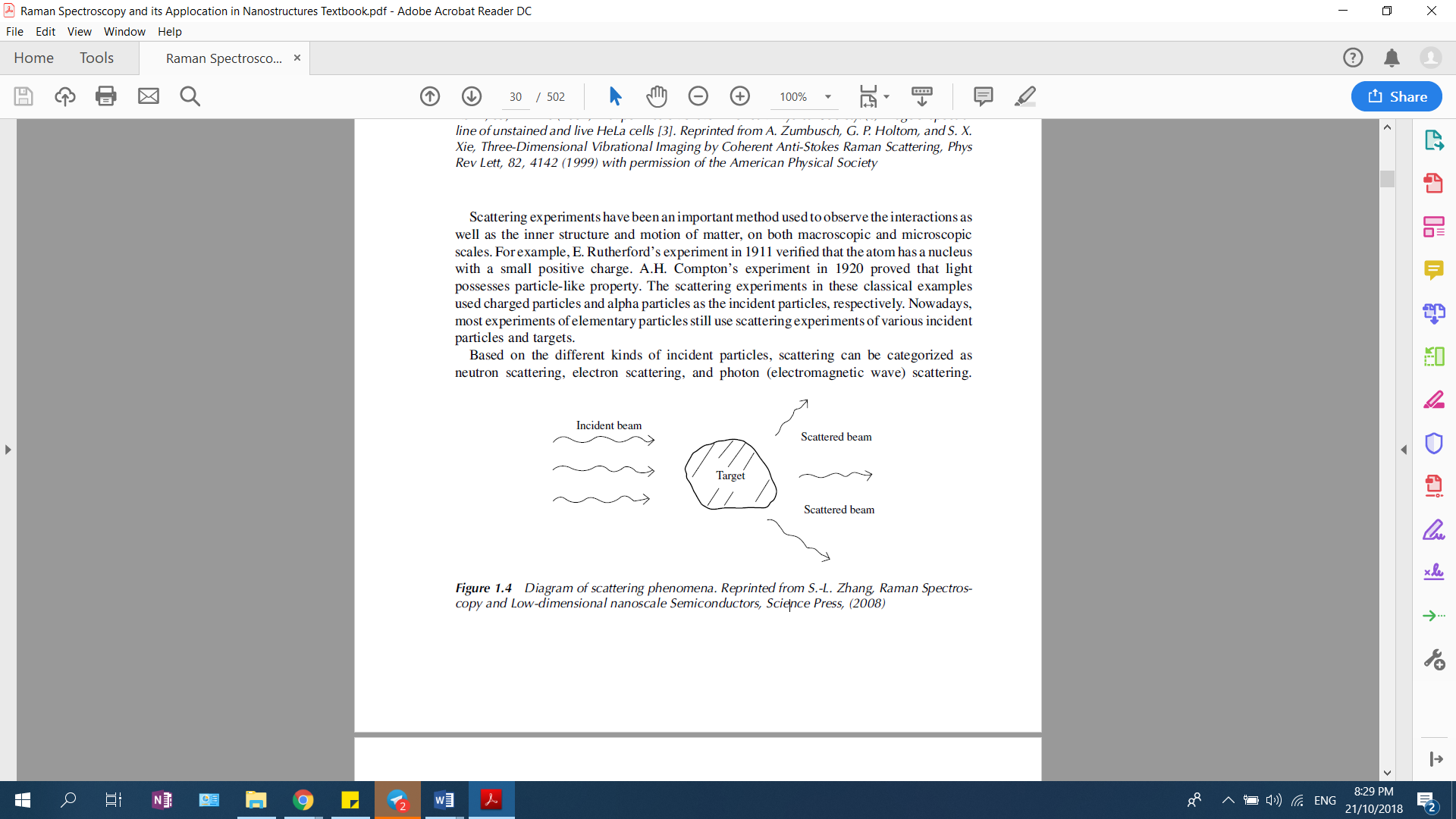
Different spectroscopy methods are often used for the classification of a wide range of samples. These methods are used for qualitative and quantitative analysis of the samples. The qualitative analysis is to establish the identity of sample while quantitative analysis is to estimate the concentration of analyte in sample. Raman spectroscopy method can be used for both qualitative and quantitative purposes. Qualitative analysis can be performed by measuring the frequency of scattered radiations while quantitative analysis can be performed by measuring the intensity of scattered radiations [1][2]. Thus, nowadays Raman spectroscopy has become highly popular for many different purposes. It is well-suited to analysis different solid, liquid or gases, depending on the set-up and it is relatively fast process. Raman spectroscopy is a technique which detects photons that have undergone Raman scattering. Raman spectroscopy can be determined by observing Raman scattering, or inelastic scattering of monochromatic light. Scattering occurs when an incident photon collides with the target molecule along the direction of it travelling (Figure 1.1). The target molecule is excited and then relaxes and emits a photon immediately. The energy and the direction of the emitted photon during the collision may change, thus causing the scattering.

Figure 1.1 Diagram of scattering phenomena. Reprinted from S.-L. Zhang, Raman Spectroscopy and Low-dimensional nanoscale Semiconductors, Science Press, (2008)

There are many different scatterings such as Rayleigh scattering, Brillouin scattering and Raman scattering. The main different between above scattering is the change of energy when the collision occur. It is known as inelastic scattering when energy of the emitted photon is either lower or higher than the incident photon. Thus, Raman scattering (Raman shift) is an inelastic scattering with the change of energy greater than 1 cm-1[1]. Raman shift is expressed in wavenumber (em­-1, wavenumber multiplied by the velocity of light, 3 X 1010 cm/sec, gives the actual frequency) [3]. As the energy change in Rayleigh scattering is caused by the recoil of the target, it is considered as elastic scattering [4].

Raman scattering spectra have their own characteristics. Usually, Raman shifts are naturally in wavenumbers, which have units of inverse length (cm-1). During scattering the frequencies emitted are used as chemical fingerprints for the identification of molecules. Raman wavenumber (R) can be calculated by using equation (1.1a), where 0 is the wavenumber of the incident light and S is the wavenumber of the Raman spectrum [4].

R = 0 – S (1.1a)

Use the following equation (1.1b) to convert between spectral wavelength and wavenumbers of shift in the Raman spectrum, where λ0 is the wavelength of the incident light and λS is the wavelength of Raman spectrum [4].

R = (1.1b)

The intensity of Raman scattering is a lot weaker than the intensity of Rayleigh scattering [4]. However, it can be enhanced using Resonance Raman Spectroscopy (RRS) and Surface Enhanced Raman Spectroscopy (SERS) [4]. SERS is a technique in which sample is adsorbed on a colloidal metallic surface such as silver, gold or copper. Hence, this improves the intensity of Raman signals [6] [7]. In addition, the low intensity can be easily improved with a notch or edge-pass filters. Similarly, recording the Raman spectrum has become easier by the advancement of Charge-Coupled Device (CCD) spectrometers.

CCD spectrometers are a multichannel detector which consists of a 2-dimensional array of light-sensitive elements. There are many different CCD spectrometers in the market. However, Compact CCD Spectrometers 100 (CCS100) by Thorlabs will be use for the implementation of the project. After considering the different parameters such as overall Size, Cost, Speed, Customization, Sensitivity, Signal-to-Noise Ratio, Dynamic range, Linearity, Thermal Stability, and Robustness CCS100 fits almost all the requirement to build a portable optical spectrometer (See Appendix B for Technical Data of CCS100).

IMPLEMENTATION

For the developers, Thorlabs provides different drivers and libraries for programming languages such as C, C++, C# and LabVIEW. It is impossible to use different language to control CS100 as without the usage of drivers and libraries it is not possible to communicating with CCS100. Hence, the choice of the programming language will be selected from C, C++, C# and LabVIEW. There are different parameters such as Cost, Speed, Size (Memory space), Resources available online and offline and Scalability to consider when choose among these four languages.

REFERENCES

[1] Skoog DA, Holler FJ, Crouch SR. Principles of instrumental analysis. 6th ed. Cengage Learning, 2006.

[2] Willard HH, Meritt Jr LL, Dean JJ, Settle Jr FA. Instrumental methods of analysis. 7th ed. New Delhi: CBS Publisher & Distributors; 1988.

[3] Wu Guozhen. RAMAN SPECTROSCOPY an Intensity Approach, Science Press, Beijing, 2014

[4] S. Zhang, Raman spectroscopy and its application in nanostructures. Hoboken, N.J.: Wiley, 7-8, 2013.

[5] Zhang, Shu-Lin. Raman Spectroscopy and Low-dimensional Nano-semiconductors, Science Press, Beijing, 2008.

[6] Settle FA. Handbook of instrumental techniques for analytical chemistry. New Jersey: Prentice, Inc., 1997.

[7] G. Bumbrah and R. Sharma, "Raman spectroscopy – Basic principle, instrumentation and selected applications for the characterization of drugs of abuse", Egyptian Journal of Forensic Sciences, vol. 6, no. 3, pp. 209-215, 2016.

Appendix A

Technical Data of CCS100

|  |  |
| --- | --- |
| Optical Specs |  |
| Wavelength Range | 350 – 700nm |
| Spectral Resolution | <0.5nm FWHM @ 435nm |
| Slit (WxH) | 20 μm x 2 mm |
| Grating | 1200 Lines/mm, 500nm Blaze |
| Sensor Specs |  |
| Detector Range (CCS Chip) | 350 - 1100nm |
| CCD Pixel Size | 8 μm x 200 μm (8 μm pitch) |
| CCD Sensitivity | 160 V / (lx · s) |
| CCD Dynamic Range | 300 |
| CCD Pixel number | 3648 |
| Resolution | 10 px/nm |
| Integration Time | 10 μs − 10 s 1 |
| Scan Rate Max. | 200 Scans/s 2 |
| S/N ratio | ≤ 2000:1 |
| External Trigger |  |
| Fibre Connector | SMA 905 |
| Trigger Input | SMB |
| Trigger Signal | TTL |
| Trigger Frequency Max. | 100 Hz |
| Trigger Pulses Length Min. | 0.5 μs |
| Trigger Delay | 8.125 μs ± 125 ns |
| General Specs |  |
| Interface | Hi-Speed USB2.0 (480 Mbit/s) |
| Dimensions (LxWxH) | 122 x 80 x 30 mm |
| Weight | < 0.4 kg |

All technical data are valid at 23 ± 5°C and 45 ± 15% rel. humidity (non-condensing)

1) integration time 5 ms

3) software allows to set up to 60 s. Hot pixels and noise may increase drastically. See section Integration Time

|  |  |
| --- | --- |
| Operating Temperature | 0 ... +40 °C |
| Storage Temperature | -40 ... +70 °C |
| Relative Humidity | Max. 80% up to 31 °C; decreasing to 50% at 40 °C |
| Operation Altitude | < 3000 m |

APPENDIX B