

TEXRAY: Textile Identification via Raman Spectroscopy

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1 Executive Summary

2 Project Description

2.1 Motivation and Background

As the 21st century consumer is becoming increasingly conscientious of their buying power in the global market, many shoppers opt to spend more in hopes of receiving a higher quality, environmentally-friendly product that makes them feel good about their purchase. More and more consumers are swearing off synthetic fabrics in favor of natural textiles only, such as 100% cotton, wool, or silk. This is due to increasing awareness of the fact that synthetic materials utilize high amounts of fossil fuels during production, and are non-biodegradable, leading to persistent environmental pollution as the fabric will never break down [1]. This change in mindset is reflected in the growth of the natural fiber market, which is projected to reach a value of 74.99 billion by 2030 [2]. This has also led to a rise in merchants misleading shoppers about the materials used in their goods, hoping to cash in on the consumer shift towards eco-friendliness without committing to such an initiative. In a report released by Applied DNA Science, the company found that of 29 products tested, 89% of them were not compliant with their labeled fiber content [3]. These kinds of deceptive practices lead to consumers buying goods that don't actually align with their personal ethical standards.

Aside from the topic of sustainability, collectors of luxury goods also have a high stake in ensuring that the products they purchase are authentic and high-quality. Many consumers buy vintage luxury goods from second-hand retailers, where the reputation of the seller is often the only indicator of authenticity they have, leaving them susceptible to buying counterfeit goods. One prominent example of this is well-known luxury consignment retailer The RealReal, which was sued by Chanel in 2018 for hosting counterfeit Chanel merchandise on their site and implying an affiliation to the official brand [4]. While real Chanel bags are made of genuine leathers with "exquisite luster and color absorption," customers unknowingly received low-quality faux leathers or synthetic materials [5]. The retailer has similarly been caught selling fake Christian Dior sneakers that a suspicious customer sent to a 3rd party to be authenticated, upon which they were declared a "lower-grade replica" [6]. Rather than authentic calfskin, the RealReal was selling knockoffs made of cheaper textiles. Such examples are abundant, and consumers are unlikely to know they've been ripped off just by visual inspection of their goods.

The bottom line is, consumers want and need to trust that the products they buy are made of the exact material they claim to be. Currently, the only way for the average consumer to verify the composition of the items they purchase is if they're willing to invest time and money into sending their goods off to an authenticator for peace of mind. This is generally impractical for most people, as well as a hassle. Though hand-held textile identification devices do exist commercially, they cost thousands of dollars and are generally not affordable. Motivated by these issues, our Senior Design group aims to create a table-top spectrometry system that can quickly and accurately identify the composition of a fabric

sample and convey this information to the user, while being more cost-effective than competing commercial products.

2.2 Current Commercial Technologies and Existing Projects

2.2.1 Sagitto

There are currently a few commercial products that are able to accurately identify textile composition without any sample preparation. One such technology is the Sagitto handheld spectrometer. This is a portable device that enables the user to simply hold the spectrometer up to the sample for a few seconds before it conveys the sample's exact material composition via the connected smartphone app. For example, if a t-shirt sample was composed of 63% polyester and 37% cotton, the app will quickly display this information to the user. This product utilizes near-infrared spectrometry to acquire the unique absorption spectrum of each test sample in the NIR range and utilize machine learning models to accurately identify the material in question within a few seconds. The Sagitto website boasts examples of this technology being applied to fabrics and textiles, plastics, kava, hop cones, and essential oils, demonstrating the variability of their device's applications. There are varying levels of specificity in the material composition and data shown to the user depending on the material the spectrometer is being used to analyze. This product costs \$2,500 commercially [7].

2.2.2 Fabritell

Similarly to Sagitto, the company Matoha has its own commercial spectrometer that can quickly identify sample composition. However, whereas Sagitto seems to advertise a single device that can identify a variety of different materials, Matoha has two separate spectrometers for sale, with one being dedicated to identifying plastic samples, and the other being dedicated to identifying fabric samples. Their fabric spectrometer, Fabritell, utilizes NIR reflectance spectrometry within a band in the 1-2 μm range combined with machine learning techniques just like the Sagitto device, displaying sample information to the user via an app. They claim their spectrometer can identify the fabric sample in .5 seconds, and the device can be powered by an adaptor or a battery pack. Both the fabric spectrometer and plastic spectrometer also come in handheld or desktop varieties. Fabritell's latest model supports the identification of 10 pure materials and 13 fabric blends, stating that it is not possible to separate chemically identical fibers such as wool vs. alpaca, though it can separate cotton vs. wool. The product site also states that the accuracy of the device depends on the correct measurement technique of the user, as well as accuracy being $\pm 10\%$ for blends and a 5-10% detection threshold for contamination in pure materials. They also state they cannot reliably identify non-uniform samples. The Fabritell desktop version retails for €2,499 whereas the handheld version goes for €3,499 [8].

2.2.3 trinamaX: Mobile NIR Spectroscopic Solution

Similarly to Sagitto and Matoha products, trinamiX creates a handheld, non-destructive, commercial spectrometer, which can be used for fabric, plastic, PV pipe, and liquid analysis. Notably, the Mobile NIR Spectroscopic Solution provides a spectroscopic material analysis on an article of clothing at “the push of a button”. The product is paired to an application which displays the data of material composition. No note was provided on the analytical method used towards the data processing. The supported textile materials of the device include: acrylic, cotton, polyamide 6/6.6, polytrimethylene terephthalate (PTT), polyester, polypropylene (PP), silk, viscose, and wool. Blended materials are typically identified if the content of the minor material is > 5%. Further specifications include a spectral range of 1450 nm to 2450 nm and a spectral resolution that is 1% of the wavelength. The detector used is a 256-pixel PbS line array detector [9].

2.2.4 OceanOptics: NIR Quest+2.5

The NIR Quest+2.5 provides high sensitivity and low noise spectral assessments for the authentication of products. The wavelength range is 900 nm to 1240 nm, with an optical resolution of 6.46 nm to 25.50 nm. Signal-to-noise ratio of a single 10 ms scan is 10:000:1. This product is applied towards not only product authentication, but for the determination of hydrocarbon solvents, plastics in recycling, and moisture in fruits and grains [10], [11].

2.2.5 Study on characterizing microplastic fibers using Raman spectroscopy

Spectroscopy published an exploration of macroscopic and microscopic Raman spectroscopy to identify different commercial microplastic fibers. This study on characterizing microplastic fibers using Raman spectroscopy is justified to account for the excess of microplastics in the form of fibers that shed from textiles. For samples larger than 1 mm macroscopic Raman spectroscopy is deemed appropriate. For samples smaller than 1 mm, or for heterogeneous samples, a Raman microscope is recommended due to its “high spatial selectivity”. Two fiber samples are used in the study. Sample 1 is a white polyester soft felt fabric made up of rayon and high quality acrylic craft felt. Sample 2 is red and white patterned that is 100% cotton. Sample 1 used a MacroRam benchtop Raman spectrometer (Horiba), equipped with a TouchRaman BallProbe (Marqmetrix). The MacroRam uses an excitation wavelength of 785 nm, which helps to suppress fluorescence that would otherwise be present at shorter laser wavelength excitation. The probe is pressed onto the sample and a spectrum is recorded. The Raman measurement confirmed the sample contained PET and there was no detection in acrylic (which would correspond to a 2240 cm^{-1} band). For sample 2, spectral measurements were taken using an XploRA Plus (Horiba) confocal Raman microscope. This system is equipped with a combination of three different excitation lasers (532 nm, 638 nm, and 785 nm), four gratings (600 gr, 1200 gr, 1800 gr, and 2400 gr), and a 100x magnification objective (numerical aperture of 0.9). The system also used a deep-cooled SynapseEM electron multiplying charge coupled device (EMCCD), for sensitivity and speed. They were able to identify PET, cellulose, and a red pigment [12].

2.2.6 Textile material identification using Shifted Excitation Raman Difference Spectroscopy

The research explored how Shifted Excitation Raman Difference Spectroscopy (SERDS) can be employed to determine the material composition of textile samples while avoiding fluorescence interference from the fiber materials and dyes. Their system uses a dual-wavelength diode laser emitting at 784.6 nm and 785.2 nm as an excitation light source. The detector used was a MityCCD H10141. SERDS was used to assess 22 dyed and undyed textiles produced from various commercially relevant textiles. For all investigated samples, SERDS was successful in separating the Raman signals of fibers and dyes from the fluorescence interference. Reliable fiber identification was sustained from SERDS derived Raman signals for undyed and light-colored textiles made of cotton, viscose, wool, and polyester. Principal component analysis (PCA) and linear discriminant analysis (LDA) allowed for a “very good” discernibility amongst the four textiles [13].

2.2.7 Raman Spectrometer General Operations

Light from a monochromatic light source is directed onto a sample. The scattered light off of the material can be defined as Rayleigh and Raman scattering. Rayleigh Scattering is of the same energy level as the incident light, where Raman scattering is of a different energy level. The whole of the scattered light is sent through a filter which will eliminate the Rayleigh signal. The Rayleigh scattering is then sent through a diffraction grating which will separate the Raman light into its constituent wavelengths, allowing us to determine how the light interacted with the sample. This separated Raman light is then directed onto a CCD. The grating used will dictate how much separation of light we see (spectral resolution). The longer the Raman range we’re looking to detect off the sample, the lower line density should be, as to not spread the light too much, impacting the received light signal. However, having a higher line density will allow for a better spectral resolution [14].

2.3 Objective and Goals

The main goal of our Senior Design project is to create a portable system that will allow the user to place a fabric sample within a designated area, upon which the device will quickly identify characteristic information about the sample, displaying this information to the user via a LCD screen (Fig. 1). It should be noted that practically all of the previously mentioned commercial products intended for fabric identification rely on NIR spectrometry, a technology that requires an InGaAs sensor as a receiver within the device. A single InGaAs photodiode array can run upwards of \$1,000, a significant factor in why these products average around \$2,500 for the consumer. Such an expensive component limits the cost-effectiveness of the device. As such, our group intends to avoid NIR spectrometry as a technique and instead rely on Raman spectrometry to achieve material identification.

We intend to develop a proof of concept for a commercial Raman-spectroscopy system that can determine the authenticity of a product and conduct a material analysis. To limit the scope of the project and avoid taking on more than we can complete within a Spring-Summer course, we will be honing in on a few particular fabrics that we aim to identify as well as separately conducting a product comparison for a few clothing items.

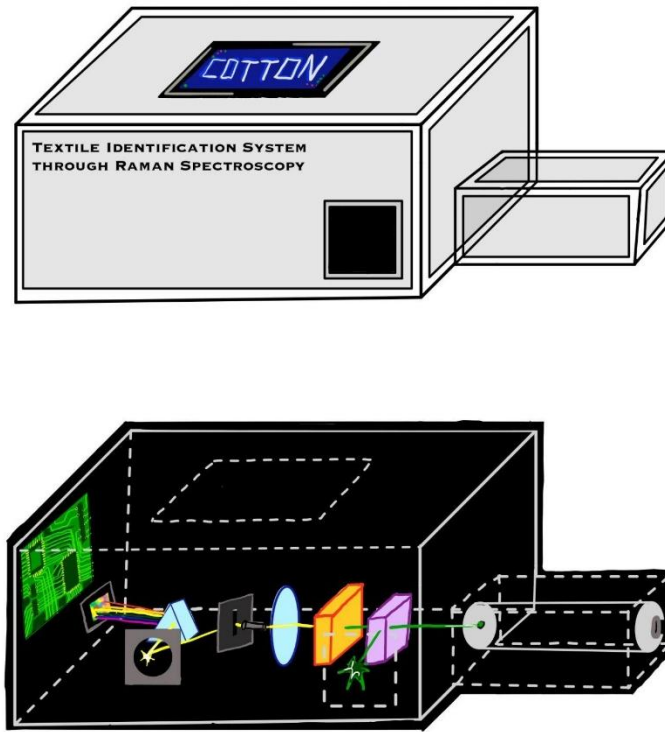


Figure 2.3.1 Textile identification system through Raman spectroscopy prototype

2.3.1 Goals

Basic goals

- The material analysis function will be able to classify 3 types of textile samples based on their spectral signature. The three textile types will be cotton, silk, and polyester. All of the samples will be undyed and unblended.
- The device will display the results of the analysis to the user via an LCD screen.

Advanced goals

- Introduce a second system functionality which would be able to determine if two clothing products are identical
 - The user will be able to select either “Material Analysis” or “Product Comparison” on the home LCD screen
 - The product comparison function will conduct a spectral comparison between a clothing sample being tested to a database of previously scanned

clothing items. If a match is found, this indicates the sample is identical to a reference clothing item.

- The scanned and stored items will not need to be undyed, unblended, or one of the three textile types from material analysis.
- The material analysis function will be able to classify 2 additional types of textile samples based on their spectral signature. The additional textile types will be nylon and wool.

Stretch Goals

- A mobile app will be integrated to replace the functions of the LCD screen.
- The material analysis function will be able to identify undyed, blended fabric samples and give portion ratios.
- The material analysis function will be able to differentiate between the key textiles regardless of whether or not the sample is dyed or undyed.

2.3.2 Objectives

Basic Objectives

- Build an effective Czerny-Turner Raman spectrometer to analyze the materials while keeping cost efficiency in mind
- Determine a lens setup to enable efficient Raman-illumination and high Raman signal acquisition from samples
- Implement an efficient power source for the system while maintaining portability
- Create a database with reference spectral signatures of cotton, polyester, and silk for comparison during material analysis
- Utilize machine learning to improve the accuracy of the material analysis comparison system

Advanced Objectives

- Create a more robust fabric analysis system to include the classification of nylon and linen.
- For the secondary product comparison feature:
 - Create a more specified fabric analysis system to determine a unique clothing item's spectral signature.
 - Implement an efficient data processing algorithm which can accurately determine the correlation between a sample clothing item and the existing items in the database to find a match.
 - Store reference clothing items into a database.

Stretch Objectives

- Determine a method utilizing machine learning to find the material ratio of blended fabrics.
- Determine a method of identifying dyed materials.
- Implement a mobile app that allows for a more user-friendly interactive display
 - Use Flutter for frontend development
 - MongoDB for database management

- Postman and visual studio code for api configuration and testing

2.4 Features and Functionality

This project will act as a proof of concept for a Raman-spectroscopy based commercial fabric scanner and will likely have limited functions compared to the commercial product alternatives that were previously discussed. However, it will display the practical features a future fully functioning product might include, while maintaining a lower total cost.

2.4.1 Optical System

The system will include a sample tray upon which the user can place their fabric sample, with no prior sample preparation. The sample will then be illuminated by a laser light source via a series of probe optics, such as one or multiple lenses and a beamsplitter, which will cause Raman scattering and Rayleigh scattering to be reflected off of the sample. The beam splitter will guide the back-reflected light back towards the collection path of the system, where a longpass filter will block all Rayleigh scattered light from continuing. This light will then be coupled into a fiber which will guide it to the spectrometry system's entrance slit. Mirrors will be used to align the Raman scattered light onto a diffraction grating which will disperse it into its constituent wavelengths. A second mirror will focus this diffracted light onto a detector.

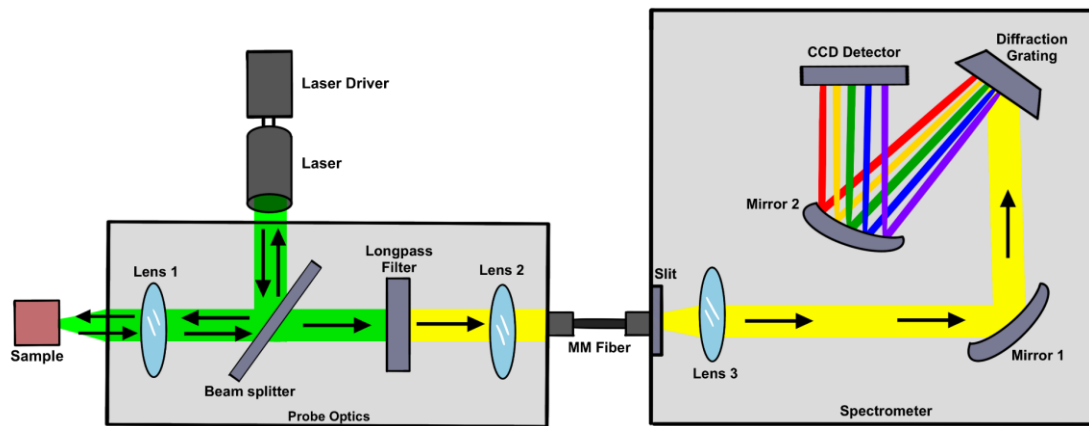


Figure 2.4.1 Preliminary design of optical system, including Raman illumination and spectroscopy. Distances will be added as the design progresses.

2.4.2 Electrical Hardware

The PCB for the system will include a battery source to power the components. In order to accomplish this, the battery source will be connected to a switch which will be wired to a 3.3V and 5V voltage regulator. From the 5V regulator voltage will be distributed to the LCD screen and to the Raspberry Pi. LEDs would be used to indicate the power is being properly distributed and they will be soldered onto the PCB and be receiving voltage from being wired to the 3.3V regulator. The laser component will be powered via a wall outlet

separate from the PCB. Once the system is powered on, the detector will then receive the spectral analysis of the sample provided by the spectrometer. The detector will be wired to the MCU to transmit the collected data for the information to be processed. Once the classification is determined by the program in the MCU, the results will be transmitted through a wire to the LCD screen and be displayed onto the screen for the user to see.

2.4.3 Software

The Raman scattering of the material will be captured by the spectrometer's detector. The captured signal is then processed by the Raspberry Pi, creating a graph to show the intensity of light at all points across the wavelength spectrum (measured in nanometers). The resulting graph will be compared to similar signatures of previous scans using methods such as dynamic time warping and k-means clustering. The user will communicate with the Raspberry Pi via a graphical user interface on the attached LCD. First, they will be prompted to select between the settings of product comparison and material analysis. In the case of product comparison, the controller will search through a numpy array of prior scanned products to find if any pass a similarity threshold designed to identify identical products. If this threshold is cleared, the user will be told through the LCD that the product is a match, listing the product from the ID label attached to the matched item inside the closet array. If there is no match detected, the user will be prompted to input a name tag for the signature so that it can be saved into the closet array as a new product for future scans. When material analysis is selected, the signature will be sorted into one of three integer arrays containing the signature data of all previous trials for a specific identified material, displaying the label of the most similar group of prior scans (cotton, polyester, silk) on the LCD as the material the sample has been matched with.

2.5 Engineering Requirement Specifications

Table 2.5.1 Engineering Requirement Specifications

Table 2.5.2 Engineering Requirement Specifications		
Parameter	Specification	Units
Material Analysis Accuracy	>90%	Percent
Total Response Time	<10	Seconds
Product Comparison Accuracy	>90%	Percent
Spectral Resolution	<12	cm ⁻¹
Spectral Range	600 – 3000	cm ⁻¹
Signal Strength	8	pW

Signal to Noise Ratio	50	N/A
Battery Life	>5	Hours
Battery Voltage	$3.7 < x < 5$	Volts
Battery Charge Capacity	>10,000	mAh
Battery Energy	≥ 37	Wh
Maximum Current Required	<2	Amps
Unit Size	<24''x18''	Inches
Unit Weight	<10	lbs
Cost	<\$2,500	USD

Table 2.5.3 Component Specifications

Table 2.5.4 Component Specifications			
Component	Parameter	Specification	Units
Plano-convex Collimating Lens DTR-G-2	a) EFL b) BFL c) Diameter d) NA e) Thickness f) Center wavelength g) Coating	a) 4 b) 2.4 c) 6.33 d) .6 e) 3 f) 445 g) AR	a) mm b) mm c) mm d) N/A e) mm f) nm g) N/A
Plano-convex Focusing Lens #48-423	a) EFL b) BFL c) Diameter d) NA e) Thickness f) Center wavelength	a) 18 b) 15.20 c) 18 d) .5 e) 5 f) 587.6	a) mm b) mm c) mm d) N/A e) mm f) nm
Plano-Convex Fiber Coupling Lens #49-879	a) EFL b) BFL c) Diameter d) NA e) Thickness	a) 45 b) 43.35 c) 15 d) .17 e) 2.5	a) mm b) mm c) mm d) N/A e) mm

	f) Center wavelength	f) 587.6	f) nm
Dichroic Mirror Chroma T525lpxr	a) Cut-on wavelength b) Transmission wavelength c) Reflection wavelength d) Diameter e) Transmittance f) Reflectance g) Thickness	a) 525 b) 525-1000 c) 390-510 d) 25 e) 96.47 f) >97 g) 3.5	a) nm b) nm c) nm d) mm e) % f) % g) mm
Laser diode ams-Osram PL 520B	a) Wavelength b) Output power (typ.) c) Current (typ.) d) Threshold current e) Voltage (typ.) f) Spectral bandwidth g) Parallel beam divergence h) Perpendicular beam divergence	a) 520 b) 80 c) 200 d) 40 e) 6 f) 1 g) 6.3 h) 22.5	a) nm b) mW c) mA d) mA e) V f) nm g) Degrees h) Degrees
Longpass Filter Chroma ET525lp	a) Cut-on wavelength b) Transmission wavelength c) Rejection wavelength d) Diameter e) Optical density f) Transmittance	a) 540 b) 529.4-900 c) 404-515 d) 20 e) 6 f) 97.73	a) nm b) nm c) nm d) mm e) OD f) %
Multimode fiber Newport F-MCC-T	a) Core diameter b) Cladding diameter c) Wavelength range d) Bandwidth e) NA	a) 200 b) 220 c) 250-1100 d) 25 e) .22	a) μm b) μm c) nm d) MHz/km e) N/A
Entrance slit DIY Optics	a) Width b) Height c) Thickness	a) 100 b) 3 c) 0.2	a) μm b) mm c) mm
Collimating Mirror Thorlabs CM254-250-E02	a) Focal length b) Radius of curvature c) Diameter	a) 250 b) 500 c) 1	a) mm b) mm c) inches
Ruled Reflection Diffraction Grating MKS Newport 33025FL01-280R	a) Groove density b) Blaze wavelength c) Blaze angle d) Size	a) 1200 b) 500 c) 14.5 d) 12.5 x 12.5	Grooves/mm mm Degrees mm

Focusing Mirror Thorlabs CM254-250-E02	a) Focal length b) Radius of curvature c) Diameter	a) 250 b) 500 c) 1	a) mm b) mm c) inches
Linear Array CCD TCD1304DG	a) Pixel amount b) Pixel size c) Detector width d) Dynamic range e) Power supply voltage f) Operating temperature	a) 3648 b) 8 x 200 c) 29.1 d) 300 e) 3 f) -25 to 60	a) N/A b) μm c) mm d) N/A e) V f) $^{\circ}\text{C}$
LCD	Resolution	800 x 480	Pixels
LCD	Screen	5.6 x 6	Inches
LCD	Color	18	Bits (262,144 total colors)
LCD	Supply Voltage	3.3	Volts
Voltage Regulator	Voltage Maintenance	3.3, 5	Volts
Raspberry Pi	RAM Capacity	4	GB
Raspberry Pi	Processing Speed	2.4	GHz

2.6 Hardware Block Diagram

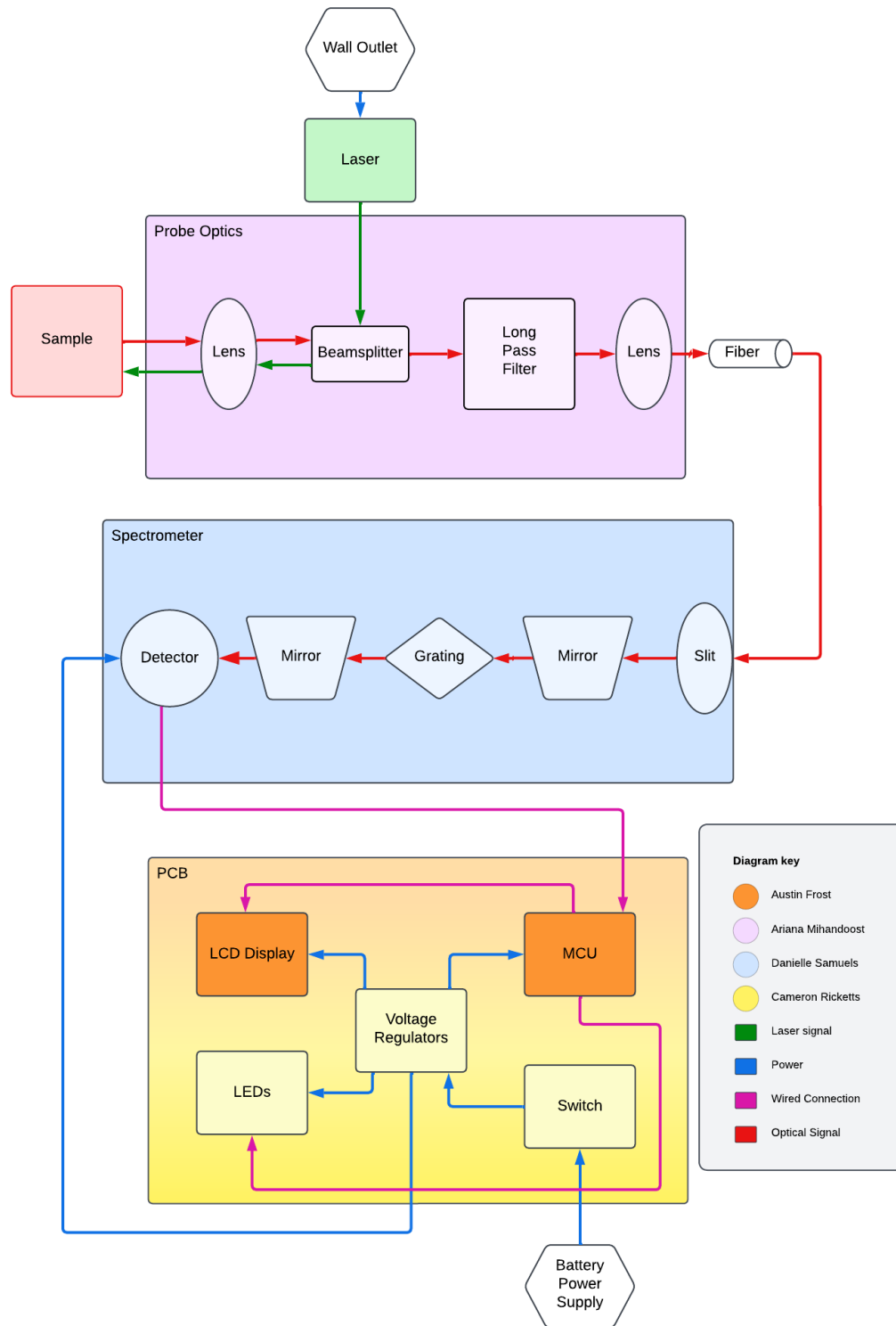


Figure 2.6.1 Hardware Block Diagram

2.7 Software Block Diagram

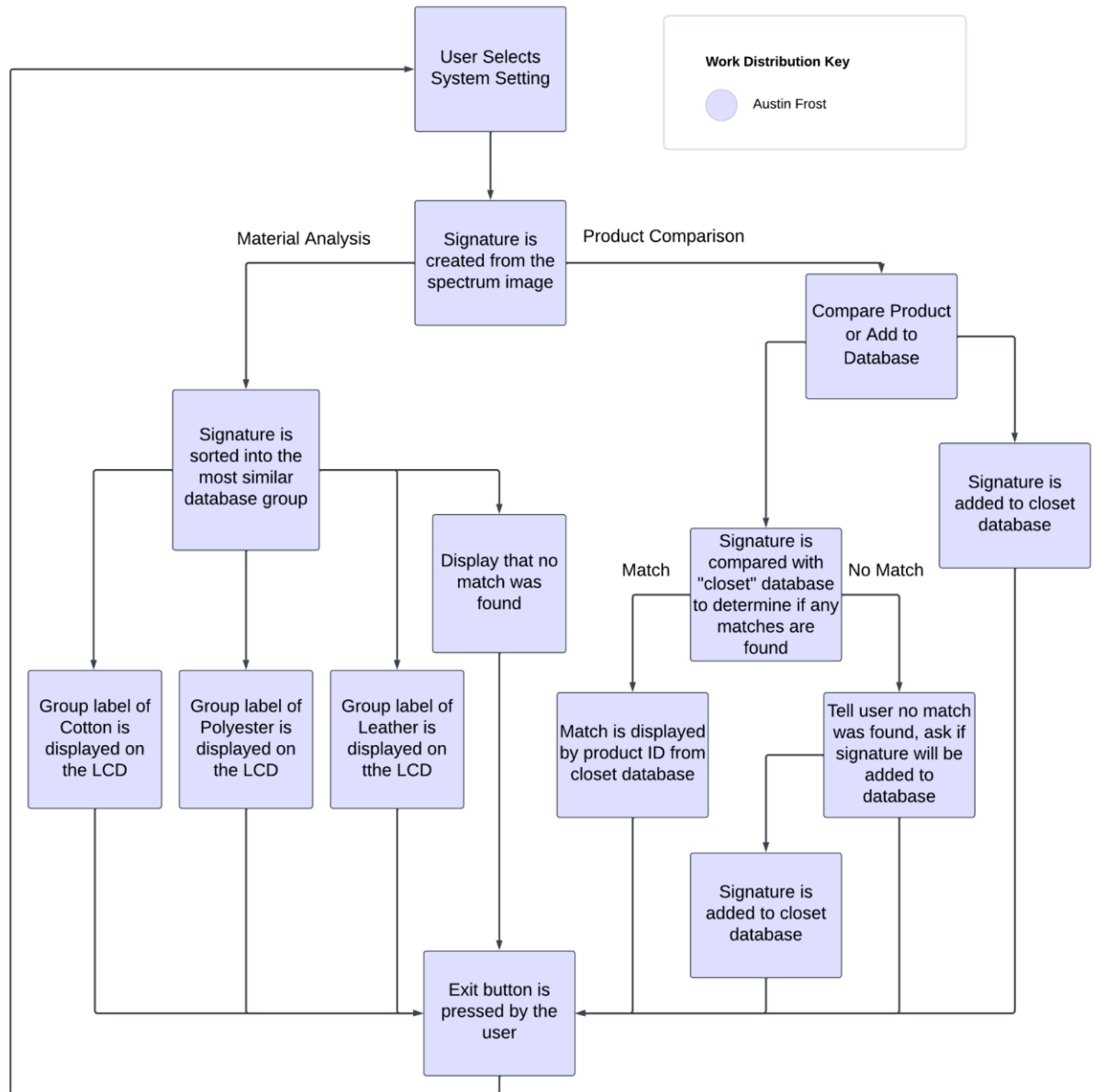


Figure 2.7.1 Software Block Diagram

2.8 House of Quality

Correlations														
Positive		+												
Negative		-												
No Correlation														
Relationships														
Strongly Positive		↑↑												
Weakly Positive		↑												
No Correlation														
Weakly Negative		↓												
Strongly Negative		↓↓												
Direction of Improvement														
Maximize		▲												
Target		◇												
Minimize		▼												
Column #		1	2	3	4	5	6	7	8	9	10	11	12	13
Customer Requirements (Explicit and Implicit)	Engineering Requirements	Maximum Cost	Material Analysis Accuracy	Total Response Time	Product Comparison Accuracy	Spectral Resolution	Laser Power	Unit Size	Unit Weight	Battery Life	Battery Voltage	Battery Charge Capacity	Battery Energy	Maximum Current Required
	Direction of Improvement	▲	▲	▼	▲	▲	◇	▼	▼	▲	◇	▲	▲	▼
	Accuracy	▲	↓	↑↑	↑↑	↑	↑							
	Speed	▲	↓↓	↑	↓↓	↑	↑							
	Performance	▲	↓↓	↑↑	↓↓	↑↑	↑↑			↑	↑	↑	↑	
	Safety	▲					↓↓							↑
	Portability	▲						↑↑	↑↑	↑↑	↑	↑	↑	
	Cost	▼	↑↑	↓↓	↓	↓↓	↓↓	↓↓	↓↓	↓↓	↓	↓↓	↓↓	↓
Target		<\$2500	>90%	<5 sec	>90%	>50 cm ⁻¹	<100 mW	Approx. 24" x 18"	<10 lbs	>5 hours	3.7 V < x < 5 V	>= 10,000 mAh	>= 37 Wh	<2 A

Figure 2.8.1 House of Quality

3 Research and Development

This chapter details the experimental methodologies and components being applied in this project to create a working prototype textile identification device.

Needed: Regulators, battery types, switches buttons physical I/O, communication protocols add serial comm in ch. 3. No info on software– packages, platforms, frameworks, environment, language etc. basics. If using matlab explain why

3.1 Electrical Hardware

3.1.1 LCD Technology Comparison

The user's interaction with the system will come through a display connected to the system's controller. From this display, the user will provide all required input beyond the sample itself, and with the display, the spectral signature and final output message can be shown. In the simplest example, this could be accomplished with a graphical user interface (GUI) in the case of a laptop computer being used as the system controller, as several GUI libraries are available in all common programming languages that would be capable of creating an interface window with all functionalities necessary for the project. However, as portability goals eliminated a laptop as a controller option for the project, a GUI is no longer possible for the system, as when using microcontrollers or single board computers, displays are separate from the controller and use communication protocols for operation.

Because of this, possible options would have to be liquid crystal displays (LCD) or light-emitting diode (LED) displays, in both cases small enough to be portable. In the end, an LCD was chosen for this project, as an LED matrix would have been more expensive on average despite being only marginally larger in screen size and providing worse image quality. The matrix spacing of LED displays makes them an ideal choice for commercial billboards or jumbotrons for sporting events, but in portable displays just a few inches in dimension, they are insufficient. LCDs, in contrast, handle this task very well, which is why most desktop monitors are liquid crystal displays, though many use LED backlighting. LCDs also provide the largest amount of options for our system, so there is very little downside.

3.1.2 LCD Selection

So the output of the system will be shown to the user on a liquid crystal display. The LCD will provide the system's setting options to the user via touchscreen functionality before displaying the system's results, namely spectral signatures and output messages of the textile material detected or the result of a duplicate item test. These functions require the LCD in question to be small enough to fit the scale of the system but also large enough for easy interaction with the user, providing enough space for simple touchscreen selection of system settings and legibility of the output results.

The first option is the standard 16 x 2 dot matrix liquid crystal display module, the cheapest and most common LCD model. It is the same type used in UCF classes from Embedded and Real Time Systems to Junior Design. This was the initial idea when an LCD was proposed early on in the project planning phase; however, as the requirements of the display grew, it became clear that the module would be insufficient in functionality to achieve what we had in mind. Without touchscreen functionality, it is unable to take any form of input from the user, and with a dot matrix, it is impossible to show the user the generated spectral signature as part of the output. These limitations made the cheaper price tag irrelevant, and so it was clear that an LCD with higher levels of functionality would be necessary.

The next option is the Hosityond touch screen, a high-resolution display developed for the Raspberry Pi. It is significantly higher priced compared the previously mentioned LCD (\$32.99 vs \$6.99) but is much better in terms of functionality. The Hosityond's display is a vast improvement in several categories, with touchscreen functionality, a resolution of 800 x 480 pixels, dimensions of 5.6 x 6 inches, and 18 bits of color (262,144 colors total). It can fulfill every function planned for the display in our system and there is such a high level of improvement over cheaper alternatives that the cost increase in this case is justified. The display being specifically developed with the Raspberry Pi in mind means that if the Raspberry Pi is chosen as the controller in our system, then the Hosityond will be seamless in its integration. The downside of the Hosityond is that, given its dependency on the Raspberry Pi, if another controller is selected, then the display will be much harder to configure, and another display will have to be used.

The third option is an LCD with a similar level of functionality as the Hosityond but developed for common microcontroller units. The LCD still has the same requirements as the Hosityond, needing both touchscreen capabilities as well as the size and pixel resolution to adequately display spectral signatures and text output. This option should also be lower in cost than the Hosityond, as due to its independent operating system, development for the Raspberry Pi is almost always more expensive than development for an MCU like the ESP32. As a result, all directly connected components like the LCD should be required to have a lower cost than the alternative raspberry pi product. The chosen LCD model for this option is the AITRIP development board smart display. The display is a touchscreen, 5.8 x 4.5 inches in dimension, has a 240 x 320 pixel display, and has a price tag of \$17.99, fulfilling all four previously stated requirements.

Table 3.1.1 Liquid Crystal Display Product Comparison

	Dot-Matrix	Hosityond Touchscreen	MCU Touchscreen
Cost	\$6.99	\$32.99	\$17.99

Touchscreen Functionality	No	Yes	Yes
Size	1.4 x 3.1 inches	5.6 x 6 inches	4.5 x 5.8 inches
Resolution	N/A	800 x 480 pixels	240 x 320 pixels
Required Supply Voltage	5V	3.3V	5V
Communication Protocol	I2C	DSI	UART, SPI, I2C

The final decision on which LCD option would be best was inherently tied to the choice of which controller would be used on the software side. While the requirements of the chosen display led to the dot-matrix LCD being eliminated, the question of whether a Raspberry Pi would be part of the system was ultimately the deciding factor on which option was chosen. If the display is connected to a Raspberry Pi, then the Hosyond is the clear choice, otherwise, the AITRIP display would be better suited for the system. The final version of the project will include a Raspberry Pi, as explained in the following section, and so the Hosyond was chosen.

3.1.3 System Controller Technology Comparison

All actions done in the software end of the project will be done through the system controller, which can be anything from a microcontroller built into the printed circuit board, to a single board computer like a Raspberry Pi, and even a laptop or desktop computer. The third example is not a real option for this project however, as even a laptop would mean the system overall is no longer viable, as a project goal is for the entire project to be small enough to be carried by one person.

At the opposite end, a microcontroller, while small enough to accomplish the goal of system portability, is insufficient for other project goals. A microcontroller does not have the technical support necessary for all aspects of the project, as while the extraction of image data, data preprocessing, signature generation, dynamic time warping, and clustering calculations are all feasible for more robust microcontrollers, running through all of these consecutively as required in this project on a microcontroller would result in unacceptable performance for the system, taking far too long to deliver to the user an output, even if the end results are found to be accurate. For these reasons single board controllers provide a preferable middle ground that can allow for all goals of the project to be achieved.

3.1.4 System Controller Selection

While the photonics side of the project can take a physical sample as input and generate a spectrum, and the printed circuit board is able to power system components such as the laser diode and the liquid crystal display, the actual goal of the project depends on the software analysis done by the controller to create the output the user is looking for. The controller's job includes graphing the spectral signature of the sample from the analog image data generated by the optical spectrometer's detector and finding a match for the signature's data from previous scans of textile groups or clothing items, depending on the user's setting selection.

The first product that came to mind was the Raspberry Pi, as the RPi is a single-circuit board computer built with an independent operating system. This means the Raspberry Pi would fit the scope of the project in terms of physical size but also in terms of complexity. The board is 2.2 x 3.35 inches in dimension and since its operating system is capable of running python code and can be used to perform machine learning methods like those possibly expected in the project, the board fulfills all requirements for consideration for the project. The series model chosen for consideration is the newest version (Fifth Gen), as while the 4B was considered since the newest generation model is still recent enough that not all common commercial accessories are compatible, the 5 is marketed with an increase of over double the CPU performance. The previously mentioned RPi 5 model comes in four variations depending on the chosen size of internal memory, available in models with two gigabytes of random access memory, four gigabytes of RAM, eight gigabytes of RAM, and a newly added sixteen gigabyte model. The price tags of these versions are \$59.99, \$69.99, \$89.99, and \$129.99, respectively. The board has forty general-purpose input and output pins, and is compatible with the Honyond liquid crystal display. The 5 model also has a 2.4 gigahertz sixty-four-bit quad core processor, a GPU frequency of eight hundred megahertz, a maximum power of fifteen watts, thirty-two giga-bytes of flash memory storage, and multiple commonly sold compatible external memory cards if the purchased version's internal memory is determined to be insufficient for the scope of the project. The RPi also has a larger amount of product documentation, example projects, open source code, and overall community resources for debugging and general support than any other system controller option. Considering all of this, the four-gigabyte 5 model is well suited for the role of system controller in this project.

The alternative to the Raspberry Pi would be to choose a more standard controller development board. However, the drawback with this approach is that true microcontrollers (boards without a built-in operating system) are likely to fall short of the project's requirements, while single-board computers like the RPi are frequently in the three-digit price range, an unnecessary expenditure for this project. There are exceptions though, products that lie in the middle range of performance and cost. One of these is the NVIDIA Jetson Nano. At \$88.99 the Nano is noticeably more expensive than the Raspberry Pi, but not outside the possible price range of this project. The development board has four gigabytes of random access memory, a 1.43 gigahertz CPU, forty general purpose input and output pins, a power range maximum of ten watts, sixteen giga-bytes of flash storage memory, is 3.95 x 3.15 inches in size, and has an improved nine hundred and twenty-one megahertz GPU over the RPi, with four hundred and seventy-two giga-floating-point operations per second. The board has quality library support, especially for Python

libraries, which is a notable upside for this project. There are, however, options with further improved performance compared to both the Raspberry Pi and Jetson Nano.

If the choice is based purely on performance, the Coral development board would be the best alternative. The largest detractor for this option is the cost, at \$129.99 for the basic model, and \$169.99 for the four giga-byte random access memory version, it is significantly more expensive than all other choices mentioned. The upside of the board is that it has the newest and most efficient processor of any option, with listed maximum capabilities of four tera-floating-point operations per second at just half a watt for every thousand operations. At two watts for four TFLOPS, the Coral development board is easily the top choice among the three options in both processing speed and energy consumption, possibly justifying the very significant price jump of \$169.99, which would be one hundred and fifteen dollars more than the Raspberry Pi, and eighty-one dollars more than NVIDIA's Jetson Nano. The board has forty general purpose input and output pins, a 1.5 gigahertz CPU, 1.6 gigahertz GPU, eight giga-bytes of flash memory storage, is 3.45 x 2.2 inches in size, and runs on the Linux-based operating system Mendel, a variant of Debian. A notable downside of the board is a lack of choices when it comes to Python packages, as many prominent libraries are unavailable, which is a considerable limitation given the asking price of the product.

Table 3.1.2 System Controller Product Comparison

	Raspberry Pi 5	NVIDIA Jetson Nano	Coral Development Board
Price	\$60.00	\$88.99	\$169.99
Floating-point Operations Per Second (FLOPS)	13.5 Giga-FLOPS	472 Giga-FLOPS	4 Tera-FLOPS
Random Access Memory	4 GB	4 GB	4 GB
GPIO Pin Count	40 pins	40 pins	40 pins
Physical Size	3.35 x 2.2 inches	3.95 x 3.15 inches	3.45 x 2.2 inches
CPU Frequency	2.4 GHz	1.43 GHz	1.5 GHz
GPU Frequency	800 MHz	921 MHz	1.6 GHz
Maximum Power Usage	15 Watts	10 Watts	2 Watts
eMMC Storage	16 GB	16 GB	8 GB

The Raspberry Pi was chosen as the best middle ground option after considering factors such as performance, flexibility, support, and cost. The RPi meets the requirements of the system on its own, but in the worst case is still capable of closing all performance gaps while maintaining an advantage in cost and support. The RPi 5 has additional first-party commercial devices that greatly expand the board's memory and processor performance. SD card add-ons increase the internal eMMC storage to thirty-two or sixty-four gigabytes for \$12.95 or \$14.95. Also, the artificial intelligence hardware attachment features a neural network accelerator with additional support, this device increases the RPi's performance capability significantly, advertised with the ability to conduct thirteen trillion floating point operations per second, more than triple that of the Coral development board, and at \$85.00, the total price of the board with the hardware attachment is still twenty-five dollars cheaper. Given this level of support in both open source software and additional hardware products, the Raspberry Pi can offer the best of both worlds while remaining the most cost-effective option.

3.1.5 Printed Circuit Board Design Software Comparison

A printed circuit board, also known as a PCB, is a structure that is used for electric assemblies using copper conductors acting as wires between components. Printed circuit boards are also used as an enclosure for housing components properly and securely while ensuring proper connections as desired. The circuit boards are typically composed of multiple layers consisting of conductive copper and electrically insulating material. The outermost layer consists of a non-conductive solder mask that allows for exposed conductive copper pads and traces where components are to be placed. These placements are done by through-hole soldering, surface-mount soldering, or a combination of the two. Through-hole soldering is the process of taking the lead pins of a component and placing them into conductive holes of the PCB and then connected with soldering wire (this method is usually for larger external components like LCDs, switches, and battery sources). Surface-mount soldering is done by placing solder paste onto the pads of the PCB followed by the components and then placed into a reflow oven (this method is often used for smaller components such as LEDs, resistors, capacitors, etc.). Both of these methods ensure proper secure connections allowing the PCB to function properly. The outer layer also contains a silk screen that is printed on top of the solder mask that will label the components as specified to help differentiate between one another when undergoing the soldering process.

For this project all the hardware components will be integrated and housed into the PCB. The battery source will be through-hole soldered into the board which will then be connected to the switch component. From the switch the connections will lead to the voltage regulators and from there voltage will be distributed to the components such as the LCD, LEDs, and microcontroller. Connections will also be made for the microcontroller to be able to communicate with the LCD and detector.

In order to obtain a PCB that meets the needs of the project, it must be customized and designed as desired. There are mediums to complete this through design softwares that specialize in PCB design. The softwares that are under consideration include SolidWorks, EAGLE, and Fusion 360. The following analysis will focus on highlighting the specialties

of the softwares to further decide which software would be chosen to design the PCB for the project.

SolidWorks

SolidWorks is a CAD software used in the industry for designs who self-proclaims it to be the best. They also make strong claims that using SolidWorks will make the user a better designer. Their main focus is being the industry standard for 3D design, mechanical CAD, and production ready documentation. With this skill set, designing capabilities are endless from structures, automobiles, to PCBs which is our focus. For creating PCBs with SolidWorks they have a subdivision called SOLIDWORKS PCB and is powered by Altium. The software claims to have an easy-to-use interface allowing PCB design to be completed quickly and efficiently. With such a broad field of expertise, this allows for ECAD and MCAD collaboration meaning collaboration between the electric design and mechanical design which can be valuable for projects that require both.

The use of the ECAD and MCAD collaboration that SOLIDWORKS PCB provides are the main backbone of the benefits they have to offer. One of the benefits stated is it enhances team efficiency by enabling seamless ECAD-MCAD collaboration for streamlined cross-discipline development. The software improves communication by providing intelligent, real-time collaboration between electrical and mechanical teams. It helps optimize project management by reducing prototyping costs and minimizing rework through accurate electromechanical integration. Additionally, its real-time visualization features prevent design flaws, ensuring proper fit of the PCB and its components inside of its mechanical enclosure before manufacturing and assembly.

EAGLE

EAGLE is the next design software under consideration. In short, EAGLE is an electronic design automation (EDA) software which is developed by Autodesk and allows users to create schematics and design PCBs. The software lets PCB designers connect their project schematic diagrams, component placement, PCB routing, and comprehensive library content. Unlike SolidWorks, EAGLE does not support 3D modeling and is primarily focused on electronic design rather than mechanical design.

For PCB design EAGLE has their own set of benefits when compared to other softwares as well. With its low requirement of disk space, EAGLE is lightweight on storage, requiring between 50 and 200 MB. The software's platform versatility gives it merit when it comes to using either MAC, Windows, and Linux. It is claimed to be the preferable tool across all PCB communities especially when sending layouts. The cost is also something to take note of due to the fact EAGLE offers a freeware version. It is believed that the features that EAGLE provides allows users to create any intermediate or simple PCB with ease for designers that are novices to PCB development.

Fusion 360

The last software under contention is Fusion 360 which is a cloud-based 3D computer-aided design (CAD), computer-aided manufacturing (CAM), computer-aided engineering (CAE), and PCB design software developed by Autodesk similar to EAGLE. Fusion 360 has gained recognition in the industry for its wide range of features and has been praised for its advanced 2D and 3D-based designing capabilities. Fusion is a fairly new program when compared to the others and has been welcomed by the industry due to its features.

Considering that Fusion 360 provides such a wide variety of features, it also has a considerable amount of benefits. Although having many functions which can be perceived as overwhelming, the user interface has maintained a reputation of being described as friendly and easy-to-use. Like SolidWorks, Fusion allows for MCAD and ECAD designing and collaborations, making projects dealing mechanical and electrical design seamless. Making the software cloud-based permits collaborators to work on projects together to complete designs and tasks which is essential for a team based project. Another useful strength the software has is its simulation feature allowing developers to test their designs to verify the product is working as desired before fabrication and while in different situations and stresses. When creating the design Fusion also takes note of the parts and components implemented into the design and in turn is able to produce a bill of material (BOM) for the parts needed for the fabrication process. Most importantly, for a group of college students is the price. Traditionally, fusion charges \$85 monthly or \$680 annually, however they offer a 3 year free trial for students to be able to make designs.

3.1.6 PCB Design Software Selection

After analyzing the benefits and attributes that the design softwares has to offer, the information noted will be used in the following chart to compare to one another to ascertain which software will be ideal for the project design.

Table 3.1.3 Design Software Comparison

Feature	EAGLE	Fusion 360	SolidWorks
Best For	Pure PCB design	PCB & Mechanical design	PCB & Mechanical design (Industrial Focused)
Primary Function	PCB schematic & Layout	3D CAD + PCB integration	Mechanical CAD with PCB add-ons
PCB Schematic & Layout	Yes	Yes	Yes with add-ons

PCB Design Tools	Dedicated tools PCB	Dedicated tools PCB	Requires add-ons
3D Modeling	No	Yes	Yes
Mechanical Integration	No	Strong	Strong
Cloud Collaboration	Some	Yes	Limited
Pricing	Freeware Version	Free for Students	\$60-\$139 for Students

After a side by side comparison, the ideal PCB design software becomes apparent. While providing many features that are valued for this project, and having much flexibility, Fusion 360 is unmatched. The main differences distinguishing it from EAGLE was the versatility, allowing for 3D modelling and mechanical integration while remaining exemplary in PCB design. Another key factor giving it edge is the cloud collaboration feature provided which is crucial for this team based project. As for SolidWorks, although having versatile and useful features, it also has its drawbacks. The fact that add-ons may be needed for efficient design and the limitation on cloud collaborations are the first handicaps observed. Also, due to the scale of the project at hand and not being an industry level project, it is not necessary to be used at the moment. Lastly, and the overall deciding factor was the disadvantage of the pricing when compared to Fusion 360. In closing, Fusion 360 has proven itself to be the best software for use to complete creating the PCB due to its features, flexibility, collaboration element, simulations, 3D modelling, and most importantly pricing.

3.1.7 Signal Analysis Methodology Comparison

Throughout the project, the values obtained from the Raman spectrum will be provided as an analog signal. An analog signal is a type of signal that continuously varies over time and holds information that can be transferred between devices, sensors, and systems. These signals are naturally produced by the entity under analysis and remain in a continuous state, both in terms of amplitude and time. In other words, analog signals are present in almost all physical phenomena, including sound waves, temperature fluctuations, and light intensity, making them fundamental in various scientific and engineering applications. In the context of this project, the materials under examination will generate analog signals when placed under the Raman spectrometer, allowing for the analysis of their spectral properties.

To accurately process the signal and extract meaningful data, it is essential to convert the given analog signal into a digital format. Digital signals are another form of electrical signal used for transmitting information between devices, sensors, and systems, but unlike analog signals, they do not exist as a continuous wave. Instead, digital signals encode information using discrete binary values, typically represented as a series of ones and zeros. This digital

representation makes processing, storage, and transmission significantly more efficient and reliable, particularly in modern computing systems. Compared to analog signals, digital signals are generally more resistant to noise and external disturbances, making them ideal for applications where precision is crucial. However, despite the reduced impact of noise, digital signals are not entirely immune to errors. The process of sampling an analog signal for digital conversion can lead to the loss of certain details, and quantization errors may occur when the signal is mapped to a finite number of discrete levels. To mitigate these issues, techniques such as antialiasing filters and higher-resolution sampling can be employed. Additionally, while digital signals offer improved accuracy and power efficiency, they often require greater bandwidth for transmission, which can be a limiting factor in some systems. Nevertheless, due to their reliability, accuracy, and ease of integration with digital processors, digital signals have largely replaced analog signals in many modern applications.

To achieve this conversion from analog to digital, an analog to digital converter (ADC) must be utilized. This is necessary because microcontrollers and most modern digital processing units cannot interpret analog signals directly, instead they require data to be in a digital format. The conversion process involves several key steps: first, the analog signal is sampled at specific intervals, determining how frequently the signal's values are recorded. Next, the sampled values are quantized, meaning they are mapped to a finite set of discrete levels, defining the resolution of the resulting digital signal. Finally, the quantized values are encoded into binary form, creating a structured digital representation of the original analog input. The accuracy of this conversion is largely dependent on the sampling rate, which dictates how often the signal is measured per unit of time. According to the Nyquist theorem, the optimal sampling rate should be at least twice the highest frequency present in the analog signal which is known as the Nyquist rate. Failing to meet this requirement can lead to aliasing, a phenomenon where high-frequency components are misrepresented in the digital domain, causing distortions in the signal. Therefore, it is crucial to use an analog to digital converter capable of supporting the necessary sampling rates to ensure precise and accurate data conversion.

Table 3.1.4 Signal Analysis Comparison

Feature	Analog Signal	Digital Signal
Type	Continuous values produced over time as a waveform	Discrete binary values represented as 1's and 0's
Application	Represents real-world phenomena as continuous values	Represents information as data in discrete numerical values
Bandwidth	No limitations	Band-limited
Disturbances	More susceptible to noise and distortion	Less susceptible to noise and distortion
Accuracy	Accuracy can be heavily affected by noise	More accurate, but may introduce quantization and sampling errors

Error correction	Once information is altered, errors cannot be easily corrected	Errors can be detected and corrected by way of encoding methods and antialiasing
Power	Higher Power Consumption	More Power Efficient at the cost of Bandwidth
Processing & storing	Harder to process and store due to continuous nature	Easier to process and store due to discrete values while allowing for easier encoding and transmission
Transmission Efficiency	Requires less bandwidth but is affected by interference	More reliable, but more bandwidth required
Requirements	Requires disturbance free setting and more power	Requires Analog-to-Digital Conversion and less power

3.1.8 Analog to Digital Converter Selection

When considering the implementation of an analog-to-digital converter (ADC) for this project, several viable options present themselves for evaluation. The three ADCs under consideration are the MCP3008, ADC0804, and ADS1115. Each of these devices has unique features, specifications, and limitations that make them suitable for different scenarios. The goal is to analyze these options based on their operational characteristics and determine which one best aligns with the requirements of this project.

MCP3008

The first candidate is the MCP3008, a 10-bit ADC that offers a practical combination of precision and flexibility. It features 8 input channels, which can either be used as 8 single-ended inputs or as 4 differential pairs. This capability allows it to support multiple signal configurations, depending on the application's needs. However, single-ended inputs are generally more susceptible to noise and environmental interference, which could affect measurement accuracy. To help mitigate this, the MCP3008 includes separate ground connections for analog and digital circuits, offering improved noise isolation and flexibility during hardware integration.

The 10-bit resolution allows for 1024 quantization levels, providing a moderate degree of precision when converting analog inputs into digital values. The device uses a 4-wire SPI (Serial Peripheral Interface) protocol for communication with microcontrollers, ensuring fast and reliable data transmission. The MCP3008 operates within a voltage range of 2.7V to 5.0V and supports a sampling rate between 75 kbps and 200 kbps. This high sampling rate enhances its suitability for applications where quick and accurate data acquisition is essential. With an operational temperature range of -40°C to 85°C, it offers adequate resilience for typical environmental conditions, making it a reliable and versatile option for general-purpose ADC tasks.

ADS1115

The second option is the ADS1115, a high-precision 16-bit ADC that significantly improves resolution and measurement detail. Out of the 16 bits, 15 are used to quantify the voltage level, while the 16th bit is a sign bit, allowing the ADC to differentiate between positive and negative voltages. This dual polarity support is particularly useful in applications requiring differential voltage readings or where signal polarity is critical.

The ADS1115 offers both single-ended and differential input modes. However, in single-ended mode, it only processes positive voltages unless the comparator mode is activated. The device communicates using the I2C protocol, which supports multiple devices on a shared bus, simplifying system integration in multi-sensor setups. Having 15-bit resolution allows for 32,768 quantization levels, the ADS1115 delivers high-resolution signal conversion, enabling accurate measurements of small voltage changes. It can handle input voltages up to 6.144V and offers a voltage resolution as low as 0.187 mV. Although its maximum sampling rate is lower at 0.86 ksp/s, this is often sufficient for low-frequency signals where precision is prioritized over speed.

One of the most beneficial features of the ADS1115 is its internal comparator function, which can detect overvoltage or undervoltage conditions and trigger alerts. This adds a layer of safety and regulation to signal monitoring. The device has an extended temperature range of -40°C to 125°C, making it suitable for more demanding environments. Overall, the ADS1115 stands out as a precise and reliable ADC, especially valuable when high resolution and signal integrity are critical.

ADC0804

The final ADC reviewed is the ADC0804, which offers an 8-bit resolution and is best suited for simpler, low-resolution applications. With only 256 quantization levels, this converter has the lowest sampling precision among the three, which could be a limiting factor in cases where more precision and differentiation in measurements is required. Nevertheless, it is a straightforward and cost-effective solution for converting analog signals between 0V and 5V into digital values.

The ADC0804 operates with a voltage supply of 2.5V to 6.5V and utilizes a Successive Approximation Register (SAR) architecture paired with a differential potentiometric ladder to perform signal conversion. It supports only a single differential analog input channel and lacks the versatility of handling multiple inputs or single-ended configurations. The maximum sampling rate is 10 ksp/s, which, while relatively low, is still usable for basic tasks that don't demand high-speed data requirements.

One of the appealing aspects of the ADC0804 is its ease of integration. It does not require complex interfacing logic with microcontrollers, making it ideal for entry-level applications or systems where simplicity is key. However, its recommended operating temperature range is limited to 0°C to 70°C, which may pose constraints in harsh environments, but may still fall within the scope of this project so it wouldn't raise too

much worry. Despite these limitations, the ADC0804 remains a practical option for low-cost, low-precision applications where basic signal conversion is sufficient.

ADC Selection

After thoroughly analyzing each analog to digital converter we can conclude each one has their own benefits as well as limitations that are specialized for different requirements. The following chart will highlight and compare the practicality of each one. This will then be used to select which ADC would be optimal and provide the desired performance.

Table 3.1.5 ADC Comparison

Feature	MCP3008	ADS1115	ADC0804
Resolution	10-bit	15-bit with sign integration	8-bit
Quantization Levels	1024	32,768	256
Input Channels	8 single-ended / 4 differential	4 single ended / 4 differential	1 differential
Input Signal Voltage range	0 to 5 volts	-6.144 volts to 6.144 volts	0 to 5 volts
Sampling Rate	75 ksp/s – 200 ksp/s	0.86 ksp/s	Max 10 ksp/s
Power supply	2.7 volts - 5 volt	2 volts – 5.5 volts	2.5 volts – 6.5
Operating Temperature	-40 degrees Celsius to 85 degrees Celsius	-40 degrees Celsius to 125 degrees Celsius	0 degrees Celsius to 70 degrees Celsius
Communication Protocol	SPI	I2C	No interfacing protocol needed
Polarity	Positive	Positive and Negative	Positive
Comparator	No	Yes	No
Input Mode	Single Ended or Differential	Single Ended or Differential with comparator	Differential
Main Benefit	High sampling rate	Comparator and quantization precision	Ease of use
Best Use	Moderate speed multi-channel readings	High-precision Low frequency readings in temperature varying locations	Simple low-precision ADC needs
Cost	~\$3	~\$4	\$2-\$5

After comparison, even though all may be effective enough to successfully implement into the project, each one's abilities and benefits are directly apparent. For this reason, the

ADS1115 would be the ideal ADC to incorporate to the system. Due to its practicality, low voltage resolution, precision, and features. Also allowing for efficient stability in different climates and conditions and providing safety and troubleshooting protocols such as the undervoltage and overvoltage detection. The only drawbacks found were the slower sampling rate and having slightly less ease of use when compared to the ADC0804. These downsides in comparison are minimalistic and won't hinder the project as a whole. Overall, this is the best possible choice for what is being offered with and coming in at a similar price to the others. Figure 3.5.6.1 shows the schematic of the ADS1115, specifically note the inner workings of the circuit.

3.1.9 Power Source Technology Comparison

We will now focus on the power supply, which plays a crucial role in ensuring consistent and proper power distribution among all components in the system. The components that require a reliable power source include the LCD display, the microcontroller, the laser source, the LEDs, the analog to digital converter (ADC), and any other devices or components that may be connected to the PCB. Given the variety of these components, it is essential to meet each of their specific voltage and power requirements to guarantee smooth and efficient operation. The following sections will evaluate different types of common power sources, namely, battery (DC) power sources, AC power sources, and solar power sources with the objective of determining the most appropriate solution for our system.

Battery Power (DC)

Starting with batteries, they provide a direct current (DC) power source. In a DC system, the current flows in a steady, singular direction, which simplifies the power delivery and ensures a consistent energy supply to the components. This simplicity makes DC a widely used and dependable option for electronics. One of the key benefits of batteries is their ability to store energy, allowing the user to harness power when it's needed without relying on an external power grid. The energy in batteries originates from chemical reactions within the cell, which convert stored chemical energy into usable electrical energy. Because of their ability to store power and function independently, batteries offer the appealing option of portability which is an important factor in the context of our Raman spectrometer project, which aims to develop a compact and mobile system.

However, the portability of batteries can be impacted by their size and weight, which varies significantly depending on the type and capacity of the battery. Larger or higher-capacity batteries may prove too bulky or heavy to support a truly mobile design. Additionally, batteries have a finite energy reserve. Once depleted, they must be either replaced or recharged, introducing the need for recurring maintenance or replacement costs. To mitigate this issue, using rechargeable batteries is a suitable and more cost-effective approach over time. Rechargeable battery systems not only help reduce waste but also enhance the practicality of using DC power in portable projects. Another advantage is that DC sources typically deliver a constant voltage level, which is ideal for powering sensitive electronics, ensuring they operate reliably without voltage fluctuations. In terms of safety,

DC sources can be considered dangerous, however, the continuous nature of the current gives individuals a better chance of letting go if contact is made, potentially making it slightly safer in specific scenarios.

AC Power

Now let's consider alternating current (AC) power sources. Unlike DC, where current flows in one direction, AC power alternates its direction periodically, forming a wave usually being sinusoidal in nature. This sinusoidal characteristic allows AC power to be transmitted more efficiently over long distances, which is why it is the standard for power distribution from power plants to homes and industries. A significant advantage of AC is that its voltage levels can be adjusted using transformers, enabling effective long range transmission while minimizing energy losses. This characteristic makes AC particularly suitable for environments where fixed settings are present, such as homes, offices, and industrial facilities.

AC power is commonly accessed via wall outlets and can deliver high amounts of energy, making it ideal for applications that demand significant power or long-term stability. However, the main drawback is that AC sources are generally stationary and are not found in portable applications. While they can be used to charge portable devices or batteries, the source itself must remain connected to a larger grid or generator. In terms of longevity, AC power sources do not rely on stored energy, so they don't deplete like batteries. Instead, their availability depends on the grid's reliability or the operation of the connected generator. In the event where AC power is not available it would be due to outlier factors such as a blown fuse or power outage, in this case maintenance would be required. This eliminates the need for recharging or replacing energy sources, making them highly convenient, although provided the system is stationary. From a safety perspective, AC can be more dangerous than DC due to higher peak voltages and its alternating nature. The human body is more susceptible to harm from AC at certain frequencies due to a lower impedance, and involuntary muscle contraction may prevent a person from letting go if shocked, increasing the overall risk associated with AC systems.

Solar Power

The third energy source under consideration is solar power. Like batteries, solar power delivers DC electricity, but the source of energy differs significantly. Instead of relying on stored chemical energy, solar energy is harvested from sunlight through the use of solar panels composed of solar cells. These cells convert sunlight into electrical energy using the photovoltaic effect, making solar energy a renewable and environmentally friendly solution. One of the greatest strengths of solar energy is its sustainability, it offers a limitless source of power that produces zero emissions during operation, aligning well with modern sustainability goals.

However, there are some practical challenges when using solar power. One major limitation is that solar panels rely on the availability of sunlight, which is not always consistent. Cloudy days, poor weather conditions, or nighttime hours severely limit or halt

power generation, making solar an unreliable source in environments without consistent sun exposure. Even though excess energy can be stored in batteries for later use, the limitation still makes a backup power supply necessary to maintain continuous system operation. Additionally, solar panels typically require a significant surface area for installation and can be difficult to position and integrate into compact systems. Their efficiency is lower compared to other forms of energy, and they generally come at a higher cost. These drawbacks must be carefully weighed when considering solar as the main power supply. However, the ability to convert solar-generated DC power into AC via inverters gives some flexibility, especially in hybrid systems that combine solar with grid power or batteries.

3.1.10 Power source selection

In conclusion, while each of the three power sources has its distinct advantages and disadvantages, the decision must be made based on the specific needs of the Raman spectrometer system with the main factors including portability, cost-efficiency, and power reliability. The below section will highlight these features against each other providing thorough comparison

Table 3.1.6 Power Source Comparison

Features	Battery (DC)	AC	Solar Power (DC)
Current type	Direct Current	Alternating Current	Direct Current
Portability	High (size and weight dependent)	Low (stationary)	Moderate (mostly stationary with exception of some portable panels)
Power Storage	Chemical energy stored	None (continuous supply)	Can store in batteries
Reliability	Great at short distances; depletion may impact	Great	Varies heavily
Ease of Use	Simple	Requires at least one outlet	complex
Stability	Very stable and constant	Fluctuates do to alternating current	Stable as DC, light intensity may cause fluctuations
Efficiency	Moderate	High	Lower
Cost	Low to moderate	Low	High
Maintenance	Medium	Low	Medium
Uses	Portable sensitive electronic devices	Stationary high demand loads	Hybrid systems

After comparing the different power supply options and evaluating their unique advantages, it becomes clear that a battery power supply is the most suitable choice for the Raman Spectrometer system. Its reliability, portability, and stability output make it the

ideal match for this application. Since one of the key goals of the project is to create a portable device, battery power directly supports this objective. Additionally, given the sensitivity of the spectrum signals being received, a stable and noise-free power source is crucial which is something battery power can provide. In contrast, AC power lacks portability and introduces potential instability. Solar power, while renewable, falls outside the scope of this project due to its complexity, unreliability, and higher cost.

3.1.11 Battery Selection

In this section, we will go in-depth on the battery selection process for TEXRAY. Choosing the right battery is a crucial step in ensuring the system operates efficiently and reliably. Several factors must be taken into account when making this decision, including the chemical composition of the battery, its portability, voltage output, and cost. Additionally, any extra benefits a specific type of battery might offer will be considered, as they may provide added value to the overall system performance. After conducting thorough research, three battery types emerged as the strongest contenders: Lithium-ion battery packs, Lithium Iron Phosphate (LiFePO₄) batteries, and Sealed Lead Acid (SLA) batteries. To determine the most suitable option, each will be examined in further detail, comparing their strengths and limitations.

Lithium-Ion Battery Pack

The first option under consideration is the Lithium-ion (Li-ion) battery pack. As the name suggests, these batteries rely on the movement of lithium ions between two electrodes—an anode (commonly made of graphite) and a cathode (often composed of lithium-based compounds). Alongside these electrodes, the third essential component is the electrolyte, which facilitates the movement of ions and enables the generation of an electric current. This current is what powers electronic devices. Li-ion batteries are widely used in portable electronics due to their rechargeable nature and high energy efficiency. Additionally, as previously discussed, they are also an effective solution for solar energy storage.

One of the standout advantages of Li-ion batteries is their high energy density, meaning they can store large amounts of energy relative to their size and weight. Compared to other battery types, they are significantly more compact and lightweight while still delivering a strong power output. They also have an impressive ability to retain charge, losing only about 1-2% of their energy per month when not in use. Another key factor is their lifespan, as they can endure between 2,000 and 5,000 charge cycles, vastly outperforming Sealed Lead Acid batteries, which typically last between 500 and 1,000 cycles. Due to their lightweight nature, they enhance portability, which is critical for the TEXRAY system.

However, Li-ion batteries are not without their drawbacks. The availability of lithium as a resource is limited, which raises concerns about long-term sustainability and cost. Additionally, proper disposal and recycling of Li-ion batteries are necessary due to environmental concerns, as improper handling can contribute to pollution. Despite these limitations, Li-ion batteries remain a top choice for a wide range of applications, including cellphones, automotive batteries, and portable electronics.

The specific Li-ion battery pack being considered for TEXRAY is an 18650 11.1V battery with a 3500mAh capacity. Based on its specifications, it operates at a peak voltage of 12.6V with a cutoff voltage of 7.5V and a maximum discharge current of 4.2A. Its physical dimensions measure 2.75 inches in length, 2.17 inches in width, and 0.8 inches in height, with a weight of 5.3 ounces. These specifications make it an excellent choice for a system requiring a balance of high voltage and portability, both of which are key requirements for TEXRAY. In terms of cost, this battery is priced at approximately \$89.99.

Lithium Iron Phosphate (LiFePO₄) Battery

The second option is Lithium Iron Phosphate (LiFePO₄) batteries, which are a variant of traditional Li-ion batteries. The main difference lies in the chemical composition, as these batteries use lithium iron phosphate as the cathode material, represented chemically as LiFePO₄. This composition prioritizes safety, stability, and longevity while maintaining a high energy density. Due to these characteristics, LiFePO₄ batteries are widely regarded as a safer alternative to standard Li-ion batteries. They have a significantly lower risk of overheating, fire hazards, or explosion, making them a more stable and reliable choice. Additionally, they are environmentally friendly, as they do not contain toxic heavy metals, reducing the negative impact of improper disposal.

Despite sharing similarities with traditional Li-ion batteries, LiFePO₄ batteries stand out due to their durability and lifespan. They typically last longer than other battery types and maintain their performance over thousands of charge cycles. Their stability under high loads and consistent voltage output make them an appealing option for applications where reliability is key. Given their environmentally friendly nature, they are often preferred in renewable energy projects, including solar power storage increasing demand for them.

The LiFePO₄ battery under consideration for TEXRAY is the Bioenno Power BLF-1206A. It operates at 12V with a capacity of 6Ah (6000mAh) and a maximum continuous discharge current of 12A, which translates to a maximum power output of 144W. The battery dimensions measure 4.4 inches in width, 2.6 inches in length, and 2.8 inches in height, with a weight of 0.7 kilograms. It also includes an integrated Protection Circuit Module (PCM), which ensures cell balancing and provides safeguards against overcurrent, short-circuiting, undervoltage, and overvoltage. This added layer of protection enhances the battery's longevity and safety, making it a strong contender. The estimated cost for this option is approximately \$79.

Sealed Lead Acid (SLA) Battery

The third and final option is the Sealed Lead Acid (SLA) battery, which is another type of rechargeable battery. These batteries use thickened sulfuric acid as the electrolyte and are designed with a sealed structure to prevent electrolyte spillage, enhancing safety and reliability. SLA batteries are known for their low maintenance requirements and long cycle life, making them a practical choice for a range of applications. However, they have a

moderate energy density, meaning they are bulkier and heavier than lithium-based alternatives.

One of the key benefits of SLA batteries is their deep discharge capability, allowing them to use a significant portion of their capacity without incurring substantial damage. Their sealed design further enhances safety by preventing leaks, while built-in safety valves help manage internal pressure. SLA batteries also have a lifespan of 3-5 years and can withstand 300-500 charge cycles, making them a reasonably durable option. Additionally, they excel in charge retention, making them ideal for backup power solutions. Their stable voltage output ensures consistent performance, making them reliable for applications requiring steady power distribution.

However, when compared to Li-ion and LiFePO₄ batteries, SLA batteries fall short in several areas. They have a lower energy density, meaning they are significantly heavier and less portable. Their lifespan and charge cycle count are also inferior, and they tend to perform poorly in extreme temperatures. Additionally, they have a higher self-discharge rate, making them less efficient over time. Despite these limitations, SLA batteries remain a cost-effective solution, often being more affordable than lithium-based options. They are commonly used in uninterruptible power supplies (UPS), solar energy storage, and emergency lighting systems.

For this comparison, the SLA battery under review is the Power Sonic PS-1270 12V 7Ah. It delivers 12V with a capacity of 7Ah and a maximum discharge current of 70A, resulting in a maximum power output of 840W. It measures 5.95 inches in length, 2.56 inches in width, and 3.7 inches in height, with a weight of 1.91 kilograms. While the larger size and heavier weight make it less ideal for portability, its affordable price of approximately \$16 makes it an attractive budget-friendly option.

Each battery type has its own advantages and trade-offs. Li-ion batteries offer high energy density, portability, and long lifespan but come at a higher cost and require proper disposal. LiFePO₄ batteries provide safety, stability, and durability while maintaining a moderate cost. SLA batteries, while more affordable, fall short in terms of energy density, lifespan, and weight. Based on the requirements for TEXRAY, the selection will ultimately depend on balancing performance, reliability, cost, and portability to ensure optimal system functionality. Below will compare the their features to isolate the best choice.

Table 3.1.7 Battery Comparison

Feature	Lithium-Ion (Li-ion)	Lithium Iron Phosphate (LiFePO ₄)	Sealed Lead Acid (SLA)
Current type	Direct Current	Alternating Current	Direct Current
Portability	High (size and weight dependent)	Low (stationary)	Moderate (mostly stationary with exception of some portable panels)
Power Storage	Chemical energy stored	None (continuous supply)	Can store in batteries
Reliability	Great at short distances; depletion may impact	Great	Varies heavily
Ease of Use	Simple	Requires at least one outlet	complex
Stability	Very stable and constant	Fluctuates do to alternating current	Stable as DC, light intensity may cause fluctuations
Efficiency	Moderate	High	Lower
Cost	Low to moderate	Low	High
Maintenance	Medium	Low	Medium
Uses	Portable sensitive electronic devices	Stationary high demand loads	Hybrid systems

3.2 Raman Background

3.2.1 Overview of Scattering

The scattering of light describes light's deviation from its original path when incident upon a medium. Scattering phenomena from light-matter interactions are primarily characterized by the fact that the energy of an incident photon does not necessarily need to be resonant with any molecular transitions—unlike in light-absorption interactions. The energy transfer of radiation due to scattering provides insightful information on the substance it interacts with.

One can analyze scattered radiation and find that its frequency content contains the frequency of the incident radiation along with the addition of new frequency pairs. These new frequency components correspond to transitions between rotational, vibrational, and electronic energy levels of the molecular structure of the substance. Scattering occurs in all directions, where the direction and polarization of the scattered radiation depends on the direction of observation. Scattered light exists in two main forms: elastic and inelastic scattering. Elastic scattering, also known as Rayleigh Scattering, describes the scattered radiation as having the same frequency as the incident radiation. Inelastic scattering, known as Raman scattering, occurs when the frequency of the scattered radiation differs from the frequency of the incident light.

3.2.2 Raman Scattering

In 1928, physicist Sir Chandrasekhara Venkata Raman and his student Sir Kariamanikkam Srinivasa Krishnan observed the first Raman scattering event from liquids. They visually noted that most of the light scattered from the sample retained the original radiation's frequency. However, upon isolating the beam path with a colored filter observed some of the scattered light was a different color. These qualitative observations alone were not sufficient. Raman replaced the eye of the observer with a quartz spectrograph, which allowed him to photograph the spectrum of the scattered light. This discovery of Raman scattering was not only significant in supporting quantum theory, but it also presented itself as a powerful tool in probing molecular structures— as Raman noted, "...the character of the scattered radiations enables us to obtain an insight into the ultimate structure of the scattering substance." Raman was awarded the 1930 Nobel Peace prize in physics for Raman scattering.

As previously mentioned, Raman-scattered light contains frequency components distinct from the frequency of the incident light. Raman scattering is considered a rare event compared to Rayleigh scattering, where approximately 1 in 10 million photons undergo Raman scattering. Raman scattering occurs when light interacts with a molecule, and the electromagnetic field of the incident photon induces a polarization to the molecule, temporarily exciting its electrons to a virtual state. Polarization in this context refers to the distortion of the negatively charged electron cloud by an incident electric field. Since this electron cloud surrounds a positively charged nucleus, this offset makes one side of the atom slightly positive and the other side slightly negative, creating an induced dipole moment. The magnitude of the dipole moment depends on the intensity of the light and the molecule's polarizability. An increased electromagnetic field strength results in an increased dipole moment, which can set the molecule into a virtual state. The virtual state is inherently unstable and the photon is re-emitted almost immediately, as scattered light. When the energy of the scattered photon differs from that of the incident photon, the process is defined as Raman scattering. The energy difference between the incident photon and the scattered photon corresponds to a vibrational mode of the molecule.

3.2.3 Stoke and Anti-Stokes Scattering

There are two distinct types of Raman scattering: Stokes scattering, where the scattering is of a lower frequency than the incident light, and anti-Stokes scattering, where the scattered light has a higher frequency than the incident light. Stokes scattering occurs when an incident photon interacts with a molecule, exciting its electrons to a higher energy virtual state. The molecule then relaxes to a higher energy vibrational state, ν_1 , rather than returning to its initial ground state, ν_0 . As a result, the energy of the emitted photon is lower than the incident photon. Conversely, anti-Stokes scattering occurs when the molecules are already in an excited vibrational state, ν_1 , before interacting with an incident photon. This excited state is often due to thermal energy. The incident photons excite the molecule to a higher energy virtual state, after which the molecule relaxes back to its ground state, ν_0 . As a result, the energy of the emitted photon has higher energy than the incident photon. Because fewer molecules naturally occupy excited vibrational states at room temperature, anti-Stokes scattering is typically weaker than Stokes scattering.

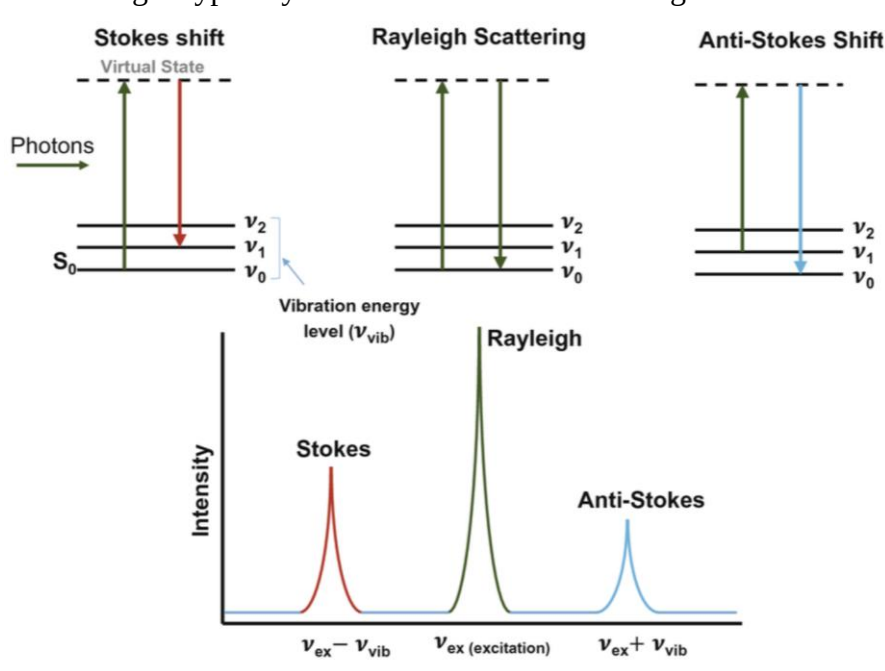


Figure 3.2.1 Demonstration of Stokes Scattering, anti-Stokes scattering, and Rayleigh Scattering

Analyzing scattered light provides useful insights about the molecular characteristics of a substance. Rayleigh scattering is not useful for standard material identification, as its elastic nature means the scattered wavelength is the same as the incident wavelength. Alternatively, Raman scattering is useful for material identification because it introduces a wavelength shift due to transitions in vibrational and rotational modes of the molecules.

3.2.4 Raman Spectroscopy

Raman spectroscopy is a primary analytical technique to assess the vibrational and rotational modes of a material through Raman scattering. It plays a crucial role in chemical sensing, biological imaging, and material science applications. Raman spectroscopy can be specifically employed to characterize materials, measure temperature, and find the crystallographic orientation of a sample by analyzing its vibrational energetic modes. The

analysis of a sample's vibrational modes serves as a molecular fingerprint, which provides distinct spectral information on the nature of a molecule.

For a material to experience Raman Scattering, it must be "Raman active". A molecule is considered Raman active if it undergoes a significant change in its polarizability during its excitation. For bonds which have a weak dipole moment, the polarizability is usually high and the vibrational states of the bond are Raman active.

Our system will leverage Raman spectroscopy to distinguish between different textile materials by analyzing their Stokes bands. Since each fabric type has distinct vibrational signatures, Raman spectroscopy serves as an effective tool for verifying material authenticity and composition. The following section will explore how Raman spectroscopy systems have been employed to discern material types.

3.2.5 Raman Spectroscopy Methods

Raman spectroscopy comes in over 25 variations. These iterations refine the Raman signal attainment process, allowing for functionalities such as cross section imaging, limiting fluorescence, assessing anti-Stokes scattering, etc. Dispersive Raman spectroscopy is the most applicable for our application due to its cost effectiveness and well attainable spectral resolution. The research we will reference uses different Raman spectroscopy techniques to assess the material characteristics of textiles. Therefore, it's relevant to assess their working principles to better understand their systems and to consider how we may need to modify our Dispersive Raman spectrometer.

Dispersive Raman Spectroscopy

Dispersive Raman spectroscopy is considered the main type of Raman spectroscopy. To observe the Raman spectra, the Raman signal must be separated into its constituent wavelengths. This is achieved through focusing the Raman signal onto a diffraction grating, which then disperses the light, allowing for the shifted Raman signals to be detected.

Raman Microscopy

Raman microspectroscopy uses the same techniques as a typical dispersive Raman spectrometer. However, it not only provides the information on the chemical fingerprint of the sample, but also an image of the internal structure. It is an ideal method for the analysis of smaller structures and for the depths of transparent structures without having to physically manipulate them. One has the ability to create a chemical image with a Raman microscope, which shows the distribution of chemicals in a sample. In a Raman microscope system, the laser is focused through an objective lens and upon interaction with the sample, induces Raman scattering. The scattered light is received back through the objective and goes through a confocal pinhole and the rest of the microscope system before reaching the spectrometer. The integration of the confocal pinhole serves as an advantage as it blocks out unfocused light from the Raman signal before it reaches the spectrometer to improve

the spatial resolution of the spectra. This design further helps limit fluorescence and allows for movement in the focal plane. Moving the focal plane allows one to assess various depths of the sample. However, this system requires tedious alignment between the confocal pinhole and the entrance slit for an acceptable microscope throughput, which describes the rate at which a microscope can process images of the sample. By accounting for this conflict and increasing the throughput by integrating a hybrid- or pseudo- confocal pinhole design, the higher spatial resolution is sacrificed.

Enhanced Raman Spectroscopy

A significant limitation in Raman spectroscopy is deriving and maintaining a substantial amount of Raman scattering. This sensitivity can be enhanced through Surface Enhanced Raman Spectroscopy (SERS), which allows for the detection of low concentration amounts. Ultimately, this sensitivity enhancement is due to a combination of the electromagnetic and resonant charge transfer effects. These effects refer to the phenomena when an electromagnetic field is tuned to the resonant frequency of a system, enhancing the transfer of electric charges between molecules or atoms within that system. In SERS, the Raman signal becomes amplified by having the sample attached to a nanostructured metallic surface— typically made of gold or silver colloids— through a process known as plasmon resonance. Through SERS, the Raman signal intensity can be 10^6 times greater than with classical Raman spectroscopy. The output signal intensity is further influenced by the character of the metal— type, roughness, size, and shape— and the intensity of the incident light. Similarly to SERS, Tip-enhanced Raman spectroscopy (TERS) intensifies the Raman signal. As opposed to the use of colloid nanoparticles, a sharp metal tip is brought close to the sample, which experiences the electromagnetic and resonant charge effects. Ultimately, SERS and TERS are specifically beneficial for assessing the Raman spectra for microscopic samples, where our system will be assessing macroscopic samples.

3.2.6 Spectrometer Configurations and Comparison

Most Raman Spectrometers are designed under the Czerny-Turner arrangement. While there are alternative Raman spectrometer designs, i.e., Littrow, and Ebert-Fastie, Czerny-Turner remains the dominant design due to its good balance of performance and cost. They are all marked by their use of reflective gratings, which advantageously avoids chromatic aberrations. However, their varying alignments and optical components dictate the quality of the received Raman spectrum. Choosing the appropriate spectrometer arrangement for our system determines our capacity to receive a high enough Raman signal off of our textile and receive a discernible Raman shift.

Littrow & Ebert-Fastie

While the Littrow spectrometer configuration is not typically found in commercial spectrometers today, it is still used to characterize diffraction gratings. It was worth considering its configuration for a fabric identifier spectrometer due to its simplicity. A reduced number of needed optical components allows for maintenance of a higher signal throughout an optical system. However, the Littrow spectrometer works best for the detection of a single wavelength. Capturing broader Raman shifts, like our system requires,

involves manually adjusting the grating. Therefore, the Littrow Configuration is ultimately not compatible with our system's needs. Similarly to Littrow spectrometers, Ebert-Faiste has fewer optical components than typical Raman spectrometers. This simplifies alignment and would ultimately be lower cost. However, we are faced with the same tradeoff, where a consequence is a limited spectral resolution.

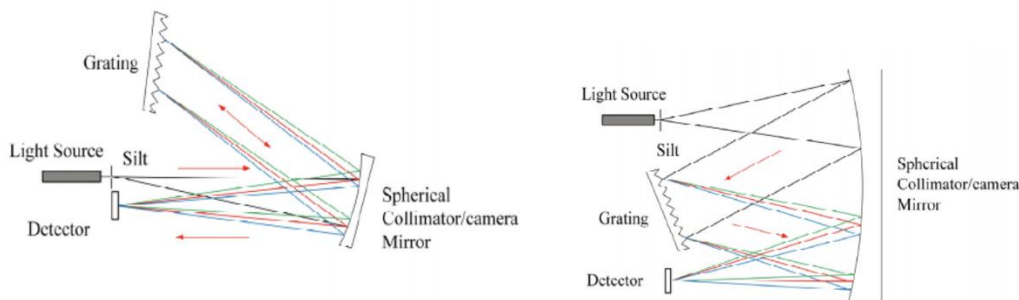


Figure 3.2.2 (Left) Littrow spectrometer. (Right) Ebert-Fastie spectrometer.

Czerny-Turner

The Czerny Turner Spectrometer design is a popular setup for dispersive spectroscopy. The Czerny-turner spectrometer configuration presents itself as the best option for our system for its capacity to detect a broader wavelength range without significant realignments, cost-effectiveness, and portability. That quality is essential for analyzing a variety of textile types with distinct Raman spectral shifts along a broad spectral range under a compact system. The two concave mirrors correct aberrations and minimizes stray light, allowing for the highest possible spectral resolution. The customizability of the spectrometer, i.e., of the excitation source wavelength, grating density, focusing optics, etc., will further allow for more specific detection of various textiles. The Czerny-Turner configuration consists of two concave mirrors and one planar, reflective diffraction grating. The fundamental working principle begins with the focused Raman radiation entering the slit. The first concave mirror collimates the light and reflects the light onto the grating. The Raman signal is dispersed into its constituent wavelength components and is reflected off of the second concave mirror. This second concave mirror focuses the light onto the detector.

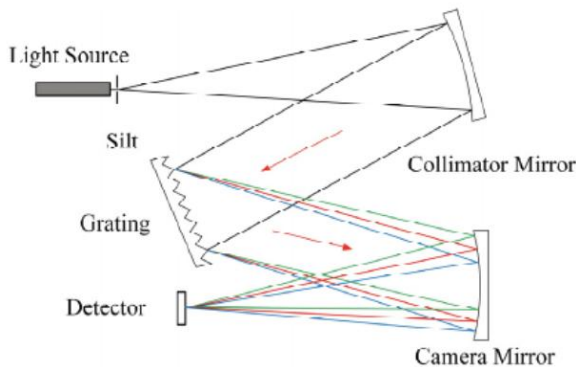


Figure 3.2.3 Czerny-Turner Spectrometer configuration.

Despite the advantages of the Czerny-Turner configuration, considerations are being made towards the possible pitfalls. While the multiple optical elements allow for the opportunity for higher resolution, the multiple reflections can attract stray light– which interferes with our signal. A very precise alignment of the gratings, mirror, and detectors is required to attain a highly resolved spectrum. Raman signal by default are of a reduced intensity, we may be faced with a limited light throughput of our signal. We must be mindful of introduced aberrations.

3.2.7 General Spectrometer Design Considerations

The following section serves as an introduction to the notable design considerations that must be held to ensure a proper functioning system. These considerations will guide our spectrometer design and will be further evaluated throughout the technical comparisons and specifications of Chapter 3. The Raman spectrometer Czerny-Turner design consists of three main components: the illumination source, beam handling optics, and a detector. Important needs are detecting and maintaining the Raman signal and receiving a highly resolved spectrum. A well operable Raman spectrometer requires the following:

Laser choice

The nonresonant Raman effect is a very weak process. The excitation source incorporated into our system will dictate the strength of our Raman signal– as the intensity of the Raman signal is inversely proportional to the fourth power of the laser wavelength (λ^4). Therefore, a monochromatic, narrow-linewidth, high-intensity laser is ideal as an excitation source to produce a quality Raman spectrum. The laser should be monochromatic since Raman scattering is measured in terms of the shift from the original excitation wavelength, and the linewidth of our laser directly influences the spectral resolution of our Raman peaks. To compensate for the use of longer wavelength sources, longer acquisition times should be considered. The laser source wavelength further dictates the amount of fluorescence emitted in the de-excitation process. These considerations will guide our laser source decision.

Filter

A filter must be integrated to eliminate Rayleigh and anti-Stokes scattering while simultaneously isolating the Raman scattering. Without a proper filter, the already limited Raman scattering would be overpowered by the spectrum of the excitation source. There are various components that could be used as a filter within the spectrometer. A dichroic mirror can be integrated that reflects respective wavelengths of light and transmits others. In this circumstance, it would reflect the source wavelength and transmit the Raman scattering. One can further integrate a notch filter or low pass filter. A notch filter has a sharp wavelength where the light is cut-off. The intention for this system would be to choose a notch filter that aligns with the excitation source wavelength, this would allow anti-Stokes and Stokes scattering to pass through. A long pass filter would block all wavelengths up to a given cut-off wavelength. Wavelengths higher than this cut-off are transmitted. Our sample will not be in an excited state before analysis; therefore, anti-

Stokes scattering should not be prevalent, and a notch filter can be considered for our application. However, a long pass filter will ultimately ensure the Raman signal is purely Stokes scattering.

Diffraction Grating

The diffraction grating plays the critical role of separating the Raman scatter into its constituent wavelengths, which will correlate to distinct molecular vibrations in the textile sample. The appropriate grating chosen based upon a given excitation source and sample. Proper incorporation of a diffraction grating determines the detection of the Raman shifts. There are four main considerations in selecting an appropriate grating: spectral resolution, spectral range, blaze wavelength, and excitation wavelength. The diffraction grating will dictate the spectral resolution through its groove density. Where the higher the groove density, the higher the spectral resolution, because the CCD will see a larger spread of the light. The groove density further dictates the discernable spectral range. The spectral range of the spectrometer is inversely proportional to the groove density. We will have to find the design balance between achieving an acceptable spectral resolution and range.

3.3 Experimental Methodologies

3.3.1 Characterization of Fiber by Raman Microprobe Spectroscopy

In the paper, Characterization of Fiber by Raman Microprobe Spectroscopy, by Imelda P. Keen et al., the researchers considered Raman spectroscopy as an alternative vibrational spectroscopic technique to infrared spectroscopy, which is widely used for fiber characterization and acts as the basis for the majority of current fiber identification technology. The researchers obtained various reference fiber samples from the Collaborative Testing Service (CTS) 1987 Reference Collection of synthetic fibers, and utilized a Renishaw Model 1000 microprobe spectrometer to obtain the Raman shift of samples in the range of $3700\text{-}200\text{ cm}^{-1}$. Two lasers, a Spectra-Physics Model HeNe laser emitting at 632.8 nm and a Renishaw semiconductor laser emitting at 780 nm, were available, both with a maximum laser power of about 20 mW at the sample. Though this system involves Raman microscopy whereas our project intends to utilize a more basic Raman spectroscopy system, the results of this experiment are still useful to analyze as Raman microscopy simply utilizes a “point and shoot” approach to Raman spectroscopy of microscopic substances, such as a strand of fiber [15]. Since our samples will be macroscopic, the microscopy aspect of the system is not necessary in our project.

The researchers first used the HeNe laser to obtain Raman spectra of a variety of fiber samples, both synthetic and natural. No sample preparation was done to obtain the spectra; the fibers were taped to a glass slide or metal plate, placed onto the Raman microscope stage, and brought into focus. The HeNe laser light was allowed to fall on the sample and the spectrum was then collected. Shown in fig. 3.1.1.1, this resulted in distinct spectrums for every single tested fiber type, demonstrating how the Raman spectra can act as a “fingerprint” unique to the vibrational modes of the tested fiber, validating the basis of our project [16]. The majority of the tested fibers only required a measurement time of 1-10

seconds to obtain high quality spectra, but weaker Raman scatterers like wool and rayon required longer measurement times of about 1 minute. The paper notes that Raman spectra tend to have fewer, but sharper and less overlapped bands than infrared spectra, demonstrating another unique advantage of using Raman Spectra as an identification tool.

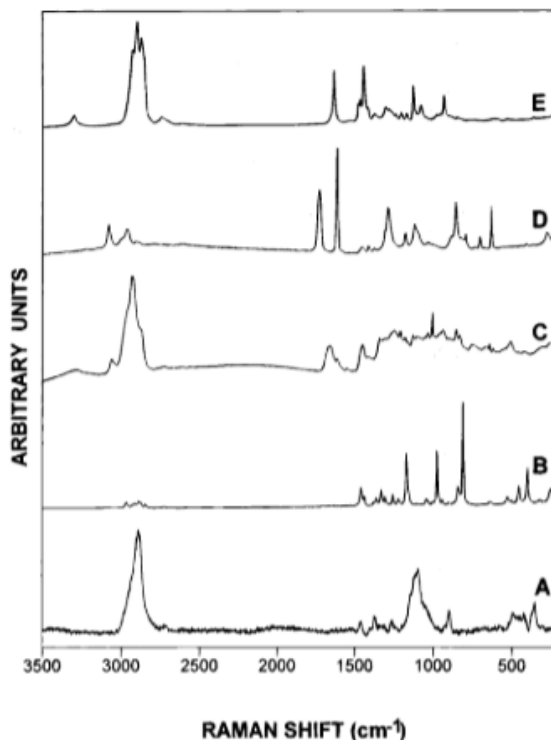


Figure 3.3.1 Raman microprobe spectra of (A) rayon; (B) polypropylene; (C) wool; (D) polyester; (E) nylon.

The paper highlights the fact that most of the CTS Reference Collection samples demonstrated little fluorescence, which could swamp the Raman signal if present. In some cases, fluorescence was visible but the Raman spectrum of the sample was still clearly distinguishable above the background, and the fluorescence would dwindle as the collection time increased due to the photodegradation of the fluorescing species. The few samples that did demonstrate significant fluorescence, such as polypropylene, to the point where the Raman spectra of the fiber was indistinguishable, were able to generate clear Raman spectra by changing the excitation wavelength to 780 nm. Further increasing the wavelength would reduce fluorescence even further, but such high wavelengths would no longer be compatible with a CCD camera, as we intend to use in our system design. The researchers suggest that the best excitation wavelength for forensic applications would be 780 nm, or an NIR laser, as few samples showed fluorescence at this energy. However, the intensity of Raman scattering is inversely related to the fourth power of the excitation wavelength [17], and thus a 780 nm laser would result in decreased signal intensity when compared to a HeNe or 532 nm laser. The paper notes that this can be compensated by increasing the measurement time by just a few seconds. These findings indicate that our team will need to find a balance between Raman signal intensity and fluorescence when choosing an excitation wavelength, and ensure that the wavelength we choose is compatible with the fluorescence bands of our chosen test samples.

If a user wanted to test the composition of two random fabric samples, there is a non-zero chance that both samples may be identical in composition but sourced from different manufacturers. For example, the samples may both be 100% polyester, but originate from different sources, resulting in slightly varied Raman signatures. The authors of this paper tested whether or not they could consistently identify polyester samples sourced from different manufacturers, shown in fig. 3.1.2. Upon testing four 100% polyester samples, four Raman spectra with identical peaks resulted, with the only variation between the spectra of the samples being the intensity of each peak. Using principal components analysis, the researchers found that the differences in the spectra were reproducible and significant enough to be able to group 4 measurements each per the four samples into consistent groups, indicating that they could identify the manufacturer of each random tested fiber based on the variations of their spectral signal. For our purposes, we do not intend to identify the manufacturer of our tested samples, however, this research indicates that we should be able to consistently identify sample composition regardless of the manufacturer being different from that of the reference sample spectra. The researchers conducted this same experiment on nylon samples from different manufacturers, leading to the same results. In the case of nylon, the researchers noted that there were many small variations between samples of the locations of the spectral peaks. For example, the C-CO stretching band position varied from 929 cm^{-1} for nylon-6 to 946 cm^{-1} for nylon 6,12. This indicates that we will need to incorporate error into our spectra-identification software such that, for example, two 100% polyester samples from different manufacturers with slight variations in peak location will still be consistently identified as polyester.

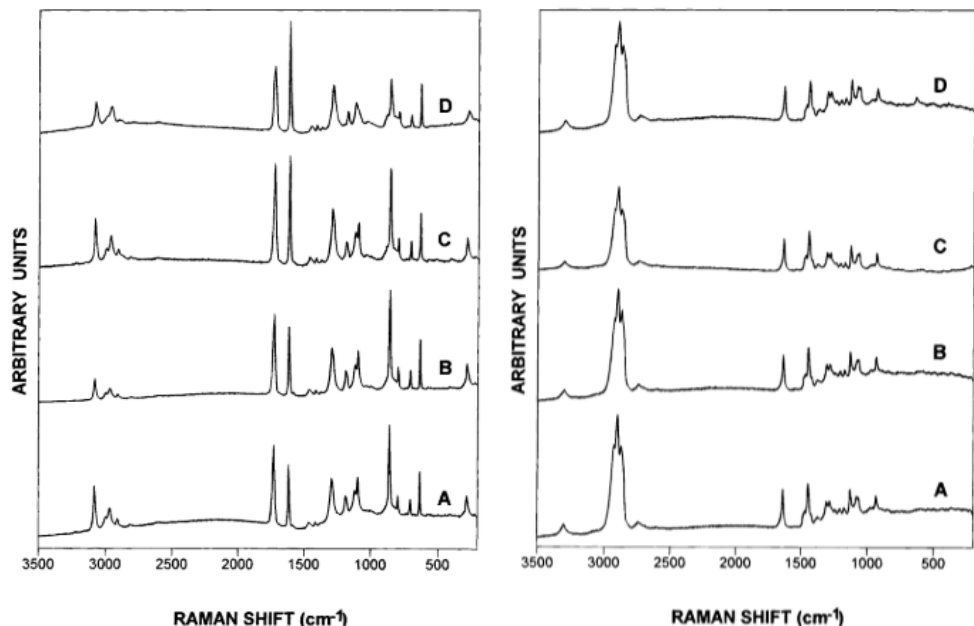


Figure 3.3.2 Raman microprobe spectra of polyester samples from four manufacturers (left). Raman microprobe spectra of nylon samples from four manufacturers (right).

3.3.2 Raman Spectra of Textile Fibers

It is important to intimately understand the composition of the fibers that will be tested in our prototype, as the different textiles will have different molecular structures and thus different vibrations modifying the polarizability of its molecules, which is what gets detected by Raman spectroscopy. The spectral range recorded must encompass the stretches and bends characteristic of the functional groups of each fiber type.

Cotton fiber is composed of over 88% cellulose, with its other organic components not exceeding 2% of its composition. The band structure of cotton informs the distinctive features of its Raman spectrum. These regions of interest are:

1. Low-Frequency Region (100 cm^{-1} to 240 cm^{-1}): This region includes small peaks at 205 cm^{-1} and 265 cm^{-1} , but otherwise has no significant identifiable features
2. Fingerprint Region (240 cm^{-1} to 1600 cm^{-1}): This region includes the most characteristic vibrations of cellulose. Key peaks are located near:
 - a. 381 cm^{-1} due to CCC ring deformation bending
 - b. 1099 cm^{-1} due to C-O-C glycoside link asymmetric ring breathing and skeletal stretching
 - c. 1125 cm^{-1} due to C-O-C glycoside link symmetric ring breathing and skeletal stretching
3. High-frequency Region (2800 cm^{-1} to 3600 cm^{-1}): After a large stretch of the spectrum being featureless, there is a characteristic peak at 2903 cm^{-1} as a result of the stretching bands of CH vibrations [18].

Polyethylene terephthalate (PET), most commonly referred to as polyester when in fiber or textile form [19], is a synthetic fiber produced through the polymerization of ethylene glycol and terephthalic acid [20]. Because textile polymers are not 100% crystalline, the Raman spectrum of PET can vary slightly based on the polymer form of the textile. If the spectrum has an intense peak at 1096 , this indicates that the PET fiber is in crystalline form and has a trans structure. The carbonyl band at 1728 is an even better marker of crystallinity, with a narrow carbonyl peak indicating a highly crystalline sample, rather than an amorphous sample[18]. Thus, regions of interest for polyester samples include:

1. Low-Frequency Region (100 cm^{-1} to 200 cm^{-1}): This region can include a band near 142 cm^{-1} belonging to TiO_2 , which is often used as a matting agent in the processing of PET fibers
2. Fingerprint Region (200 cm^{-1} to 1750 cm^{-1}): This region includes the most characteristic vibrations of PET fibers. Key peaks are located near:
 - a. 278 cm^{-1} due to deformation skeletal C-C band
 - b. 632 cm^{-1} due to the in-plane ring bend
 - c. 1289 cm^{-1} due to CO-O stretching
 - d. 1615 cm^{-1} has the highest intensity peak in the spectrum due to the C-C aromatic ring stretching
 - e. 1728 cm^{-1} due to carbonyl C=O stretching, with peak width varying as a result of crystalline or amorphous structure
3. High-frequency Region (1750 cm^{-1} to 3100 cm^{-1}): Two minor spectral peaks are located near 3081 cm^{-1} and 2966 cm^{-1} , but are not crucial to the identification of PET [18], [21], [22]

While cotton is a natural plant fiber, wool is an animal protein fiber mainly consisting of keratin, a sulfur possessing protein. Wool keratin is composed of 11.9% glutamic acid, 10.4% serine, 10.3% cysteine, 8.4% glycine, 7.7% leucine, 6.9% arginine, 6.6% proline, as well as other amino acids. Silk, being another animal protein fiber, shares very similar characteristics to wool. Silk fibroin is composed of 44.1% alanine, 26.5% glycine, 11.8% serine, 4.9% tyrosine, 4.7% aspartic acid, and 2.6% arginine, with other amino acids not exceeding 1% [23]. Noticeably, both wool and silk share multiple amino acids in their composition, but the differences in sequence and amount of each amino acid enables Raman spectroscopy to distinguish the two fibers. While two Raman spectra of wool and silk visually share many close peaks, they have substantially different fingerprint characteristics. The defining band characteristics of the Raman spectrum of wool are:

1. Low-Frequency Region (100 cm^{-1} to 400 cm^{-1}): There is one key peak at 116 cm^{-1} with more significant intensity than any other peaks in the spectrum
2. Fingerprint Region (400 cm^{-1} to 1670 cm^{-1}): The most important defining characteristic of wool is a band at 512 cm^{-1} due to an S-S disulphide bridge resulting from cysteine, an amino acid silk completely lacks. Other notable peaks include:
 - a. 925 cm^{-1} due to C-C skeletal bending
 - b. 1311 cm^{-1} , 1463 cm^{-1} due to CH_2 and COO^- bending, respectively
 - c. 1665 cm^{-1} due to C=O AND COO^- stretching resulting from Amide I
3. High-frequency Region (1670 cm^{-1} to 3000 cm^{-1}): Two peaks exist at 2931 cm^{-1} and 2959 cm^{-1} as a result of CH stretching[24]

Silk has a few key peaks that aid in discerning it from wool. These include:

1. Low-Frequency Region (100 cm^{-1} to 500 cm^{-1}): Silk has characteristic skeletal vibrations in this region (117 cm^{-1} , 249 cm^{-1} , 271 cm^{-1} , 339 cm^{-1} , 414 cm^{-1} , 499 cm^{-1}) as a result of combinations of backbone deformations with pendant chains
2. Fingerprint Region (500 cm^{-1} to 1670 cm^{-1}): While lacking the characteristic 512 cm^{-1} band of wool, silk uniquely has a dominating band of amide CH_2 bending at 1228 cm^{-1} . Silk also notably has bands at 1085 cm^{-1} due to CC skeletal vibrations and at 1667 cm^{-1} due to Amide I.
3. High-frequency Region (1670 cm^{-1} to 3000 cm^{-1}): Similarly to wool, silk has a band at 2935 cm^{-1} , but it is due to CH stretching in this case

Nylon, the final fabric of interest for our project, is a semicrystalline polyamide. A polyamide is a polymer in which an amide group joins the monomer units, with the most commercially relevant textile polyamides being Polyamide 6 and Polyamide 6.6. While the two polyamides have some differences in structural formula and thus Raman spectra, they share many bands that may allow our system to recognize both types of polyamides as “nylon.” Such bands include:

1. Low-Frequency Region (100 cm^{-1} to 200 cm^{-1}): Only Polyamide 6.6 has a band near 142 cm^{-1} belonging to TiO_2 , but it is important to mention as PET fiber shares this characteristic as well.
2. Fingerprint Region (500 cm^{-1} to 1670 cm^{-1}):
 - a. 643 cm^{-1} due to CC deformation
 - b. 930 cm^{-1} - 950 cm^{-1} due to CCO stretching
 - c. 1132 cm^{-1} due to CC skeletal stretching

- d. 1302 cm^{-1} due to twisting
 - e. 1448 cm^{-1} due to CH_2 bending
 - f. 1643 cm^{-1} due to $\text{C}=\text{O}$ stretching
3. High-frequency Region(1670 cm^{-1} to 3000 cm^{-1}): Both polyamides have a band at 2942 cm^{-1} as a result of CH stretching [18]

While the National Institute of Standards and Technology (NIST) does not have a comprehensive list of standard Raman spectra for textiles, it does have a standard set of Raman peaks corresponding to various molecular vibrational frequencies. Comparing the molecular vibrational frequencies for each key fabric discussed above to these NIST standards ensures the accuracy and reliability of the characteristic Raman spectra data acquired from various sources and listed in this section. Some of these Raman shifts are displayed in Appendix B, Table 1.

3.4 Excitation Wavelength and Laser Selection

3.4.1 Addressing Fluorescence via Horiba LabRAM HR Evolution Nano Confocal Raman Microscope Readings

The NanoScience Technology Center at the University of Central Florida houses the Horiba LabRAM HR Evolution Nano Confocal Raman Microscope. As a proof of concept for our project, we used this system to validate the Raman Spectra of various fabric types and observe spectrum quality obtained by various excitation wavelengths. We used the confocal Raman/PL spectroscopy function, which has 473 nm, 532 nm, 633 nm, 785 nm, and 1064 nm excitation wavelengths available, with their specifications detailed in table 3.2.1.1. The imaging spectrometer was of a Czerny-Turner configuration with a focal length of 800 nm. The diffraction grating used in this experiment had 300 grooves/mm. The findings of the Horiba LabRAM HR are being applied towards guiding the optical hardware we should integrate, specifically the excitation wavelength we will implement into our system. Since fluorescence is far more likely to occur than Raman scattering, and thus can effectively swamp any meaningful Raman signal, it is in our best interest to choose an excitation wavelength which offers low fluorescence while maintaining high Raman intensity [25].

Table 3.4.1 Specifications of laser available in Horiba LabRAM HR

Table 3.4.2 Specifications of laser available in Horiba LabRAM HR							
Medium	Class	Type	Wavelength (nm)	Max Output (W)	Manufacturer	Model	Serial

Diode	3B	CW	473	0.026	Hubner Photonics	0473-04-01-0025-700	16067
Nd:YAG	3B	CW	532	0.105	Horiba Scientific	LCX-532S-100-CSB-PPF-001	LAS06445
HeNe	3B	CW	633	0.017	Horiba Scientific	300995	IGM43-2
Diode	3B	CW	785	0.103	IPS Photonics	I0785SHO O98-IS-TH-L-Hoiba	27801

Our team exposed a variety of different textiles to the 473 nm, 532 nm, and 785 nm excitation wavelengths to examine how the different samples fluoresce under these lasers of interest. Due to limited materials at the time of testing, out of our five materials of interest we only tested 100% bleached cotton, 100% polyester, and 100% wool, all of which were undyed. When testing the cotton sample with an acquisition time of 10 seconds, 3 accumulations, 50% laser power, and an aperture size of 100 , we found that the signal was exceedingly clear at both the 532 nm and 473 nm incident wavelengths, with no considerable advantage of one wavelength over the other in terms of minimizing fluorescence. Both spectra clearly demonstrated the key peaks of cotton as described in section 3.1.2. The 785 nm incident laser led to significant fluorescence and did not yield an identifiable Raman spectrum of cotton.

When testing the polyester sample, we found that the spectrum was significantly clearer and with less noise at 473 nm compared to 532 nm. The spectrum at 473 nm incident wavelength and an acquisition time of 10 seconds and 3 accumulations clearly correlated to the anticipated key peaks of polyester, whereas the spectrum at 532 nm demonstrated extreme fluorescence to the point where no Raman signal could be recovered. After reducing the acquisition time to .5 seconds with 10 accumulations, the Raman signal could somewhat be recovered. There was still a significant amount of fluorescence, but the characteristic peaks of polyester were identifiable above this noise and thus the textile type could theoretically be distinguished from this result. Testing the 785 nm wavelength at a 10 second acquisition time and 3 accumulations enabled a decent resulting spectrum, with all the characteristic peaks of polyester being clearly identifiable with minimal fluorescence until 1800 cm^{-1} . However, the signal began to degrade after this point, demonstrating significant noise.

Due to time constraints our team was only able to test the 532 nm wavelength on the wool sample, with an acquisition time of 10 seconds and 5 accumulations. The aperture size had also been reduced by 50% compared to the other tests. These conditions led to a fairly good

Raman spectrum as the key peaks of wool were easily identifiable and little if any fluorescence was present.

3.4.2 Supplementation of Testing Results via Literature

Though we were unable to test all of our samples of interest to see what wavelengths suited them best for reducing fluorescence, literature exists documenting this kind of testing. For example, Jasco Spectroscopy Group tested their NRS series of Raman spectrometers fitted with a 457 nm laser for the measurement of samples that tend to exhibit fluorescence, in order to determine if this wavelength is more effective than red and NIR lasers. They found that using the 532 nm and 785 nm excitation wavelengths on their sample resulted in strong fluorescence and unidentifiable signals. However, the 457 nm wavelength reduced fluorescence significantly and the resulting spectrum was correctly identified as nylon-6 when compared to a database library spectrum. These findings indicate that 457 nm, close to 473 nm used in our tests, would be a suitable excitation wavelength for nylon [26].

There is also much literature that supports our already existing findings from our personal experiment. In the paper “Application of Raman Spectroscopy for Differentiation Among Cotton and Viscose Fibers Dyed with Several Dye Classes,” by J. Was-Gulaba and W. Machnowski, the researchers obtained the Raman spectra for uncolored cotton at the excitation lines 514 nm, 633 nm, and 785 nm. They found that there was no difference in the number of bands, and that the resulting spectra could only be shifted by 5 cm^{-1} between wavelengths. All of the resulting spectra were high quality and demonstrated little fluorescence [27]. This further supports the idea that we should be able to obtain a distinguishable Raman spectrum for cotton at either blue or green excitation wavelengths, as we found in our own experiment. Likely, had we adjusted the acquisition time and various other parameters of our test, we would have been able to produce a distinguishable spectrum at 785 nm as well.

In the study, “Evaluation of Raman spectroscopy for the analysis of colored fibers: a collaborative study,” by G. Massonnet et. al, members of the European Network of Forensic Science Institutes European Fibres Group on three types of dyed fibers: two red acrylic and one red wool. They tested Raman instruments from six different manufacturers and nine different laser wavelengths ranging from 458 nm to 1064 nm. The researchers found that for the chosen fiber and dye samples, red lasers gave the worst spectral quality whereas blue (458 nm), green (514 nm), and NIR (785, 830, and 1064 nm) lasers resulted in average spectral quality. Notably, they found that blue (488 nm) and green (532 nm) lasers globally produced the best quality spectra [28].

This study, combined with the other cited literature as well as our own findings, point towards green and blue excitation wavelengths being optimal for reducing fluorescence while maintaining a strong Raman signal. Both blue and green wavelengths provided distinguishable spectra for the majority of our samples. However, because Raman scattering is proportional to λ^{-4} , where λ represents laser wavelength, a blue laser would result in a stronger Raman signal than a green laser [25]. Additionally, the 473 nm excitation wavelength yielded better results for the polyester sample than the 532 nm laser.

This indicates that a 473 nm laser would potentially be the best excitation source for our system to reduce fluorescence and maximize Raman signal strength.

3.4.3 Laser Comparison and Selection

Though testing and literature point towards the 473 nm laser being the best option for our samples, we must consider the current market and our budget constraints before we finalize the laser wavelength choice. Because Raman signal strength is directly proportional to laser power, our system would be most optimized with a high power excitation source. However, if the power is too high, it could burn the fabric samples, ruining the Raman shift data and no longer enabling non-destructive textile identification. As shorter wavelength lasers have a higher energy and generate more Raman scattering, there will be different power requirements between the blue and green lasers when attempting to generate sufficient Raman signal while simultaneously avoiding sample destruction. These differences will also affect the cost comparison between laser choices [29]. Table 3.2.3.1 details a variety of blue and green excitation laser choices, including a variety of specification details such as wavelength, spectral linewidth, output power, operating current, operating voltage, beam divergence, and cost. All of the listed options are single transverse mode laser diodes.

Table 3.4.3 Comparison of various single transverse mode laser diodes.

Table 3.4.4 Comparison of various single transverse mode laser diodes							
Specification		Thorlabs DJ532-40	ams-OSRAM PL 520B	Thorlabs L520P50	Thorlabs L473P100	Thorlabs L450G3	Civil Laser GH04580A2G
Peak Wavelength		532	520	520	473	450	450
Output Power (mW)		40	80	45	100	100	80
Operating Current (mA)		330	200	150	120	80	110
Threshold Current (mA)		160	40	45	20	12	22
Operating Voltage (V)		1.9	6	7	5.7	5.2	5.3
	Parallel	.69°	6.3°	7°	10°	8.4°	10°

Beam Divergence	Perp.	.69°	22.5°	22°	24°	21.5°	24°
Spectral Linewidth		.0283 pm	1 nm	1.3 nm	1.25 nm	1.25 nm	N/A
Price		\$212.64	\$46.00	\$76.61	\$3,032.68	\$138.57	\$9 (min. 10 purchase)

After sorting through various sites and listings of laser diodes, these options seemed the most suited to our project. Just by looking at the table it is clear that, on average, blue laser diodes are generally much harder to find at a reasonable price point than green laser diodes. In particular, finding laser diodes or laser modules at 473 nm is very challenging, as the majority of the products at this wavelength cost hundreds to thousands of dollars. One of the few TO can style laser diodes at 473 nm we were able to find was the Thorlabs L473P100, which cost \$3,032.68. This is obviously nonviable for our system, as the cost of the diode alone outweighs the cost of buying one of the fabric analyzers already on the market. As a result, we tried to find other blue wavelengths that were a bit more affordable, such as the 450 nm options listed. However, of these two options, one of them was sourced from Civil Laser, which has mixed reviews with regards to the quality of their lasers and the consistency of their products with their spec sheets. In a Raman spectrometry system, it is imperative that the laser specs are precise and behave exactly as anticipated, which discourages us from purchasing from Civil Laser.

Aside from cost, the affordable blue lasers tended to have much higher output powers than the selected green lasers, which is an issue when combined with the already higher energy of the low-wavelength blue lasers. This could lead to sample destruction if the power of the laser is not impeded by some external optics. Additionally, 450 nm is a bit lower than the wavelengths at which we tested our samples at the Nanoscience center, and as previously mentioned, lower excitation wavelengths can lead to greater sample fluorescence. Though a 23 nm difference is not much, blue wavelengths are already more prone to fluorescence, and pushing the wavelength even lower than 473 nm could lead to unexpected spectrum flooding that we are not prepared to deal with. Bearing in mind these various factors, we think it would be best to use a green laser as the excitation source for our system.

When choosing a laser source for a Raman spectroscopy system, there are a few key considerations that need to be made with regards to the laser specifications. One such factor is the laser power density at the sample. High brightness lasers with tight focus allow for improved Raman scatter “yield” at a given laser power, improving signal collection. However, this factor can be adjusted via lenses and external optics, and thus doesn’t necessarily impact laser selection [29]. Another consideration, which definitely impacts laser selection, is the spectral linewidth of the laser. This is the full-width half-max of the

laser's optical spectrum, dictating the monochromaticity of the emitted light and the range of wavelengths that the laser can emit. This factor can influence the spectral resolution of the collected Raman signal, as a narrower laser linewidth allows you to have a better distinction between the Raman peaks of a signal. Thus, the laser linewidth should be narrower than the spectral resolution of the spectrometer, so as to never be the limiting factor for the system's overall spectral resolution and to maximize the signal-to-noise ratio of the system [30], [31].

Of our selected green laser options, the 532 nm DJ532-40 has the smallest spectral linewidth, which would enable very high spectral resolution should we pair it with a spectrometer of 1 nm or lower resolution. However, as we are not particularly aiming for such a high resolution spectrometer build, the other green laser options also have acceptable linewidths of around 1 nm or less. The 532 nm diode also has the least beam divergence when compared to the other two green lasers, but most beam divergence can be mitigated via external focusing optics, and thus isn't such an important factor to consider. On the other hand, the 520 nm ams-OSRAM PL 520B is significantly cheaper than the other green laser diodes, while also having the lowest threshold current, and having the highest output power of 80 mW, which will ensure high Raman signal generation. For these reasons, we believe the ams-OSRAM PL 520B would be the best choice for the excitation source of our system. In the case that this option does not pan out somehow, we can consider the Thorlabs DJ532-40 as our backup option.

3.5 Excitation and Collection Setup

3.5.1 Beam Splitting Technology Comparison

Raman spectrometers can employ a variety of probe optic geometries for signal collection, with the most common geometry being the backscattered configuration. In this configuration, the excitation laser is collimated and directed towards a beamsplitter, which separates the excitation path from the collection path in the system [32]. This is advantageous because it enables the use of a single objective lens that both focuses excitation light onto the sample as well as collects backscattered radiation from the sample, rather than needing two separate lenses [33]. This radiation, which is a combination of Rayleigh scattered and Raman scattered light, is then passed back through the beam splitter which is followed by an optical filter, isolating the Raman scattered light before it is collected by the spectrometer [34].

In this configuration, the beamsplitter is integral for proper alignment of the beam so as to minimize the number of focusing lenses required. However, assuming a 50:50 beamsplitter is employed, the laser power will be evenly divided between the two emerging beams. As a result, the excitation power reaching the sample will be substantially diminished, leading to weaker Raman signal generation, as its intensity is directly proportional to the laser power. Not only will the generated signal be weaker overall, but as the scattered light is collected by the focusing lens and sent back through the beamsplitter, the Raman signal will be even further reduced as it is split among the two paths. Considering the fact that Raman scattering is already millions of times less likely to occur than Rayleigh scattering

[35], it is not ideal to have this much signal loss before even reaching the spectrometer setup.

One alternative option to a traditional beamsplitter is a dichroic mirror, which is simply a wavelength-selective beamsplitter. Dichroic mirrors use alternating layers of high and low refractive index dielectric films, causing the incident beam to superimpose with itself to achieve destructive interference and selectively suppress certain wavelength bands [36], [37]. The result is a mirror that preferentially reflects a specific wavelength while allowing other wavelengths to transmit through. When considering the proposed backscattered collection configuration, a dichroic mirror presents significant advantages over a traditional beamsplitter, which splits light indiscriminately.

The dichroic mirror will allow for almost all of the laser light to be reflected towards the focusing lens and sample with little transmission power loss, facilitating greater Raman signal generation. Simultaneously, because the dichroic mirror essentially acts as a bandpass filter and will only reflect light in a narrow band around 520 nm, any stray wavelengths resulting from the laser pump or other factors will be eliminated. This improvement in the monochromaticity of the laser source facilitates a higher spectral resolution in the Raman shift measurements [31]. This same property of the mirror allows it to block Rayleigh scattered light from passing through, as Rayleigh scattering is elastic and shares a wavelength with the laser source, and thus will get reflected upon hitting the dichroic mirror. Meanwhile, the Raman scattered light is allowed to fully transmit through the mirror rather than having a portion of it reflected and lost, as would happen with a traditional beamsplitter. Therefore, the dichroic mirror not only eliminates the power loss issues of traditional beamsplitters, but it also acts as a type of optical filter, mitigating some of the noise in the collected Raman signal. However, it is important to note that though dichroic mirrors do contribute to Rayleigh scattering rejection in the Raman collection setup, 1-2% of green scattered light will still pass through the mirror. Though 1% seems negligible, it is much bigger than the percentage of photons converted to higher wavelengths via the Raman effect [38], and thus the system still requires a secondary optical filter in the system to further reduce noise [39].

Due to the fact that Raman signal generation is proportional to laser power, it is important for the optical components in the collection setup to be able to withstand high intensity lasers. Dichroic mirrors are typically able to withstand high incident laser powers more effectively than regular beamsplitters, as thermal damage usually occurs as a result of significant absorption. The hard dielectric films applied to dichroic mirrors lend them high durability and thermal stability, and when combined with the fact that they reflect unwanted wavelengths rather than absorbing them [40], dichroic mirrors are generally well-compatible with high intensity light sources and can avoid heating well [41]. On the other hand, the metal coatings used on traditional beamsplitters tend to be very absorbent and thus result in fractures due to thermal stress, limiting their damage thresholds [42]. Of course, coatings and materials can vary from product to product resulting in some dichroic mirrors having high thermal absorbance or some beamsplitters having low absorbance, but in general dichroic mirrors often have high damage thresholds when compared to beamsplitters, making them more suitable for use with high power laser sources. For this

reason, as well as those outlined above, a dichroic mirror is the ideal choice for our Raman spectroscopy system.

3.5.2 Dichroic Mirror Selection

There are various factors to consider when choosing a dichroic mirror suitable for our optical system. As a preliminary choice, there are multiple types of dichroic mirrors: hot and cold, short pass, longpass, and multi-band. Hot and cold mirrors are a specific type of dichroic mirror that are designed to block infrared radiation while transmitting visible light, enabling temperature management of the system in applications where heat control is crucial. Shortpass dichroic mirrors enable the transmission of short wavelengths and filter out longer wavelengths, characterized by a “cut-off” wavelength that defines the transition between the reflective and transmissive regions. Longpass dichroic mirrors behave oppositely, transmitting longer wavelengths while reflecting short wavelengths, with the “cut-on” wavelength defining the separation of the two behaviors. On the other hand, multi-band dichroic mirrors have multiple “cut-on” and “cut-off” wavelengths and thus multiple transmission and reflection bands, enabling multi-color laser beam splitting [41], [43]. For our purposes, we will need to block out the 520 nm source by reflection while allowing the higher wavelength Stokes scattered light to pass through. Due to the fact that lower wavelength Anti-Stokes scattering is even less likely to occur than Stokes scattering, it makes up a negligible portion of the Raman scattered signal, and thus can be ignored when considering what wavelengths will be blocked and transmitted. For this reason, it makes the most sense to implement a longpass dichroic mirror into our setup, as there is no real need to implement a more expensive and complicated multi-band mirror for the sake of recovering a miniscule Anti-stokes signal. The longpass dichroic mirror will be able to effectively block out the excitation source wavelength as well as backscattered Rayleigh light, while allowing the Stokes wavelengths to pass through.

Aside from ensuring the proper wavelength range is selected, it is important to ensure that the chosen longpass dichroic mirror has a sufficient laser damage threshold, as was mentioned previously. The goal for our system is to maintain a continuous-wave laser power below 100 mW so as to avoid sample damage. The laser damage threshold for CW lasers is a linear power density which decreases as exposure time increases. The exposure time is the interval for which the optic is subjected to the source laser’s power [44]. The goal for our system is to have an exposure time of 10 seconds or less so as to ensure that the user receives an output quickly on the LCD screen. The sample also must be given enough rest time to fully thermally relax between tests, so that consecutive tests do not become progressively more difficult on the sample. Additionally, because the damage threshold is a power density, the beam diameter of the excitation laser must be taken into account. Because our selected 520 nm laser source has significant beam divergence, the beam diameter at the sample surface is a factor that will be influenced by the focusing optics used to collimate the beam. These factors must be considered when determining if the damage threshold of the proposed longpass dichroic mirrors are sufficient for our application [44], [45].

Our system intends to implement a 45 angle of incidence onto the dichroic mirror as is integrated into most backscattering geometries. Taking this, as well as the above factors into consideration, a few dichroic mirrors of choice have been compiled into table 3.3.2.1 for comparison and selection. Key specifications include: cut-on wavelength, transmission wavelength, reflection wavelength, diameter, thickness, transmittance, angle of incidence, clear aperture, and damage threshold.

Table 3.5.1 Comparison of prospective dichroic mirrors

Table 3.5.2 Comparison of prospective dichroic mirrors				
	MKS Newport DCM13	Chroma T525lpxr	Edmund Optics #86-393 / #86-386	Thorlabs DMLP550 / DMLP550T
Cut-on wavelength (nm)	552	525	552	550
Transmission wavelength (nm)	561.4-790	525 - 1000	561.4-790	565-800
Reflection Wavelength (nm)	514.5-543.5	390 - 510	514.5-543.5	380-533
Diameter (mm)	25	25	25 / 12.5	25.4 / 12.7
Thickness (mm)	3.5	1	3.5	3
Reflectance	>98%	>97%	>98%	>90%
Transmittance	>95%	96.47%	>95%	>85%
Angle of Incidence	45°	45°	45°	45°
Clear aperture diameter (mm)	22	25.4	21.33 / 8.8	>22.9 / > 11.4
Damage threshold (J/cm ²)	N/A	N/A	N/A	.5
Cost	\$359	\$250	\$280 / \$202	\$200.76 / \$134.24

It should be noted that the cut-on wavelength of a longpass dichroic mirror indicates the threshold at which transmission of that wavelength is roughly 50%. Knowing this, then just a glance at the table would indicate the Chroma T525lpxr being the best option, as it is the closest to our excitation source of 520 nm, and would effectively block out the laser photons without reflecting too many Raman shifted photons on the lower end of the Raman spectrum. All other three options have a cut-on wavelength of around 550 nm, meaning that though the laser source will be almost fully reflected, they will also reflect some of the photons on the lower end of the Raman spectrum, as a peak at 550 nm with a 520 nm source corresponds to a Raman shift of 1048 cm^{-1} . This means that any peaks below 1048 cm^{-1} will experience significant light loss, which could be detrimental to textile identification when considering some of our chosen textiles have pivotal peaks before this point, such as wool having a characteristic peak at 512 cm^{-1} . Better alternatives to the 550 nm cut-on wavelength mirrors would have been mirrors with cut-on wavelengths closer to 532 nm, however, it would seem that all dichroic mirrors with cut-on wavelengths in this range cost significantly more than the currently presented options, often being between \$600-700.

Unfortunately, the Chroma T525lpxr did not have a very comprehensive datasheet, and thus was lacking some critical information, such as damage threshold and whether or not the back side of the mirror had an anti-reflective coating. In dichroic mirrors, having a backside anti-reflective coating is important for achieving maximum transmission, as it can reduce unwanted reflections from the backside of the substrate and prevent stray light from entering the optical system. This means an improved signal-to-noise ratio in the system as residual reflections are minimized [43], [46]. Notably, both the Thorlabs and Edmund Optics dichroic mirrors were stated to have anti-reflection coatings, demonstrating high quality manufacturing and suggesting they would contribute to a high system SNR.

Only one of the datasheets for these presented options provided the damage threshold for the dichroic mirror, with the Thorlabs mirror having a damage threshold of $.5\text{ J/cm}^2$. It can be somewhat difficult to calculate how the optic will withstand the CW laser under the conditions we previously described, but IDEX provides a laser damage threshold calculator on their website compatible with Semrock's line of optical components [47]. This calculator indicates that a 532 nm CW laser with a 40 mW average power and an assumed beam diameter of 2 mm would not be likely to produce damage within a $.1\text{ J/cm}^2$ dichroic mirror from their line of products, reasonably indicating that a $.5\text{ J/cm}^2$ mirror would hold up perfectly fine under these same conditions. This comparison cannot be made for the other components, whose damage thresholds were not provided. Consequently, if we choose to purchase them, we must assume they will withstand these conditions until testing can confirm their suitability. Though the MKS Newport mirror did not specify the damage threshold, it is stated to have been manufactured via ion-beam sputtering, which involves bombarding a material with high-energy ions, causing its atoms to be ejected and deposited onto the substrate for the mirror. This technique ensures high durability and low absorption dichroic mirrors [43], implying that the MKS mirror may still have sufficient thermal resistance for our system.

The Edmund Optics and Thorlabs dichroic mirrors both come with smaller diameter variants which otherwise share the same specifications as their larger diameter

counterparts. It is worth noting that the larger, 25 mm diameter optics would have better light collection efficiency and thus may be worth paying extra for. The collimated beam of our back-reflected Raman scattered light must have a smaller diameter than the dichroic mirror to ensure the full Raman signal is captured. Though we would ideally aim for a beam of 1-2 mm, it could be beneficial to opt for a larger lens in the case of experimental difficulties preventing us from achieving such a diameter.

Considering all of the pros and cons of these prospective dichroic mirrors, we believe the best choice for our system will be the Chroma T525lpxr. Though it is unfortunate that no information was provided regarding an AR coating or damage threshold, this option has the closest cut-on wavelength to our chosen laser diode source. As a result, this dichroic mirror will ideally result in the least amount of Raman signal being reflected as it passes through, as the difference between the source and cut-on wavelength of the mirror is only 5 nm, corresponding to a Raman shift of 183.15 cm^{-1} . There were few characteristic peaks of our key textiles in this region, and thus not much valuable information will be lost. As for the damage threshold, because our system is not intended to have a source with power greater than 100 mW, we believe it is unlikely that we will near the incident powers necessary to damage the optic, as we would need a power on the order of kilowatts to reach the damage threshold of most optics according to the IDEX calculator mentioned above. The Chroma dichroic mirror also has a large diameter of 25 mm, having comparable collection efficiency to the other three provided options, as well as having very high reflectance and transmittance at the respective bands. For these reasons, we plan to implement the Chroma T525lpxr into our system.

3.5.3 Filter Technology Comparison

As previously stated, the dichroic mirror alone is not sufficient to effectively eliminate the laser line as well as Rayleigh scattering. A secondary filter must be implemented into the Raman collection system in order to ensure the Stokes scattered signal is not flooded by stray light. There are a couple of options in terms of filters that can effectively achieve this.

Fiber Bragg gratings are short segments of optical fibers in which there is a periodic alternation of the refractive index of the fiber core. This alternation results in the reflection of wavelengths of light which satisfy the Bragg condition, with such wavelengths being characterized as,

$$\lambda = 2n_{eff}\Lambda$$

Equation 3.5.1 Maximum reflectivity at Bragg wavelength

where Λ is the grating period, n_{eff} is the refractive index of light in the fiber, and λ is the wavelength of light being reflected by the fiber bragg grating [48]. These fibers can be utilized in Raman spectroscopy systems such that the filtered signal from the dichroic mirror is coupled into the fiber, which will act as a wavelength-selective filter that reflects light at the Bragg wavelength (in our case, the laser line), while transmitting all other wavelengths (Raman scattered light) through the fiber. This fiber can then lead the Raman scattered light to the spectrometer setup where the Raman spectrum will be analyzed [49]. However, as these devices are somewhat specialized, it can be difficult to find FBGs with

the center wavelength of 520-532 nm we are looking for, or to find a tunable FBG that is within our price range.

An alternative option for a secondary filter is a notch filter, also known as a band-reject filter. Notch filters are designed to attenuate light within a specific wavelength range to a very low level, while enabling all other wavelengths to pass through with minimal attenuation. Similarly to FBGs, this enables notch filters centered at the laser line to block Rayleigh scattering while allowing both Stokes and Anti-stokes scattering to pass through without significant loss. Notch filters are also highly tunable, as they are a type of dielectric stack filter. Dielectric stack filters, and thus notch filters, have stop bands dependent on the angle of incidence of the sample light. As the angle of incidence increases, the center wavelength of the stop band shifts to shorter wavelengths [50]. This means that a notch filter could be angled so as to precisely block out our preferred laser line, ensuring high signal-to-noise ratio of Raman to Rayleigh scattered light. However, one potential downside of notch filters is that they tend to have rejection bandwidths ranging from one to tens of nm, as the transition width between the stopband and the passband can be somewhat gradual [51]. This means that some Raman shifted light near the center wavelength will be rejected and lost, reducing our workable signal.

In contrast to notch filters and FBGs, longpass filters are a type of edge filter in which all wavelengths of light below the laser line wavelength are rejected, and the cut-on wavelength denotes the threshold corresponding to 50% transmittance. Longpass filters reject almost all light below the cut-on wavelength, meaning it can reject all Rayleigh scattered and laser-line light and enable only Raman scattered light to remain in the system for analysis by the spectrometer [52]. However, this means that the longpass filter will reject all Anti-Stokes scattered light since it is below the laser wavelength, and the remaining signal will be composed of only Stokes scattering. This could mean attenuation of our already weak Raman signal. One advantage of the longpass filter compared to the notch filter, however, is that longpass filters have very sharp transition widths, generally steeper than notch filters. This means that fewer wavelengths above the intended laser line will get rejected, minimizing loss of Stokes scattered light near the laser wavelength. Though longpass filters are not as tunable as notch filters, they are available in many popular laser wavelengths, including around 520 nm, 532 nm, and 550 nm [51].

Considering the potential filter options, we believe a longpass filter will be the best choice for our Raman spectrometry system. Though longpass filters block out Anti-Stokes scattered light, our system will already produce very minimal amounts of Anti-Stokes scattering, if any at all. Along with this, any Anti-Stokes scattering that may be produced by our system will have already been filtered out by the dichroic mirror by the time of reaching the secondary filter, making it negligible to our choice of filter selection. Thus, the sharper edge transition between reflection and transmission compels us to implement a longpass filter into our signal collection system, as this will maximize the Stokes scattering coupled into our spectrometer component and improve the overall signal-to-noise ratio of our system.

3.5.4 Filter Selection

Table 3.3.4.1 compares important parameters of various longpass filters from different manufacturers to determine which filter is most suitable for our Raman spectroscopy system. Such parameters include cut-on wavelength, rejection wavelength, transmission wavelength, optical density, diameter, and cost.

Table 3.5.3 Comparison of prospective longpass filters

<i>Table 3.5.4 Comparison of prospective longpass filters</i>					
	Semrock BLP01-514R-25	Chroma ET525lp	Edmund Optics #84-744 / #84-738	Edmund Optics #29-191	MKS Newport 10CGA-530
Cut-on wavelength (nm)	526	540	525	525 ± 10.5	530 ± 5
Rejection wavelength (nm)	404 - 515	300 - 522	200 - 515	441.8 - 506.8	N/A
Transmission wavelength (nm)	529.4 - 900	540 - 1000	534- 1650	543.5-1100	N/A
Transmission (%)	> 93	97.73	> 91	> 85	> 90
Optical density OD (average)	> 6	6	> 4	> 4	> 5
Thickness (mm)	3.5 ± .1	N/A	3 ± .1 / 2 ± .1	.3	1.1 ± .1
Diameter (mm)	25	20	25 / 12.5	12.45	25.4
Cost	\$405.00	\$365.00	\$255.00	\$140.00	\$47

The most important factors when choosing a longpass filter for our system is the rejection and transmission wavelengths. Ideally, the longpass filter implemented will enable near 100% rejection of light at or below 520 nm, while rejecting minimal amounts of light above the laser wavelength so as to preserve as much Raman signal as possible. This requires a sharp edge transition and high transmission at the passband. Considering the filters

presented in the above table, it would seem only the Chroma filter meets this requirement as it is the only filter to state in the specifications that it blocks 520 nm light. When the raw data for the filter is viewed on the product webpage, it is shown that this filter has near 0% transmission until 520 nm, with 50% transmission occurring at 525 nm and 97% transmission being maintained at and above approximately 526 nm. It should be noted that though the datasheet for this filter defines the cut-on wavelength as 540 nm, this seems to be referring to the point of full transmission rather than the threshold of 50% transmission, as is the traditional definition. Thus, the transmission curve of the Chroma filter demonstrates a very sharp edge transition that perfectly blocks the wavelengths of interest for our system.

Though the Semrock filter states that the rejection bandwidth only extends to 515 nm, a more detailed transmission curve is available on the product webpage that demonstrates full rejection until 522 nm, just like the Chroma filter. Half transmission is achieved around 526 nm, according to the traditional definition of cut-on wavelength and as defined in the specifications of the filter. Approximately 95% transmission is achieved around 528 nm, making the edge transition of this filter similarly steep compared to the Chroma filter. However, the Chroma filter seems to achieve higher transmission in the passband, which is important for maintaining Raman signal intensity.

The Edmund Optics filters similarly do not appear to have a rejection bandwidth that would effectively block our laser line. However, upon requesting more detailed transmission curve information from them, it is shown that both filters could potentially be suitable for our system. The Everix #29-191 is shown to have 7% transmission at 520 nm, reaching 50% transmission at the cut-on wavelength of 525 nm and a maximum transmission of approximately 90% around 532 nm. Having 7% transmission at the laser line may seem minimal, but it could potentially be too much noise compared to our Raman signal, flooding out any meaningful signal we collect and making our system useless. On the other hand, the #84-744 is shown to have .53% transmission at 520 nm, almost completely blocking out any signal at this wavelength. Half-transmission occurs at the cut-on wavelength of 525 nm, and the maximum transmission of approximately 95% occurs around 530 nm. This is comparable to the Chroma filter and is perfectly suited to the rejection and transmission bands needed for our system. The MKS Newport filter did not have any more detailed curve information available, and thus it should be assumed that based on the specifications it is not suitable for our system.

One critical parameter of longpass filters is their optical density. Optical density refers to the light blocking ability of a filter, as it is a logarithmic measure of how much energy the filter rejects [53], [54]. It is defined as the logarithm of the ratio of transmitted to incident power. For example, increasing the optical density by .5 signals a transmission loss of 5 dB. Generally, optical densities of 6 or higher are necessary for extreme blocking applications, a common one being Raman spectroscopy. [55]. Of the filters presented in the table, only the Semrock and Chroma filters have optical densities of 6 or greater. Both Edmund Optics filters have average optical densities of 4, indicating they may not be the best choice for Raman spectroscopy applications. The MKS Newport having an OD of 5 may be passable, had the rejection band been clearly defined to block 520 nm light.

Taking all of these factors into consideration, it seems that the best choice of longpass filter for our system is the Chroma ET525lp. Though the Semrock filter also met all of the system requirements, the Chroma filter is somewhat cheaper, while also having higher transmission in the passband. This will ensure that as little of our Raman signal is lost as possible before reaching the spectrometer, and maintain a high signal-to-noise ratio for our system. The Edmund Optics #84-744 has a perfect transmission curve for our system, but has a less ideal minimum optical density of 4, making the Chroma the best filter choice for our system.

3.6 Spectrometer Setup

3.6.1 Spectral Resolution

The spectral resolution of the spectrometer defines its ability to distinguish closely spaced wavelength peaks. If two spectral lines are closer than the spectrometer's resolution, they will merge and appear as a single peak. Raman spectroscopy requires a smaller spectral resolution and high frequency precision since we're observing small frequency shifts from the excitation frequency. Raman spectroscopy experiments used to identify the vibrational modes of cotton and polyester typically use a spectral resolution of 3 cm^{-1} to 10 cm^{-1} to differentiate the vibrational modes. This is further justified through the separation of relevant peaks, which could range from as little as 10 cm^{-1} to 30 cm^{-1} . A higher spectral resolution comes at the cost of a lowered spectral range and lower received signal intensity.

The four main criteria that determine the spectral resolution of a spectrometer are the slit width, grating line density, spectrometer focal length, and the detector format. Reducing the slit width improves the spectral resolution, but decreases the received Raman signal intensity. Increasing the grating line density spreads the signal over a wider angular range, improving the signal resolution. However, less light reaches the individual detector pixels, and we lose some of the signal intensity. The spectrometer focal length defines the length over which our dispersed wavelengths spread. A longer focal length corresponds to a wider separation of light; however this results in a reduced received Raman signal due to the increased size of the system. The spectrometer's focal length further defines the spectral resolution from defining the separation of wavelengths. The detector format regards the active size of the detector, pixels, and efficiency of the detector. All of which determine how much of the Raman signal is received and how much dispersed Raman shifts could be differentiated from one another.

Considering the contributions from various optical components and alignments to the spectral resolution, one can assess the Instrumental Line Width (ILW) to define the spectral resolution of a spectrometer. The ILW examines the inherent broadening effect an infinitely narrow Raman signal would get from the spectrometer due to dispersion and the pixel size of a detector. The observed bandwidth of this signal is equal to the Full Width at Half Maximum (FWHM). We can consider the Nyquist limit in determining an appropriate spectral resolution of our spectrometer, where the sampling rate must be two times the highest frequency component. If our smallest gap is 10 cm^{-1} , choosing a spectral resolution

half of the gap, 5cm^{-1} , can ensure that the FWHM of the band won't overlap with the FWHM of the band beside it. This concept is further developed by the Rayleigh criteria. The Rayleigh Criteria explains that two peaks are considered resolved if the maximum of one peak corresponds with the minimum of another peak.

3.6.2 Spectral Range

The spectral range of the Raman spectrometer refers to the range of wavenumbers that can be detected by our system. It specifically defines the highest and lowest vibrational frequencies that will be observed from the Raman spectrum. Section 3.1.2 discussed the relative descriptions of the vibrational modes per molecule seen in different textile types. Across cotton and polyester we see a large active range for Raman shifts from 3500 cm^{-1} to 100 cm^{-1} . The most prominent vibrational bands occur in the fingerprint region, 300 cm^{-1} to 1800 cm^{-1} , which will define our Raman spectrometer's ideal spectral range.

The spectral range of the Raman spectrometer is dictated by the spectral dispersion from the diffraction grating and by the focal length of the spectrometer. The following calculation will convert our spectral range of 300 cm^{-1} to 1800 cm^{-1} defined in wavenumbers into wavelengths to guide our filter, grating, detector selections.

$$\Delta\nu = \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_s}\right) \times 10^7$$

Equation 3.6.1 Raman shift (cm^{-1}) to wavelength

Where, $\Delta\nu$ = the Raman shift (cm^{-1}), λ_0 = Excitation wavelength (nm), and λ_s = Raman scatter wavelength (nm). Using Equation 3.4.2.1 results in $300\text{ cm}^{-1} = 540.6\text{ nm}$, $1800\text{ cm}^{-1} = 588.3\text{ nm}$, and $3000\text{ cm}^{-1} = 633\text{ nm}$. Therefore, our primary desired spectral range in wavelengths is 540 nm to 588 nm. As we make component selections for the illumination optics and the spectrometer, we must take this quantity into consideration. Generally, a greater spectral range comes at the expense of our spectral resolution.

3.6.3 Slit Source

The entrance slit of the spectrometer controls how much light enters the spectrometer. As previously mentioned, the width of the slit significantly impacts the spectral resolution of our Raman signal. A wider slit allows for more light collection, yet lowers the spectral resolution. A narrower slit allows for a higher spectral resolution yet lowers the signal intensity.

3.6.4 Diffraction Grating Comparison

The diffraction grating is the defining component of a dispersive Raman spectrometer as it is responsible for separating the Raman signal into its constituent wavelength components. This allows us to discern each Raman shift that corresponds to the vibrational mode of the chemicals in the respective fabric types. Diffraction gratings are repetitive arrays of diffractive elements, apertures, that produce periodic changes in the phase, amplitude, or

both, of an emergent wave. The angle of diffraction will depend on the wavelength of the incident light, this results in a linear spread of wavelengths at the focal plane of the spectrometer. However, since the dispersed Raman shift is expressed as wavenumbers, we receive a nonlinear dispersion. For example, the difference between 800 nm - 810 nm is 10 nm and 154 cm^{-1} , where the difference between 1000 nm - 1010 nm is 10 nm and 99 cm^{-1} . As a result, the detector at the focal plane will collect a constant range of wavelengths, but a nonconstant range of the Raman shifts.

Dispersive optics can come in the form of gratings and prisms. However, diffraction gratings are the prominent technology used in dispersive Raman spectroscopy. Therefore, this initial technology comparison will discuss different types of diffraction gratings.

Ruled Gratings vs. Holographic Gratings

First characteristic of the diffraction grating to consider is whether to use a ruled or holographic grating. Ruled gratings are mechanically manufactured through burnishing grooves into a thin coating using a diamond tip. The resulting groove profile is sawtooth-shaped, and when mounted at a specific angle (blaze angle) it has maximum dispersive efficiency at a specific wavelength (blaze wavelength). Holographic gratings are manufactured photolithographically, where an interference pattern of two standing waves is imprinted onto a layer of photoresist. The resulting groove pattern is sinusoidal, which is ultimately less efficient at blazing than the saw-toothed ruled grating. However, when the groove spacing to wavelength ratio is nearly one, holographic gratings have virtually the same efficiency as ruled gratings. Stray light can be produced from the manufactured irregularities of ruled gratings. This stray light can result in an oversaturated Raman signal. Properly manufactured holographic gratings are free of random groove placement errors found in ruled diffraction gratings. This is due to all of the grooves being formed simultaneously as opposed to one after the other, like in the manufacturing process of a ruled grating. Holographic gratings are typically advised for usage in Raman spectroscopy as the reduced stray light helps maximize the signal-to-noise ratio, therefore improving the spectral resolution. However, we see more usage of ruled gratings in commercially available spectrometers. With the increased efficiency of ruled gratings compared to holographic gratings, paired with our need to limit stray light, a ruled grating will be used in our system.

Reflection Gratings vs. Transmission Gratings

The second characteristic to consider is the method of dispersion, with either transmission or reflection of our Raman signal. A transmission grating passes and disperses light through the material where the grating is etched. Transmission gratings are subject to low alignment sensitivity, which can help eliminate alignment errors in our spectrometer. In reflection gratings, diffracted orders reflect off of the grating at different angles. In the Czerny-Turner spectrometer configuration, reflective gratings are typically used. The reflective grating allows for a more compact system by folding the beam path, and further contributes to a higher resolving power compared to similar transmission gratings. Raman spectrometer designs which use transmissive gratings benefit from a higher optical throughput, this is

due to the robustness in the alignment and the minimized stray light. Transmission gratings typically display comparable efficiencies to reflection gratings, however, maintaining higher efficiencies require lower groove densities. As the diffraction angle increases with an increased groove density, the refractive properties of the substrate material limits the transmission at the higher wavelengths. We will require higher groove densities for better spectral resolution. Therefore, our spectrometer design will incorporate a reflective grating due to its standard usage in the Czerny-Turner configuration and higher efficiencies under increased groove densities.

3.6.5 Diffraction Grating Selection

In selecting the planar, ruled, reflective diffraction grating the next major distinction is the groove density and blazed wavelength. The characteristics of the gratings are comparable across companies as seen in Table 3.4.5.1. We will assess which groove density would be most compatible with our desired spectral resolution, spectral range, blaze wavelength, and excitation wavelength.

Table 3.6.1 Diffraction Grating Product Comparison

Table 3.6.2 Diffraction Grating Product Comparison				
	Thorlabs GR13-1205	MKS Newport 33025FL01-280R	Edmund Optics 43-751	MKS Newport 3025FL01-266R
Groove density (grooves/mm)	1200	1200	1200	900
Blaze Wavelength	500 nm	500 nm	500 nm	550 nm
Blaze angle	17° 27'	17.5°	17.45°	14.3°
Efficiency	~90%	~ 95%	~85%	~90%
Size (mm)	12.7 x 12.7	12.5 x 12.5	12.7 x 12.7	12.5 x 12.5
Price	\$78.11	\$94	\$81	\$155

As specified previously, the ideal spectral range contains the Raman shifts from 300 cm^{-1} to at least 1800 cm^{-1} . This corresponds in wavelength to 540.6 nm to 588.3 nm, and at most 633 nm. For the full Raman shift range to be detected on the CCD, having a lower line density with a weaker dispersion effect is ideal. For better spectral resolution, we must use a greater line density with a higher dispersive effect. Our desired range is ultimately narrow, which makes a higher spectral resolution more desirable. Higher groove density

gratings offer high dispersion and resolution, and are efficient in the UV, VIS, and NIR spectral regions. However, we see less diffracted orders. This consequence is acceptable for our system because we are only looking to assess the first order. Lower groove densities have many diffracted orders, offer good performance with ruled gratings, and have a wider wavelength operational range. Consequently, they offer lower dispersion and lower resolution.

Light incident upon a grating that is diffracted is defined by the following equation,

$$m\lambda = d(\sin\alpha + \sin\beta)$$

Equation 3.6.2 Grating equation

Where m is an integer value describing the diffraction (or spectral) order, λ is the light's wavelength, d is the spacing between grooves on the grating, α is the incident angle of light, and β is the diffracted angle of light leaving the grating. $1/d$ is the groove density. Considering an incident angle of 30° , which is typical of Czerny-Turner spectrometer configurations, we can determine the diffraction angle for each wavelength given a respective groove density using Equation 3.4.5.1. This would ensure that the groove density can compensate for the dispersion in our desired spectral range. We see that 1200 lines/mm diffracts 540 nm at 8.5° and diffracts 633 nm at 15.04° . A 900 lines/mm grating diffracts 540 nm at -0.802° and diffracts 633 nm at 3.99° . While a 600 lines/mm grating would still offer dispersion of our desired spectral range, it would offer less spectral resolution than a grating at 1200 lines/mm. This theoretically coordinates with higher groove densities corresponding to higher groove densities.

The resolving power of a diffraction grating is provided by the Rayleigh criteria,

$$R = \frac{\lambda}{\Delta\lambda} = nN \quad 1$$

Equation 3.6.3 Chromatic resolving power of a spectrometer and diffraction grating

Where n is the order of diffraction, N is the number of grooves in a grating that are illuminated by the source, $\Delta\lambda$ is the spectral resolution, which will be expressed in wavenumbers, and λ is the Raman shifted wavelength. The theoretical resolving power of a 1,200 lines/mm grating is 1,200 (in a 1 mm space). If we illuminated the full 12.5 mm width of the considered gratings, the resolving power is 15,000. Let's consider a desired spectral resolution of 4 cm^{-1} . Converting this quantity to wavelength using Equation 3.4.2.1 corresponds to a resolution of 0.11 nm. Using Equation 3.4.5.2, we determine that the resolving power at 540 nm is 4,909, the resolving power of 570 nm is 518, and at 633 nm is 5754. The theoretical resolving power of a 900 lines/mm grating is 900 (in a 1 mm space). Illuminating the full 12.5 mm width provides a resolving power of 11,250. Therefore, in even lighting a portion of the grating for a 1200 lines/mm and 900 lines/mm groove density, our desired spectral resolution can be met.

The blaze wavelength, as discussed previously, describes which wavelength of the diffracted spectrum will have the highest efficiency. The blaze wavelength of

commercially available diffraction gratings is typically specified at 500 nm. However, MKS Newport offers a blazed wavelength of 550 nm. Carefully assessing the efficiency graphs of each respective grating, we see that the efficiency is relatively maintained across our desired spectral range. Since we can attain a desirable diffraction efficiency with a 500 nm blazed diffraction grating for less cost and with a greater spectral resolution, our spectrometer's diffraction grating will be the MKS Newport grating (33025FL01-280R).

3.6.6 Detector Technology Comparison

Avalanche Photodiode (APD)

The Avalanche Photodiode (APD) is a single channel, modified photodiode. Traditional photodiodes operate in linear mode, which results in a relatively small output current and limited gain. Avalanche photodiodes operate in reverse bias and amplify weak signals with avalanche breakdowns. The signal is amplified because once the photoelectron is detected it is accelerated by the high voltage and generates secondary electrons by impact ionization. The resulting gain reaches levels of amplification of 50 to 350 times per photoelectron and the output signal is proportional to the wavelength of the incident photons. The quantum efficiency is characterized by the silicon region and is generally above 80% from 400 nm to 950 nm. Sufficiently sized detection areas of about 5 mm to 20 mm in diameter are compatible for Raman spectroscopy applications. Consequently, the thermally generated and amplified electrons do contribute to a high dark signal, this can be compensated for with cooling. Due to its capacity to detect low intensity signals, it is worth considering integrating into our system. However, APD's are most suited for single wavelength detection. In our system's intention of identifying a spectral range, this system would be best integrated through a scanning system.

Complementary Metal-Oxide semiconductor (CMOS)

Complementary Metal-Oxide Semiconductor image sensors convert incident light into digital images. CMOS sensors are an all inclusive component, where an amplifier and analog to digital converter is incorporated into each pixel of the sensor. While this quality results in lower power consumption and quicker signal processing compared to CCDs, it is consequently vulnerable to noise in the output image. Having a low noise detector is critical as to not to over saturate the Raman signal. Generally, the miniaturization, on-chip functionality, and cost effectiveness of CMOS sensors have positioned them as the standard for imaging applications. Recent developments in complementary metal oxide semiconductor (CMOS) sensors have allowed them to be considered for Raman spectroscopy applications.

Charged Coupled Device (CCD)

The dominant multichannel detector used in Raman spectroscopy is the Charged Coupled Device (CCD). It is a semiconductor image sensor which converts photons into electric charges. The one dimensional CCD is linear and the two dimensional CCD is an area array. Each channel within the CCD is a photodiode pixel which generates an electric charge that

is proportional to the number of absorbed photons. Light in the 200 nm to 1100 nm range generates photoelectrons in the silicon with a probability that varies with wavelength and determines the quantum efficiency. Each pixel corresponds to a different Raman shift. The vertical pixels detect the spectral range, where the first pixel detects the low wavenumber shift (purple) and the last detects high wavenumber shift (red). The CCD position can be calibrated in terms of the Raman shift, and the resulting spectrum is a plot of electrons vs. shift. A more intense light source or longer interaction time contributes to more registered charges. The CCD can be further characterized into two types: front-illuminated CCD (FI CCD) and back-illuminated CCD (BI CCD). They dictate the direction in which photons interact with the detector, and ultimately result in varying QE curves. BI CCD's typically display a higher QE as the photosensitive region is directly exposed before passing through the electrode and insulating structure, unlike the opposite occurring in FI CCDs.

The CCD is suited for Raman spectroscopy applications for its high sensitivity, which is especially important for the low intensity nature of Raman scattering. The multiple channel availability allows for the detection of a larger spectral range without the need for additional hardware components to implement a scanning system. Therefore, a CCD will be the detection hardware of choice for our Raman spectrometer.

3.6.7 CCD Selection

The role of the detector is to convert the Raman scattered photons into an electrical signal that would allow for further qualitative and quantitative assessment. Detecting the low intensity signal of the Raman scattering requires a sensitive, low-noise detector. The following discussion will assess detector properties critical to high yield sensing of our Raman signal.

Quantum efficiency

The QE of a detector defines the ability of a detector to detect photons. It is a ratio of the number of electrons generated to the number of photons absorbed. The QE of a detector varies with wavelength; therefore, we must choose a detector with a high QE from 540 nm to 633 nm.

Physical Constraints

We will evaluate detectors based on their sensitivity to incident light and their operational spectral range. Detectors have a fundamentally limited spectral range and resolution due to their material characteristics. As we will be assessing fabric samples distinct chemical compositions, we must ensure the detector can compensate for both spectral readings. The physical criteria of the detector relevant to receiving a resolved Raman signal is the photosensitive area, number of channels, and pixel size. The photosensitive area defines the amount of light that can be collected, where a larger active area collects more of the Raman signal. The dispersed light passed the grating will physically spread across the vertical of the detector, a larger area would allow for a larger spectral range to be captured. Having too large of a detector area leads to unnecessary costs and does not contribute to

better efficiency. The number of channels is defined by the number of pixels along the wavelength axis. This quality characterizes the detector as single channel or multichannel. Multichannel detectors (simultaneous acquisition channels) can increase the signal-to-noise ratio. As we increase the number of channels, the size of each detector element must decrease to avoid an unnecessary detector size. The pixel size directly impacts the spectral resolution of the data. The smaller the pixels, the higher the spectral resolution. However, similarly to the other physical constraints, it limits the received signal intensity.

Noise

The noise of the detector determines the quality of our received signal, higher noise levels will overcome the Raman signal. Dark noise, readout noise, and shot noise are relevant to the detector and must be accounted for when purchasing the CCD. The dark signal of a detector refers to the rate of spontaneous generation of electrons in the detector, it specifically refers to the signal when no light is present. This dark signal is generally enhanced by the thermal generation of electrons within the solid-state detector. Readout occurs in the process of converting electrons from the detector to its digital value. It is quantified as the standard deviation associated with the analog-to-digital conversion of the current from electrons in the CCD. Since the detector noise is not dependent on the laser intensity or sample, we can run the spectrometer with the laser off and observe the detector to determine the readout noise. Shot noise is caused by the random arrival of photons at the detector.

Overcoming noise

The total noise can be quantified as,

$$I = \sqrt{shot^2 + dark^2 + readout^2}$$

Equation 3.6.4 Total noise

This total noise, as determined by Equation 3.4.7.1 establishes a “noise floor”. If the Raman signal is smaller than the total noise, it will become overcome by the noise and indiscernible. Shot noise cannot be compensated for. However, dark noise and readout noise can be compensated for in our detector decision. A longer wavelength excitation source, and thus lower energy light, requires detectors that are more prone to thermally generated dark signals. This determines a general operating standard in which the longer the wavelength, the colder the operating temperature detector must be, resulting in a larger dark noise signal. To account for the excess electron generation due to thermal fluctuations, we can cool the CCD. However, this lowers the quantum efficiency of the CCD. -100°C to -60°C defines the range of temperatures which would allow us to maintain the optimal signal-to-noise ratio. Compensating for lower readout noise also involves cooling the CCD.

3.7 Software Technologies

3.7.1 Software Platforms

The Raspberry Pi has multiple options available for its operating system, including one developed specifically for the RPi. Raspbian, or Raspberry Pi OS, is an open-source operating system built on Debian Linux in 2012, and remains consistently updated today. It is developed by the same company as the Raspberry Pi itself and is the official operating system for the RPi. Raspbian is also the OS with the highest level of support of all available options, as it is the most commonly used OS for the system, and is the easiest option for possible troubleshooting and example codes, with a large outright majority of projects and programs published online being built with the Raspbian OS specifically in mind.

There are, however, still other options. One such option is DietPi, a lightweight OS, built upon the Raspbian OS previously mentioned, with the goal of limiting software bloating to streamline RPi performance. This is done mainly through a more condensed operating system footprint, as well as further resource utilization. The system advertises itself as the most user friendly lightweight OS for the RPi, however, it should be noted that the OS is not the same as Raspbian OS and that troubleshooting solutions or open-source projects are not guaranteed to overlap between the two, and in fact it is very common that they do not. Given the fairly controllable size of the base Raspbian OS, this flaw represents a significant drawback of DietPi, and in the circumstance of this project, restricts it to a last resort option for potential RAM difficulties later on.

On the other side of the spectrum is Ubuntu, which is available as an OS option in its latest version for the Raspberry Pi. Ubuntu is a Debian Linux based OS found around the world, and is likely the most widely used Linux OS in existence. While Raspbian might have the highest level of support in RPi troubleshooting and open-source projects, Ubuntu has the largest support of any OS option when considering non-RPi systems running on OS, of which there are countless. And as troubleshooting and public code is not something inherently restricted to the original device, this provides a significant upside for our system. It is, however, larger than almost every OS developed for the RPi, and with a number of technical restrictions for our system, this makes the OS more difficult to implement in our project. And so the Raspbian OS was chosen as our platform.

Table 3.7.1 Software Platform Selection

	Raspbian	DietPi	Ubuntu
Memory (non-volatile)	8 GB	4 GB	16 GB
Developer	Raspberry Pi Foundation	MichaelNG	Canonical Ltd.
Latest Release	November 19, 2024	February 23, 2025	October 10, 2024
Open Source	Yes	Yes	Yes

3.7.2 Software Language

While several languages were considered for the project, the most realistic options for the project were Python, C++, and Node.js. C++ offers potentially the highest performance of the three and is likely the best option for hardware communication. C++ allows for direct control of hardware communication as well as of memory management, something crucial in this project, given the hard cap on random access memory available. This is in addition to access to object-oriented functionality, unlike in C, which ensures all aspects of the project are definitely possible using C++. The drawbacks of C++ include rigid coding flexibility, repetitive functionality, and longer expected development time.

Node.js works as an alternative with strong RPi support, though not to the same level as the others, and all functionalities necessary for the project. It is also effective in performance when operating in user-prompted systems, bounded by input and output, which this system is. However, given its development for web based projects it is not the best option given the technical constraints of the RPi's CPU and RAM when compared to usual JavaScript projects.

The only language that is better suited for the project is Python, due to the largest library support of the available options and comparable performance to C++. Python is the most flexible coding alternative and has the widest field of open-source resources. Given its flexibility, it also has the quickest development time and holds an advantage in its ability to support machine learning methods, a possible aspect of future development in the project. It will likely be slower than C++ and could be a burden on the CPU in worst cases, but the advantages outweigh the drawbacks, so Python was chosen.

Table 3.7.2 Software Language Selection

	Python	C++	NodeJS
Object-Oriented or Procedural	Object-Oriented (w/ Procedural support)	Procedural (w/ OOP support)	Object-Oriented (w/ Procedural support)
Performance	Slowest	Fastest	Moderate
Memory Management	Automated	Manual	Automated
Development Speed	Fastest	Slowest	Moderate
Compilation vs Interpretation	Interpretation	Compilation	Interpreation
Familiarity	Stronger	Moderate	Strongest

3.7.3 Python Packages

Serial

This package allows for easy GPIO communication, letting the RPi communicate high and low states of the CCD sensor's pins with simple one line functions.

PyPlot

Taken from the MatLab python library, PyPlot allows for easy line graph creation with a number of functions related to title formatting, axis calibration, and data point plotting.

Time

This package contains more detailed measurement functions to ensure precise processes, such as data extraction with the analog-to-digital converter, do not fail due to miscalculations.

NumPy

NumPy or numpy is an array and matrices analysis library, with data shaping and a variety of mathematical functions included. It is the most robust array library in Python. It is also open source and highly recommended for any data analysis involving arrays, as it speeds up all processes significantly.

FastDTW

FastDTW is a lightweight dynamic time warping function that can provide the full process and results of DTW in a singular function, only requiring two arrays and a listed distance metric as parameters. The arrays are inherently required to be of differing dimensions and the distance metric will in all useful cases be a separate package, but the function is the simplest method of implementing DTW, it is user-friendly, accurate, and efficient.

Euclidean

This subpackage of SciPy, itself the most common scientific computing package in Python, provides the ability for seamless Euclidean distance calculation, whether as a function or as a parameter. The package can be listed in the fastdtw function as a parameter and provide accurate results without any added processing time, and like fastdtw is inherently easy to use.

KMeans

K-Means is one of multiple clustering algorithms inside SciKit-Learn's cluster subpackage, and is often the most widely ranging in its effectiveness. In this project's case it works well as an easily fitted clustering algorithm to sort and analyze the altered dimensional array of similarity results after dynamic time warping.

4 Standards and Design Constraints

This chapter details relevant industry standards and design constraints that our team must take into account when designing our system.

<https://nvlpubs.nist.gov/nistpubs/Legacy/NSRDS/nbsnsrds17.pdf> FIND BONDS AND ADD TO STANDARDS

More Electrical standards

4.1 Industry Standards

Before outlining any design constraints specific to our system and timeline, it is vital to first identify any industry standards we must consider when implementing such constraints. It is important to consider these standards so that our system does not break any safety protocols and can be easily integrated into other systems that utilize industry standards. The majority of our project relies on the application of optics technologies and principles, and thus these related industry standards will be discussed first. Paying attention to industry standards is especially important in our project due to the use of lasers that have the potential for human injury upon contact, among other systems that could potentially pose a hazard.

4.1.1 Laser Standards

The standards set by ANSI Z136.1 - 2022 lay guidelines for the safe use of lasers operating between 180 nm and 1000 μm . It defines the qualifications for each class of laser, separating lasers based on their potential for biological harm [56]. Laser classes range from 1 to 4 and are divided into M, R, and B subclasses. In order of ascending hazard level, the laser classes are 1, 1M, 2, 2M, 3R, 3B, 4.

Class 1: This class characterizes lasers of the lowest level of potential biological harm, which are considered incapable of producing damaging laser radiation during normal operation. Class 1 lasers emit less than .39 mW or are otherwise located inside of a device such that the beam of any power level is not accessible during device operation. These lasers are safe for long term, intentional viewing and are not considered to be an eye hazard [57]. They are thus exempt from any control operation and do not require particular safety measures to be taken [58].

Class 1M: Like Class 1 lasers, lasers of this class are safe for long-term direct eye contact, but they can potentially become dangerous when viewed through optical instruments such as binoculars or magnifying glasses.

Class 2: These lasers must emit a visible beam of less than 1 mW of power; infrared or ultraviolet beams cannot be Class 2 or 2M. They are not safe for continuous viewing, as prolonged staring into the beam can be hazardous and damaging to the eye. However, Class 2 lasers are safe for unintentional viewing for less than $\frac{1}{4}$ of a second, and thus the natural aversion response of someone blinking away from a bright light is considered enough protection against this class of lasers.

Class 2M: These lasers are similar to Class 2 lasers in that they are safe for unintentional viewing for less than $\frac{1}{4}$ of a second. However, they can become hazardous in less exposure time should these lasers be viewed with a magnifier or similar optical instrument.

Class 3R: This class includes all visible light lasers emitting beams between 1 and 4.99 mW of power. Though it is not safe to purposefully stare into the laser for longer than $\frac{1}{4}$ of a second, accidental exposure to a direct or reflected beam is unlikely to cause significant damage. There is no eye risk associated with a diffused beam from a Class 3R laser.

Class 3B: Lasers in this class are defined as having between 5 to 499.9 mW of output power in the visible region of light, under pulsed or continuous wave operation. These lasers pose an eye hazard upon any exposure to the beam, whether direct or reflected into the eye. Humans' natural aversion response is not enough to protect the eye from direct radiation from these lasers. Diffuse reflections, however, are generally considered safe so long as the laser spot is not stared at for a prolonged period at close range. Class 3B lasers can burn skin and other materials if they are held for long enough at a close enough range. Protection from these lasers involves the use of safety eye glasses specialized for the wavelength of light being used.

Class 4: This class denotes the highest laser hazard level, and is a label applied to continuous wave lasers capable of producing greater than 500 mW of power and pulsed lasers capable of producing over 125 mJ in under .25 seconds [58]. It also applies to lasers that may generate hazardous airborne contaminants during operation. These lasers pose a severe eye hazard from direct and reflected beams, and a person should not even stare at the laser dot on a surface so as to avoid injury. Class 4 lasers can instantly burn skin and other materials upon direct contact. These lasers require safety eyewear in combination with barriers for safe operation [57].

Our system intends to utilize a laser that produces under 100 mW of power, classifying it as a Class 3B laser. It is important to keep in mind these safety standards when working with our laser; even though we are not working with a Class 4 laser, there is still potential for harm if the laser is handled improperly. According to the Class 3B safety standards, we must take caution to avoid staring at the laser dot as it rests on the sample fabric, and also monitor our sample closely such that prolonged laser exposure does not cause the sample to catch fire.

4.1.2 Optics Testing Standards

ISO 10110 is a set of standardized notations used for specification of optical elements and systems. It lays out a comprehensive list of parameters which can be used for describing optical components such as lenses, prisms, filters, mirrors, and others. These include dimensional parameters, describing the physical size of an element, such as diameter, thickness, and curvature of a lens. There are also surface quality parameters, which can convey the roughness, scratches, and irregularities of the optic's surface. Tolerance specifications indicate acceptable deviations from the dimensional parameters, ensuring a predictable amount of variability in component performance. Coating specifications

describe the material composition, thickness, reflectance/transmittance, and spectral characteristic requirements for optical coatings. All of these parameters are conveyed through a structured series of symbols and numerical codes, providing a uniform way for manufacturers to express the optical requirements met by their products [59].

This standard is important to our system as it will help us determine whether the components we've selected are acceptable for the specifications of our project. Every component in the Raman signal collection setup, from the lenses to the filters to the dichroic mirror, is applicable to this set of standards. Thus, having an understanding of this standardized notation being used will allow us to quickly and clearly understand whether or not the optics chosen for our system meet a high level of quality just by glancing at the manufacturing information. This will ensure our system is of the highest quality performance and build for our budget.

4.1.3 Communication Standards

Inter-Integrated Circuit

Since the analog-to-digital converter being used in this project is the ADS1115, the communication protocol used between the ADC and the Raspberry Pi system controller is an inter-integrated circuit (I2C). I2C is one of the most frequently used industry standards for synchronous serial communication, the other being a serial peripheral interface (SPI). I2C can often be found within a printed circuit board, acting as the communication bus for the microcontroller unit in order to interact with other components on the board. It is usually chosen due to the simplicity of its design, as while it is capable of connecting several devices at once, it only requires two pins. These two pins are for the clock (SCL) and data (SDA) lines. This differentiates I2C from SPI, as due to a requirement of support for full duplex communication, a serial peripheral interface has four wires. Because of this, I2C is not an option in systems requiring either half or full duplex communication, but in systems that have no such requirement I2C offers a simpler alternative. I2C also functions as an alternative to a universal asynchronous receiver and transmitter (UART), with the advantage of being a synchronous communication bus, because as the UART name suggests, it is asynchronous. These advantages make I2C ideal for systems that require the synchronous capabilities found in SPI, but wish to maintain the simplicity of the two wire systems seen in asynchronous serial communication buses such as UART. I2C is also capable of supporting multiple master devices within its system, unlike buses such as SPI. There is, however, a drawback when comparing I2C to SPI in terms of rates of data transmission, as while I2C places ahead of asynchronous serial communication in this regard, it is still slower than more complex systems like SPI. Standard I2C allows for 100 kHz for data transfer and 7 bit addresses, but usually includes a faster system mode of 400 kHz data transfer and space for 10 bit addresses. I2C operates based on the previously mentioned two wire signals, SDA and SCL, with pull-up resistors on both to control their states. Messages are sent in two segments, first the address frame to indicate which device the message is meant for, then the frames in which the message data is held. These messages travel through the SDA line when the SCL is initially set to low, and the address or message data is then sampled by the receiving or transmitting device once the SCL is

set to high. The SDA line is set to low prior to the SCL doing the same to indicate the beginning data transmission, followed by the SCL then being set to high for each bit as mentioned before. First, this will take in the address data, then one bit to indicate if the message is requesting or sending data, and if so, then next the message data is sent, before finally a stop signal is indicated by the SCL line being set to high and followed by the SDA.

4.2 Constraints

System constraints further dictate the functionality and design of our Raman spectrometer. The previously assessed system standards designate the more formal constraints of our project. The constraints that will be discussed here present themselves due to the nature of our project and from the general expectations outlined in the course.

4.2.1 Time Constraints

One of the biggest factors our team must take into consideration as we design and test our system are the inherent time constraints involved in Senior Design as a capstone course. Though Senior Design is typically a two semester class, our class in particular takes place over the Spring-Summer semesters. This means we have approximately 28 weeks to fully design and implement our Raman spectroscopy system compared to the typical 32 week Fall-Spring capstone course. Considering this reduced timeline, along with the very technical nature of our project, it is important for our group to maintain strict personal deadlines aside from those set by the course leaders. Doing so is the only way to ensure we deliver a working product by the end of the Senior Design course.

The first 6-8 weeks of research for our project was mostly dedicated to understanding the principles of Raman spectroscopy and how they apply to specification of textiles, as well as selecting the integral components needed to build a successful Raman spectrometer. Our team upheld weekly progress deadlines throughout this process to ensure that all members are equally contributing and documenting their design process without falling behind schedule, which would be detrimental to the completion of our system. Following the research phase is the design and testing phase, which requires even more strict enforcement of weekly plans.

The majority of the time constraints for our project are involved in the testing phase. Due to the expensive nature of optical components, it is important to do thorough testing prior to purchasing the most expensive parts so as to ensure that the components we do purchase are compatible with each other and lend themselves to a high-performance system. However, testing can be quite time consuming and thus any delays in testing could lead to delays in purchasing parts or ordering the PCB, which would prevent us from finishing our project on time. Because of this, it is important for the team to enforce a strict testing schedule and address all bugs and roadblocks as quickly as we possibly can. Doing testing early on will give us more leeway when it comes to solving technical errors, and more time to speak with our accomplished reviewers and professors who could help us work through issues more efficiently.

Another factor to consider regarding the timeline is the time it takes for parts to be shipped or for custom components to be fabricated and sent to us. This is especially important when it comes to the PCB, as custom PCBs could take 1-2 weeks to arrive, meaning any issues encountered too late into our project would leave us with little time to address them and order a new PCB. Issues like this could potentially be circumvented by designing our PCB to be flexible and prepare for unforeseen mistakes. These time constraints also apply to any other optical or electrical components should they have an extended shipping time, such as 2-5 weeks. As such, it is important to order parts well in advance so that if we were to run into design errors or a part became broken, we would be able to replace it and run tests with the new component well in advance of our final presentation.

4.2.2 Economic Constraints

Raman spectroscopy naturally lends itself to economic constraints. Being that we are a student led senior design team, cost is a major consideration in our project and largely guides our decision making. Apart from the general need to be economically mindful due to our personal budgets, creating a cost effective Raman spectrometer is part of our greater objectives. When exploring means of performing textile identification via spectroscopy, we came across commercial products that were upwards of \$2500 dollars. These spectrometers typically operate in the NIR region and use costly InGaAs detectors. Our main leverage to commercial products, and justification for completing these projects is rooted in the cost efficiency of TEXRAY.

All of the specific optical components used in a Raman spectrometer contribute to the quality of our received signal. By nature of the low intensity of Raman scattering, the components that we implement must contribute to suppressing noise and ensuring our signal is receivable. Components that cater to producing a high quality Raman signal are generally more expensive. Our first major confrontations with this tradeoff guided our excitation source and detector type selection. Using a visible wavelength excitation source avoids the need for costly IR laser source and InGaAs detectors. Even with that initial cost deducing compromise, the economic constraints still poses itself. CCD detectors typically used in visible Raman spectroscopy contain a cooling unit to increase the efficiency of the detector. However, these CCD's are more costly than other commercial detectors. We must consider whether to abandon the cooler or implement it for increased efficiency. This dynamic and compromising for cost efficiency and quality will continually show itself in the design process.

Dealing with the economic constraints involves careful planning and testing to ensure we create an economical, quality Raman spectrometer. Part of this process occurred in technical specifications of Chapter 3. Extensive considerations were made for each hardware component, where we contemplated their functionality and price points. Decisions were justified based upon the prices and functionalities of the component and how they contributed to the overall operation of the system. In further catering to the economic constraints, we explore all sources of hardware purchasing. A large part of the economical optical market comes from ambiguous resellers on Amazon and Ebay. The prices of optical and electrical components on these sites are compelling, yet we must

approach these sources discerningly. Despite careful planning, testing is ultimately a different matter. While we may make all of the necessary considerations on proper integration of optical and electrical components, we may run into malfunctions. This contributes to the economic constraints as it requires the purchasing of duplicates of the material.

Despite the compromises that are made due to the economic constraints faced throughout this project, it reflects the economic constraints that are dealt with in industry. Limited budgets present themselves in a majority of engineering projects. There is a constant clash of increasing cost effectiveness while catering to other system expectations from the customer. Therefore, while the economic constraint is uncomfortably restricting, it serves as an opportunity to perform Raman spectroscopy—a highly technical and demanding task—as economically as possible.

4.2.3 Material Preservation Constraints

An attractive quality of Raman spectroscopy is its ability to perform a nondestructive chemical analysis on a subject. Specifically regarding product identification and comparisons contexts—whether it be for forensic, environmental, preservation, or authentication purposes—the capacity to test on fabrics without reducing its chemical makeup is highly sought after. This is why we chose Raman spectroscopy as a means to perform fabric material identification and comparisons. However, despite Raman spectroscopy's inherent nondestructive nature, there are still system considerations that must be made to ensure the preservation of our fabric samples. Further, there are intrinsic qualities of our material that dictated our Raman Spectrometer design.

The laser wavelength and power level, paired with the system's acquisition time play a prominent role in the quality of our Raman spectrum and in the material subject. While higher laser power or longer acquisition times may increase the spectral resolution of our received Raman signal, it can simultaneously degrade the quality of our fabric samples. A 30mW 520nm laser incident upon a sample does not have the capacity to noticeably physically diminish the sample. However, this deduction might prove itself differently if we performed Raman spectroscopy on the same spot numerous times. The basic and advanced goal of the functionality of TEXRAY involves the product identification of non dyed, homogeneous samples of cotton and polyester. The product comparison function, as part of our advanced goal, involves performing Raman spectroscopy on a non dyed, homogeneous sample. We must ensure extra care towards these samples to preserve their material integrity.

Another critical consideration is the interference of the Raman signal from fluorescence of our fabric samples. Fluorescence is a common occurrence amongst fabric materials, an effect which is exacerbated for dyed subjects. While fluorescence of fabric under our system's design is not inherently destructive to the sample, it does alter the quality of our received Raman signal. Extensive considerations on the implications of fluorescence in our system was discussed in Section 3.2.1. As a brief review, the characteristic of fluorescence in fabric samples paired with the tests completed with the Horiba LabRAM Evolution Nano

Confocal Raman Microscope, dictated our 520 nm laser excitation source selection and system's functionality. As opposed to being able to create a universal textile identifier system that could identify the material composition of more diverse fabric sample types, we are limited to the identification of undyed samples for the most accurate results.

4.2.4 Manufacturing Constraints

The manufacturing constraints of the system are expected and stem from understandable reasons such as cost, available resources, unforeseen issues during assembly, and general availability of parts. Given the complexity of the project and the specialized equipment involved, these limitations are realistic and should be considered throughout the development process to allow for practical and efficient planning.

Component costs vary widely, and as prices rise, the likelihood of incorporating those parts into the system decreases. Since we are working within a limited budget, this could prevent us from using the ideal combination of parts for a flawless setup. Some of the most reliable or accurate components may be out of our price range, forcing us to opt for more affordable alternatives, possibly requiring additional components to compensate for the performance gap. We've identified which parts will likely be on the expensive side and have communicated that clearly within the group, giving everyone time to prepare and manage their contributions accordingly.

During system assembly, it's almost inevitable that something will go wrong at some stage. Taking the PCB as an example, unexpected issues can arise that aren't easily fixed on the fly, which would require us to reevaluate the design. That's why it's highly recommended to have the PCB in hand and tested early in the process, to confirm the design works as expected and to allow time for any needed revisions. When it comes to housing, ideally everything would fit together seamlessly, but minor dimensional discrepancies can throw that off. To stay ahead of this, once all components are available, the housing design should be near completion so we can test how well everything fits and is properly aligned and adjust if necessary.

When ordering parts and equipment, availability is always something to keep in mind. Items may be out of stock or on backorder, and planning for this in advance is important. If a part is unavailable with no imminent restock date, an alternative needs to be seriously considered. Substituting parts may change certain specifications of the system, so careful research is needed to make sure replacements are still compatible. Another factor is shipping time, delivery estimates need to be built into our overall timeline to avoid delays. Ideally, we don't want to rely on components that will arrive outside of the time allotted for manufacturing.

Since this is a two-semester capstone project and not a full-scale industry effort, some resource limitations are expected. That said, we still have access to solid tools and support through the University, which should allow us to confidently move forward and complete the project. However, there may be a few cases where industry-grade equipment could have been beneficial but simply isn't available to us.

5 Comparison of ChatGPT with other Similar Platforms

How does chat gpt relate to our project

Large Language Learning Models (LLMs) now hold a ubiquitous role in the research, design, and workflow process of a 21st century professional and academic. While LLMs are valuable as assistive tools, their use comes with rewards, risks, and responsibilities that must be taken under serious consideration. As engineering students, we are accountable for the work submitted, regardless of AI assistance. While LLMs can provide quick and concise responses, we must be mindful of its limitations, critically evaluate its outputs, and recognize the importance of producing individual work. This chapter will serve as an ethical survey on the use of LLMs for the development of TEXRAY through various examples.

Large language models are machine learning systems that predict and generate plausible language. These models estimate the probability of a token, or of a sequence of tokens. Tokens can be a word, character, or subwords and represent the fundamental unit that LLMs train with. The overall training scheme works by inputting all but the last token amongst a set of tokens. For example, let's regard the saying by William Shakespeare, "To be or not to be". A data scientist would input, "To be or not to ____". The model will make a prediction on what the last word should be based upon the probability of a selection of words. The model's prediction will be compared to what the true last word is, "be". Through an algorithmic process called back propagation, it will evaluate the decision and parameters to make the model more likely to choose the correct word. The capacity of LLMs the past couple of years have far extended the last few decades of development and research. As computer memory, dataset sizes, and processing power continue to increase, more effective techniques for modeling larger text sequences will be developed.

Despite their capabilities, LLMs have notable limitations. If used carelessly without regard to its restraints, the integrity of the work produced could be compromised. They are prone to generating false information, known as hallucinations. Hallucinations generally occur due to insufficient data on the subject or biases in the data used to train the model. Further, AI models have a lack of information. They only "know" what tokens they are trained on, and recent models lack recently developed information. They additionally hold limited reasoning skills. On a more subjective note, a dependence on LLMs can hinder the learning process that comes with investigating a research topic. The extent of understanding of a topic varies when interacting with a topic through a quick transaction with an LLM versus having to thoroughly explore different sources. Overall, we are carefully considering the limitations in the functioning capabilities of LLMs when using them as assistive tools for research purposes.

5.1 ChatGPT Evaluation

ChatGPT is undeniably the first LLM that any student might think of when asked to discuss the pros and cons of utilizing AI for research. ChatGPT was first released as an early demo in November 2022 and quickly went viral due to its extensive capabilities at the time. However, the first version of ChatGPT was GPT-1 which was introduced in June 2018. GPT itself stands for generative pre-trained transformer, and this initial version of the model consisted of 117 million parameters [60], which are the settings that control and optimize how the model generates responses to a user's input [61]. Parameters help the model generate responses that are coherent and contextually accurate; meaning, the more parameters a model has, the more effectively it can discern complex patterns in the data and provide more precise responses [62]. Currently, GPT-4 is estimated to have approximately 1.76 trillion parameters, and is predicted to be a mixture-of-experts model.

This model type has multiple MoE layers, in which each layer has a certain number of “experts,” where each expert is a neural network. This is in combination with a gate network or router for every layer, which determines which tokens are sent to which network or networks. This router is composed of learned parameters and is pre-trained with the rest of the network. This model type enables more efficient pretraining and faster response inferencing than other models, but it generally struggles with fine-tuning the details, leading to overfitting. This is a phenomenon in which the machine learning model cannot generalize to all types of data within its domain and instead fits too closely to its training dataset, causing it to not give accurate predictions for new data [63]. Another limitation of the MoE model is that only some of the many parameters within the model are used during inference, leading to faster inferences but higher memory requirements, as all parameters still need to be loaded in RAM [64].

This model type being utilized for ChatGPT-4 has many advantages, especially regarding Senior Design. The trillions of parameters ensure that the model can comprehend a variety of different types of prompts and questions, leading to more precise answers in a more natural, human voice. This could be useful for gathering general information regarding our senior design project quickly when manual research would be more convoluted and time consuming. However, ChatGPT uses the “token” method of response as previously discussed, in which it pieces together responses to your prompt based on the most likely tokens, which are trained solely on the system's training dataset rather than searching the internet for every response[65]. This means that if there is false or outdated information in the dataset it was trained on, it would provide an incorrect answer with full confidence, confusing your research and potentially extending your workload by forcing you to fact check whether or not the information provided is true. Because of this, ChatGPT is likely not very suitable for research-based tasks in niche topics like Raman spectroscopy, as it is likely for it to provide false or misconstrued information based on its training set.

5.1.1 Example 1

In this case, it may be more useful for the purposes of Senior Design to utilize ChatGPT solely for prompts that do require searching the internet and retrieving simple resources, as

these can be quickly and easily fact-checked. For example, when asking ChatGPT the following prompt: “Provide me with a longpass filter that will effectively block out 520 nm light, has greater than 90% transmission at 530 nm, and has an optical density of at least 4.” The full response to this prompt can be found in Appendix A under Output 1. ChatGPT was able to provide a list of three longpass filters which seemingly met the specifications we had set. The first option it provided was actually in the product line in which the Edmund Optics #84-744 is included, which was one of the filters under consideration in section 3.3.4. This demonstrates its ability to accurately determine a product line that suits the constraints I had set for it, indicating that asking ChatGPT such questions can significantly reduce the time spent searching for suitable components for our system. However, it should be noted that though ChatGPT did provide links to these resources, the links were sometimes nonsensical and irrelevant. For example, when discussing the Edmund Optics filter, the model attached one link that led to the Schneider Kreuznach website, which does not distribute the filter that was in discussion. The second link under the discussion of filter #84-744, however, did properly link to the Edmund Optics page and to the location of the specific filters which met our constraints.

This example demonstrates how though ChatGPT can certainly be useful in quickly and precisely retrieving simple resources off the internet, it is important to double check the information provided. Users must ensure that not only do the answers provided actually meet their specifications, but also that the attached references are not randomly pulled or nonsensical with regards to their topic, as this is a very common possibility with ChatGPT. Utilizing ChatGPT in this manner would likely be the most efficient and beneficial way of integrating AI into Senior Design research and development.

5.1.2 Example 2

Mathematical analysis is a significant part of our project. A regular computation we make is the conversion of a Raman shifted value (in wavenumbers) to wavelengths. I asked ChatGPT when given a 520 nm laser excitation source, to convert the 1000 cm^{-1} Raman shifted value from wavenumbers to wavelengths. The result it provided was 548.8 nm, where the actual answer is 548.52 nm. While ChatGPT’s output made a disclaimer that the result was an approximation, a rounding error to that extent could be detrimental to certain design efforts. I have seen ChatGPT continually miscalculate on analytical mathematical problems. Example 3 explores the wider use of ChatGPT through providing the required equations and optimizing the calculation process. The full interaction can be found in Appendix A under Prompt 2 and Output 2.

5.1.3 Example 3

MATLAB is a high-level programming language and numerical computing platform designed for data analysis, algorithm development, and creating models and applications. MATLAB is particularly useful for the analysis and design portion of creating the spectrometer portion of our system. There are many variables which govern the spectral range and resolution of our spectrometer, so it’s quite useful to have an optimized way of testing different values for the variables at once, as opposed to completing many iterations

of hand calculations. Prompt 3 asked ChatGPT to create a MATLAB code that could tabulate the spectral dispersion of a Raman signal at 100 cm^{-1} , 1500 cm^{-1} , and 3000 cm^{-1} . It considered an excitation wavelength of 520 nm, four different groove densities: 300, 600, 1200, and 1800 grooves/mm, and four different focal lengths: 100, 250, 500, and 1000 mm. I provided the required equations and other given variables. To reference the output, I used *Raman Spectroscopy for Chemical Analysis*, by Richard L. McCreery. The full interaction can be found in Appendix A under Prompt 3, Output 3, Prompt 4, Output 4.

The first MATLAB script prompted the following error:

```
Error using ()
The number of table variables in an assignment must match.
```

I pasted this error into ChatGPT and I received the following second error message:

```
The VariableNames property must contain one name for each variable in the table.
```

I disregarded tabulating the data and asked for the derivations in list format. The code ran with no error messages, I received the following results. The units were off.

```
Groove Density: 1200 gr/mm, Focal Length: 100 mm
Raman Shift: 100 cm-1 -> Dispersion: 3.11579 cm-1/mm
Raman Shift: 1500 cm-1 -> Dispersion: 2.68094 cm-1/mm
Raman Shift: 3000 cm-1 -> Dispersion: 2.25128 cm-1/mm
```

Prompt 4 asked to carefully consider the units in the dispersion calculations and provide a new MATLAB script. The new MATLAB script provided the same results. This is despite the inclusion of a new script and with an explanation which implied careful considerations were made for the units. Therefore, I manually went through the code and changed the calculations to receive the proper results.

```
Groove Density: 1200 gr/mm, Focal Length: 100 mm
Raman Shift: 100 cm-1 -> Dispersion: 311.57856 cm-1/mm
Raman Shift: 1500 cm-1 -> Dispersion: 268.09376 cm-1/mm
Raman Shift: 3000 cm-1 -> Dispersion: 225.12789 cm-1/mm
```

ChatGPT displayed acceptable sensibilities when it came to creating code. While it had issues tabulating the data, that is permissible in this context as the table was simply for readability in the output. Continuously iterating through ChatGPT to create a tabulated output would contradict the optimization efforts. Therefore, after two error messages I sought to simplify my output that would be more compatible with ChatGPT's abilities. ChatGPT created workable code that was compatible with MATLAB. However, as explored in Example 2, ChatGPT proves to lack in the analytical sector. After prompting for a new script which account for units, it could not deliver. Without providing the specific equation and variables, one could expect the resulting MATLAB code to be considerably

more corrupted. With this detriment taken under consideration, ChatGPT has ultimately proven itself useful in our project as a means of rendering code that can help optimize the analysis process.

5.2 DeepSeek

DeepSeek, a Chinese AI research company, is a relatively new contender in the artificial intelligence space but is quickly building a name for itself. Its mission is ambitious which is to close the gap between itself and major industry leaders like OpenAI's ChatGPT, specifically targeting its newer model, o1, with the ultimate goal of becoming a top competitor, or even dethroning it entirely. What gives DeepSeek an edge in this pursuit is its strong focus on machine reasoning and code generation, with continued development aiming to bring it on par with the best technologies available today.

One of DeepSeek's standout goals is its emphasis on open-source development and research transparency, setting it apart from more closed-off competitors. The company has released multiple versions of its AI models, including DeepSeek V2 and the more recent DeepSeek R1-Lite-Preview, which is marketed as a reasoning-focused model. This type of model aims to generate solutions and responses that resemble that of human-style reasoning. Based on testing, DeepSeek has demonstrated promising results, solving math problems accurately, writing code effectively, and even performing creative tasks. Some testing comparisons have even suggested it outperformed OpenAI's o1 model in certain areas.

Another factor in DeepSeek's rise is its efficient use of memory, which significantly reduces operating costs for users. This combination of performance and affordability helped the app gain massive traction quickly, becoming the most downloaded free app in the United States upon its release. The surge in popularity even caused surge in the tech industry, leading to a noticeable dip in U.S. tech stocks.

However, this rapid success hasn't come without setbacks. Despite its popularity, DeepSeek has already faced performance issues and outages. Additionally, some countries, including Australia and Italy, have taken preemptive action by blocking access to the app. The concern from these regions revolves around potential national security risks and the possibility that users' personal data could be collected and stored without sufficient provisions.

Now turning to a more direct comparison between DeepSeek and ChatGPT, this is where the evaluation becomes more refined. In our own testing, we gave both AI systems the same prompt and reviewed their responses side by side. ChatGPT's response was clear, useful, and provided solid direction for our project. It also took the time to explain its reasoning, which added value to the solution. DeepSeek's response was noticeably less accurate, misguided, and ultimately not usable for our intended purpose. Based on this comparison, ChatGPT still stands out as the more refined and reliable AI platform when it comes to delivering useful and well-explained content.

Beyond personal testing, DeepSeek is reported to have similar limitations as ChatGPT when it comes to restricting politically sensitive content. But on the contrary, concerns about data privacy breaches remain higher. Unlike ChatGPT, which has had years to build its reputation and trust amongst users, DeepSeek is still new and hasn't yet earned the same level of trust from its users. This makes users more cautious, especially in political settings.

To improve the user experience with DeepSeek, one strategy is to test it across various topics and compare its outputs to those generated by ChatGPT. Doing this can help identify the areas where DeepSeek excels and may prove useful, while also highlighting where it still needs improvement. Overall, while DeepSeek has room to grow, especially in terms of reliability, security, and overall trust, it shows real promise. It'll be interesting to watch how this software develops and whether it can eventually stand toe-to-toe with the industry's biggest names.

6 Hardware Design

6.1 Excitation and Collection Design

This section will outline the finer details involved in the design of a functional Raman signal collection optical system and discuss the specifics of integrating the optical components selected in Chapter 3.

Referencing the collection configuration outlined in Figure 2.4.3, and as previously discussed in Chapter 3, the signal collection optical system will be comprised of a laser diode which will be collimated by a single biconvex lens, upon which it will be directed onto a dichroic mirror. The dichroic mirror will selectively reflect the laser line towards a focusing lens, which will illuminate the sample with the focused beam. This interaction will cause Raman shifted photons to be scattered in all directions, upon which Lens 1 will re-collimate as much of this scattered light as it can accept, redirecting it back towards the dichroic mirror. The dichroic mirror will again selectively block the laser line, allowing only Raman scattered light to pass through to the long pass filter. This filter will further eliminate the laser line, upon which the collimated beam will then be focused by Lens 2 and coupled into a multimode fiber, carrying the Raman signal to the spectrometer setup.

6.1.1 Collimating the Laser Diode Beam

The first lens in the system that will be used to collimate the laser diode's beam must be strategically selected such that the collimated beam diameter is suitable for Raman spectroscopy. As previously discussed, Raman signal strength is directly proportional to laser power at the sample. Intuitively, laser power density, or laser intensity, at the sample is just as important to generating a strong signal [29]. In order to ensure high laser intensity at the sample, Raman spectrometer systems typically limit their spot size to between .5-10 μm , noting that the minimum achievable spot size is diffraction limited. Due to the complex optical processes that occur during Raman spectroscopy, it can be difficult to approach the diffraction limit [66]. For this reason, our system will aim to achieve a maximum spot size

nearing approximately 10 μm in diameter, which in combination with our high power laser diode will still ensure significant Raman signal generation.

Because laser diodes are highly divergent, our beam must first be collimated to an appropriate diameter before it can be focused to a 10 μm spot. Understanding that a lens essentially conducts a Fourier transform on incoming light, and that the inverse Fourier transform of an extremely narrow beam is a very wide beam, it is inherent that to achieve such a tight spot size our collimated beam needs to be relatively wide. For our purposes, it should be sufficient to aim for a 3 mm collimated beam diameter, when assuming the $1/e^2$ definition of beam diameter. This defines the beam diameter of a Gaussian beam as the distance between the two points where the intensity is $1/e^2$, or 13.6%, of the peak value [67]. Taking the beam diameter at this point encompasses 87% of the beam's total energy [68], ensuring that we account for as much of the signal as possible and thus generate as many Raman shifted photons as possible. To determine the appropriate focal length lens needed to achieve a 3 mm collimated beam, the following formula can be used:

$$f = \frac{\frac{\emptyset_{\perp}}{2}}{\tan\left(\frac{\theta_{\perp}}{2}\right)}$$

Equation 6.1.1 Focal length of collimating lens

where f is the focal length needed to produce our desired beam diameter, and $\emptyset_{\perp}$ is the beam diameter, and $\theta_{\perp}$ is the divergence angle of our laser diode [69]. Because the divergence angles of our laser diode are not equal and the beam will be elliptical, this formula should be used with respect to the largest divergence angle so as to collect as much light as possible. In the specification sheet for the ams-OSRAM PL 520B, the parallel divergence angle (FWHM) is defined as 6.3° and the perpendicular divergence angle (FWHM) is defined as 22.5° . Because these angles are defined in terms of full-width half max and not $1/e^2$, we must convert our desired diameter to FWHM for the purposes of our calculation. This can be done quite simply [70]:

$$\begin{aligned} d_{\frac{1}{e^2}} &\approx 1.7 d_{FWHM} \\ d_{FWHM} &\approx \frac{3 \text{ mm}}{1.7} = 1.76 \text{ mm} \end{aligned}$$

Equation 6.1.2 Conversion of beam diameter definition

Now, inserting this FWHM beam diameter into equation 6.1.1 along with the perpendicular divergence angle of 22.5° , we can find the ideal focal length of our lens:

$$f = \frac{\frac{1.76 \text{ mm}}{2}}{\tan\left(\frac{22.5^{\circ}}{2}\right)} = 4.435 \text{ mm}$$

Equation 6.1.3 Calculation of focal length for collimation

Thus, our collimating lens must have a focal length of approximately 4.435 mm. It is also important that the numerical aperture of our lens is greater than the numerical aperture of the laser diode so that it can efficiently capture the entire beam. It is best practice to choose a lens that has approximately twice the NA of the laser diode, which is:

$$NA_{diode} = \sin\left(\frac{\theta_{\perp}}{2}\right) = \sin\left(\frac{22.5^{\circ}}{2}\right) = .195$$

Equation 6.1.4 NA of laser diode

For this reason, we have selected Edmund Optics #45-077 as our collimating lens. This standard plano-convex lens has a numerical aperture of .6 and a focal length of 4 mm, which is very close to our calculated ideal focal length. However, since it is not the exact same focal length, we will need to calculate our new actual beam diameter:

$$d = (4 \text{ mm}) \times \tan\left(\frac{22.5^{\circ}}{2}\right) \times 2 = 1.591$$

$$d_{\frac{1}{e^2}} = 1.7(1.591) = 4.057 \text{ mm}$$

Equation 6.1.5 Actual collimated beam diameter

However, the focal length of this lens was defined for a wavelength of 445 nm. Because we are not operating at this wavelength, to more accurately predict how the laser diode will react to our chosen lens, a simple simulation using the lens parameters was run in Ansys Zemax OpticStudio, defining the beam divergence as 22.5°:

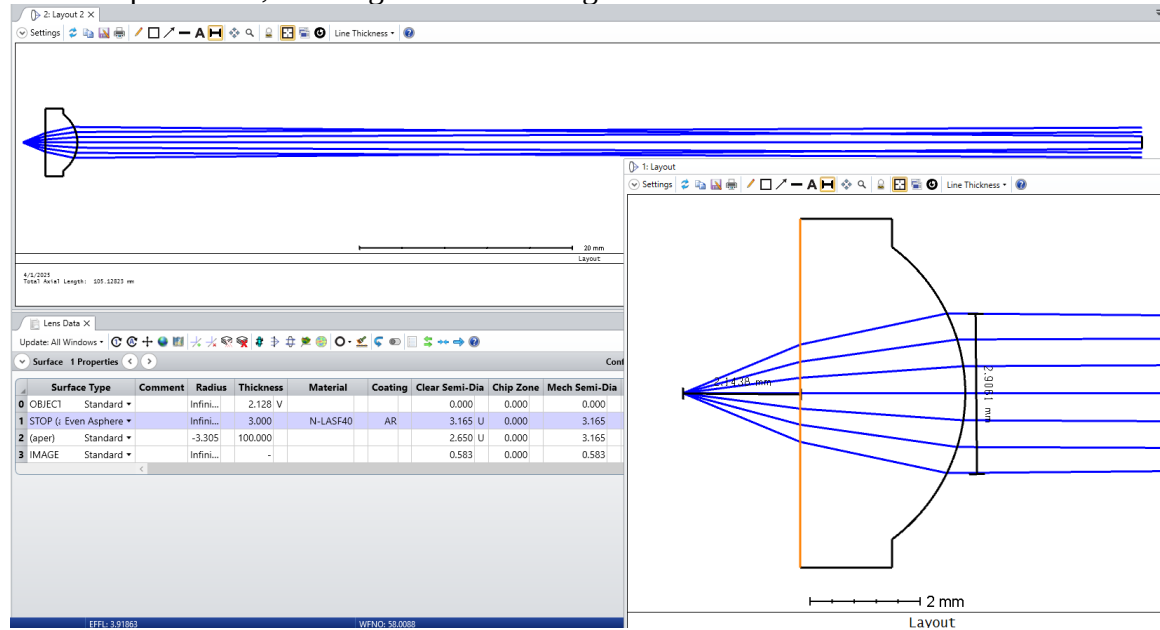


Figure 6.1.1 Zemax simulation of the chosen collimating lens

This simulation indicates that in order to collimate our 520 nm light with a divergence angle of 22.5°, the lens will need to be placed at a back focal length of approximately 2.1 mm, producing a collimated beam diameter of approximately 2.9 mm. This diameter differs very slightly from the calculation due to the difference in focal length caused by our laser wavelength, as well as due to the divergence of the laser diode beam. It should also be noted that though the center rays are perfectly collimated, the farther off-axis the rays are the more spherical aberration is present, causing the “dips” in the edge rays. This shouldn’t matter much for our purposes as beam quality isn’t a large factor in Raman spectroscopy.

6.1.2 Focusing the Collimated Beam

Once the collimated laser line is reflected by the beam splitter towards the sample, it must be focused into a spot size of near 10 μm to ensure high intensity incident upon our sample. To be idealistic, we can aim for a spot size of 5 μm , as the smaller the spot size is, the better. Knowing our ideal spot size, we can then use the following equation to estimate the appropriate focal length needed in our focusing lens [71]:

$$f = \frac{2\omega_0\pi D}{4M^2\lambda}$$

Equation 6.1.6 Laser beam spot size equation, rearranged

where f is the focal length of the lens, ω_0 is the beam waist at the sample (2.5 μm , in our case), D is the collimated beam diameter at the focusing lens, and M^2 is the beam quality parameter, which quantifies how far the beam diverges from an ideal Gaussian beam [72]. We can assume our laser diode has an M^2 value of 1.2, and knowing from our previous simulation that our collimated beam diameter will be approximately 2.9 mm, we can solve for the focal length:

$$f = \frac{2(2.5 \mu\text{m})\pi(2.9 \text{ mm})}{4(1.2)(520 \text{ nm})} = 18.25 \text{ mm}$$

Equation 6.1.7 Focusing lens focal length calculation

Now, we know that in order to achieve a maximum spot size of approximately 5 μm , we must have a lens with at most a focal length of 18.25 mm. Meaning, if we use a lens with an even shorter focal length, we can achieve an even tighter focus. This is beneficial in two ways; it increases the intensity incident on the sample while also enabling the lens to be closer to the sample, meaning it can more efficiently collect the randomly scattered Raman-shifted light. For this same reason, it is important for the lens used to focus the laser beam to have a high numerical aperture and large radius, as this would allow it to collect as much light as possible, strengthening our Raman signal. For these reasons we have chosen to use Edmund Optics #48-423 as our focusing lens. This lens has a diameter of 18 mm and a NA of .5. Though it would've been ideal to have a diameter of 25 mm, matching that of our dichroic mirror and enabling the maximum possible light collection, 18 mm should still be sufficient. This lens also has a focal length of 18 mm, slightly shorter than our calculated value, meaning our spot size should ideally be able to focus to even smaller than 5 μm . After having chosen this lens, we can calculate our new anticipated spot size:

$$2\omega_0 = \frac{4M^2\lambda f}{\pi D} = \frac{4(1.2)(520 \text{ nm})(18 \text{ mm})}{\pi(2.9 \text{ mm})} = 4.93 \mu\text{m}$$

Equation 6.1.8 Calculation of new spot size

Thus, in a perfect scenario, our focused spot diameter should be approximately 4.93 μm , a perfect spot size for Raman spectroscopy. However, like the collimating lens we've chosen, this lens is designed for a different wavelength of 587.6 nm, and thus the focal length is similarly defined for the specific wavelength of this lens. Because our laser line is 520 nm, the effective focal length of our lens may not be exactly 18 mm. Aside from this, imperfect real world conditions may also contribute to our actual beam diameter differing from our calculated ideal. To get a better estimate of what our focused beam diameter may be, a simple simulation using the Zemax file for our lens was carried out, setting the aperture size to 2.9 mm:

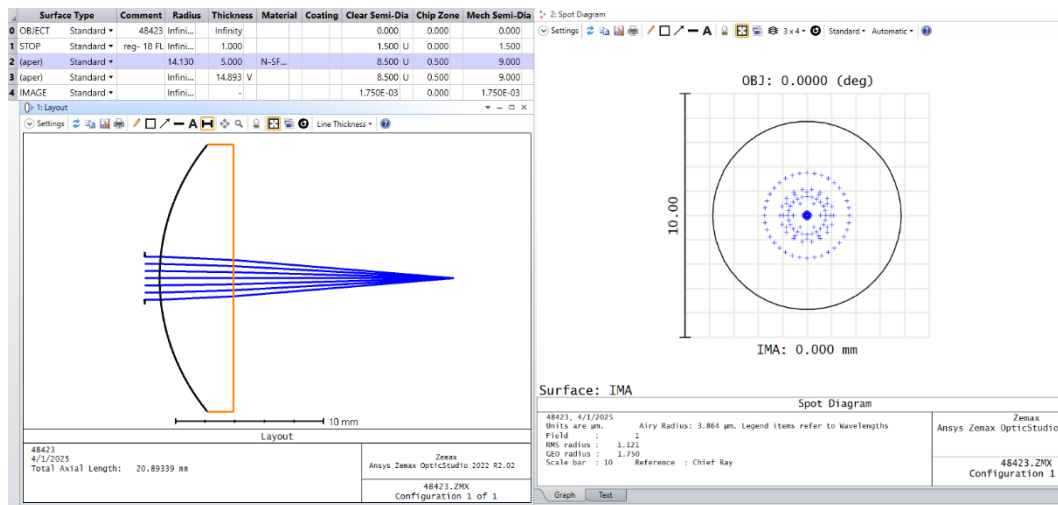


Figure 6.1.2 Zemax simulation of focusing lens effects

As is shown by the simulation, our actual beam diameter will not be exactly $3\ \mu\text{m}$. In fact, the diffraction-limited spot size (airy disk) is almost $8\ \mu\text{m}$, meaning even if we had a perfect diffraction-less system we would not be able to achieve such a small spot size. Our ideal spot size is simulated to be approximately $3.5\ \mu\text{m}$, which is close to our calculation, however, because the predicted geometric radius is less than the airy radius, our spot size is limited to the airy disk diameter. This diameter of $8\ \mu\text{m}$ is closer to our original goal of a $10\ \mu\text{m}$ spot size, so it should still be small enough to achieve high Raman excitation at our sample. The simulation also demonstrates how our actual focal length will differ from the $18\ \text{mm}$ predicted for a $587.5\ \text{nm}$ beam. Using the measure tool, the actual EFL for $520\ \text{nm}$ light is estimated to be approximately $17.7\ \text{mm}$, the back focal length is estimated to be approximately $14.9\ \text{mm}$, and the front focal length is approximately $19.9\ \text{mm}$. Implementing these parameters into our design will enable us to achieve a tight spot size suitable for Raman spectroscopy.

6.1.3 Coupling to Multimode Fiber

After our laser line is focused into a tight spot size, Raman shifted photons will scatter off the sample in all directions, and the photons that our focusing lens is able to capture will be re-collimated and directed back towards the dichroic beamsplitter. The beamsplitter will then reflect most of the laser line, allowing the Raman signal to pass through, which will then pass through the longpass filter and all remaining Rayleigh scattered light will be eliminated. This beam must then pass through another focusing lens, which would normally focus the laser down to a suitable spot size for the slit, but in our case will be used to couple our Raman signal into a multimode fiber which will carry our signal to the spectrometer component. In coupling light from a lens to a fiber, the most important factor is that the NA of the lens must be less than or equal to the NA of the fiber. This is because if the entrance angle of light into the fiber is too large, the light will not be reflected at the interface between the core and the cladding, but will instead leak outside the fiber and be lost. It is equally important to ensure that the spot size of the light focused by the lens is equal to or less than the diameter of the fiber, so as to avoid any Raman signal being wasted.

Understanding these factors, the following formula can be utilized to determine a suitable focal length for the coupling lens:

$$EFL_{lens} = \frac{\phi_{beam}}{2 \times NA_{fiber}}$$

Equation 6.1.9 EFL for coupling light from lens into fiber

where ϕ_{beam} is the diameter of the beam at/before the focusing lens. In our case, because Raman scattered light bounces off the sample in all directions, and we want to gather as much of that light as possible, the diameter of the collimated beam at the focusing lens is equal to the full clearance of lens 1, which we have previously defined to be 18 mm. We must also know the numerical aperture of our fiber in order to do this calculation. The fiber we have chosen for our system is the **Newport F-MCC-T multimode fiber**. Because multimode fibers typically have larger core diameters compared to singlemode fibers, they are generally easier to couple light into, and thus have higher coupling efficiency. This is ideal for a Raman system in which we want to waste as little light as possible. The chosen **fiber has a core diameter of 200 μ m, and a numerical aperture of .22**. Now knowing this information, we can use equation 6.1.9 to determine the ideal effective focal length of our coupling lens:

$$EFL_{lens} = \frac{18 \text{ mm}}{2 \times .22} = 40.91 \text{ mm}$$

Equation 6.1.10 Calculation of EFL for coupling lens

So, in order to achieve effective coupling between the lens and the fiber, we should use a lens with a focal length of about 40 mm. Granted, this equation is more important for singlemode fibers than multimode fibers, it won't hurt to have a lens close to this focal length to capture the most light possible.

The lens we have chosen to implement is the **MKS Newport KPX382-C**. This lens has a focal length of 50 mm, which is somewhat off from the calculated ideal focal length. However, this lens has a diameter of 20 mm, meaning it can capture all of the collimated Raman signal passed through lens 1 (18 mm dia.), and it also has a numerical aperture of .2, which is very close to the fiber NA of .22. In coupling multimode fibers to lenses, matching their NA's as closely as possible is the most important factor to high coupling efficiency.

To ensure our chosen lens will enable high coupling efficiency and carry as much Raman signal as possible to the spectrometer setup, a simple simulation was run in Zemax. The MKS Newport lens was modeled with an aperture of 18 mm (the clearance of lens 1) and utilized to simulate coupling into a multimode fiber. To enable this simulation, the clear semi-diameter of the image plane was set to the core radius of the fiber (.1 μ m). In the Geometric Image Analysis tab, the NA of the fiber is set to .22 and the settings are saved so that the IMAE operator in the Merit Function Editor can utilize these settings. The thickness of surface 3 is set to a variable such that the Merit Function Editor can be used to optimize the distance between the lens and the fiber for maximum coupling efficiency. To do so, the optimize function was used with the Damped Least Squares algorithm. This also enables a more accurate coupling efficiency to be displayed in the Merit Function Editor. Finally, the image plane material was designated as pure silica to emulate the fiber material. This step ensures that Fresnel reflections are accounted for in the model. By

saving these settings and reloading the Merit Function Editor, a more accurate coupling efficiency is displayed.

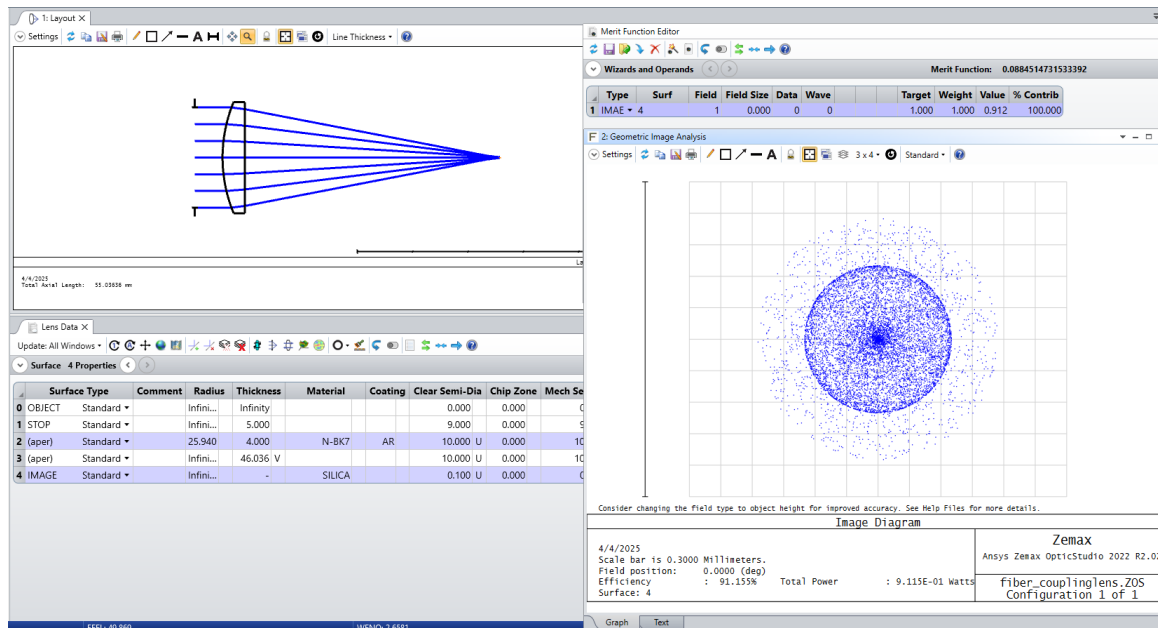


Figure 6.1.3 Simulation of coupling light into fiber via lens

As demonstrated by the simulation, the coupling efficiency when using this lens and fiber setup should be approximately 91.2%, meaning that ideally only about 9% of the Raman signal will be lost via transmission through the fiber. This is not too bad of a loss, and assuming we can recreate these ideal conditions in a real-world setup, almost all of our Raman signal should be able to make it to our spectrometer configuration, demonstrating that our chosen lens is suitable for our collection system.

6.2 Spectrometer Design

This section will be a discussion on the hardware components and design that will be implemented into the spectrometer portion of TEXRAY.

As discussed in Chapter 3, a Czerny-Turner spectrometer configuration will be used in our system. The Czerny-Turner configuration consists of two concave mirrors and one planar, reflective diffraction grating. With careful selection of our optical components and consideration of our design constraints—the two concave mirrors paired with the reflection grating will allow for the detection of our desired spectral range with the highest possible spectral resolution. The fundamental working principle begins with the focused Raman signal entering the slit. This initial slit determines how much light will enter the spectrometer. The first concave mirror collimates the light and reflects the light onto the diffraction grating. The Raman signal is dispersed into its constituent wavelength components and is reflected off the grating onto the second concave mirror. This second concave mirror will focus the light onto the CCD.

Chapter 3 further included discussions on the components of the spectrometer, the decision of which were governed by design considerations such as the focal length of the spectrometer.

7 Software Design

7.1 Software Block Diagram

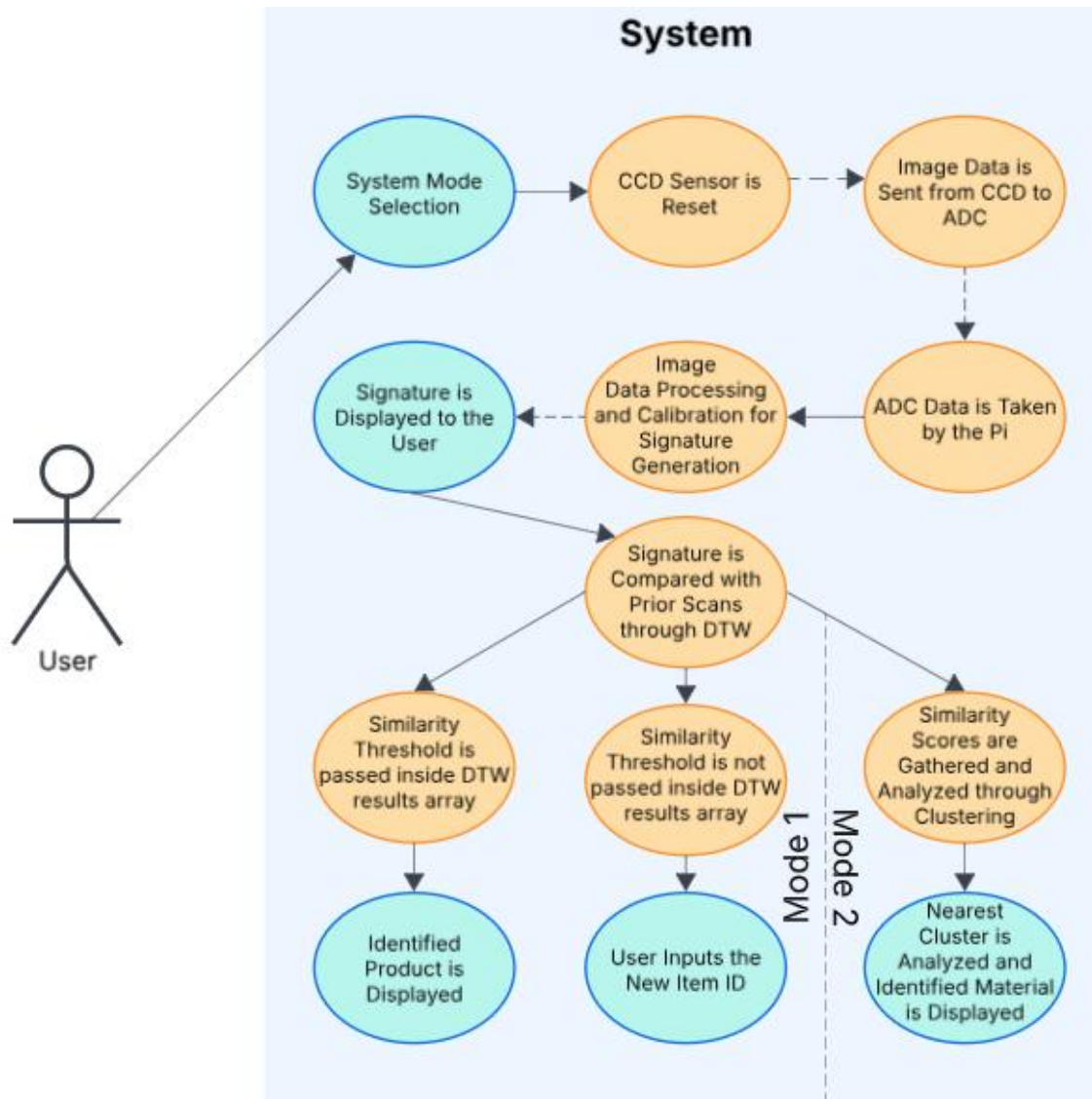


Figure 7.1 Software Block Diagram

7.2 Software Summary

The user's interaction with the system begins with the sample fabric being placed in position for analysis, after this point all input from the user comes in the form of selecting options on the liquid crystal display. The first of which is selecting the mode of the system, choosing between settings of "Material Analysis" and "Product Comparison" (Figure 7.2.1).

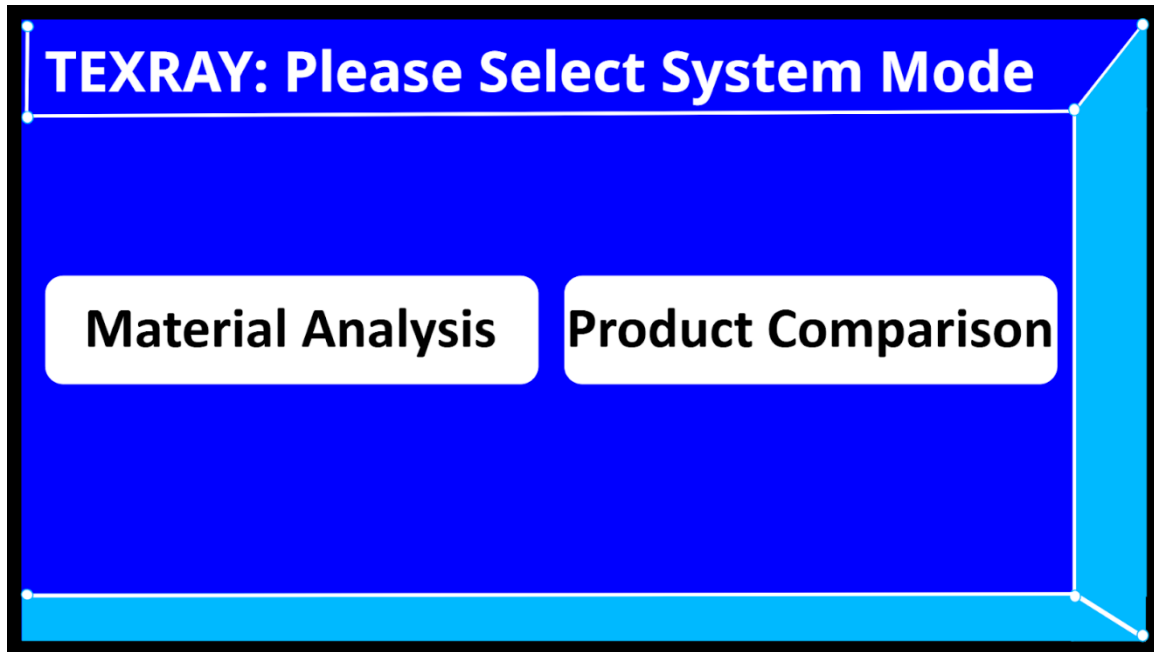


Figure 7.2.1: Initial LCD Screen Layout

Once the selection is made the Raspberry Pi, which is connected directly to the LCD, will communicate with the CCD detector inside the optical spectrometer to obtain an image of the spectrum to analyze and convert into a spectral signature. Several steps are necessary to do this, first off the detector being used is the TCD1304DG, which is an analog CCD, meaning the output of the optical spectrometer is an analog signal, the Raspberry Pi cannot analyze an analog signal like this directly, so an analog to digital converter (ADC) is required. This converter will work as a go-between for the CCD detector and RPi controller. The CCD has no means of digital communication like a serial peripheral interface or inter-integrated circuit protocol, it is a sensor that captures an image as input and sends out a series of analog voltage signals telling the intensity of light for each specific pixel in the image. This is done by representing each pixel with a photodiode, photon-sensitive semiconductor diodes held within the device, the photodiodes store incoming photons and convert them into electrical charges that are sent out as data through the analog voltage signals, this data will then be received by the ADC (ADS1115) to be made readable by the RPi controller. Once the analog signal is converted into a digital format it is sent to the RPi where it can finally be analyzed. However, the method in which this is carried out is not as straightforward as described. While the role of each component is exactly what has been stated, there are more steps necessary to integrate this process into the overall system as designed. A CCD sensor does not function the same as a commercial camera, it is not separate from the rest of the system and does not wait on the user once powered on

before capturing a singular image to look at, instead it is the output of the optical spectrometer system and once setup is constantly sending a steady flow of data as its output signal. This means that to use the CCD as a camera from the perspective of the software, a few additional steps have to be taken. The end goal of the relationship between the RPi and the CCD is to obtain the data of a singular spectral image from the optical spectrometer once prompted by the user, however, given the constant flow of data from the CCD much more closely resembles a video feed than a camera image there must be a level of control exerted on the CCD and ADC. This control will ensure that the RPi will only accept data when asked for it by the user and when accepting it will only take input data from one singular image and cut off anything else being sent. An analogy for this process would be attempting to grab a singular frame from a video feed, but instead of being done with a video editing software the process is done through pin and bus communication. Mostly the initial steps are done through general purpose input and output (GPIO) pins on the RPi communicating directly with the CCD detector, sending activation pulses to specific pins on the CCD to synchronize the output of the spectrometer and the data being taken by the RPi to ensure that only what is wanted is being received. The reason these actions must be done through pin activation on the CCD is that these specific steps cannot be taken with any other connection or communication system between the devices. The relationship between the CCD and the ADC involves no communication, the ADC's role starts and ends as an intermediary, collecting any output that comes from the CCD and processing it to be outputted in a digital format, effectively acting as an extension of the CCD that waits for an on or off switch to be flipped by the RPi to send a flow of digitally formatted spectrometer output data. This switch comes in the form of bus communication established between the RPi and the ADC, as the RPi supports both Inter-Integrated Circuit (I2C) and Serial Peripheral Interface (SPI) communication. Nowhere in this process is there room for actions to control the CCD and manage the flow of the spectrometer output, so this must be done manually through voltage pulses sent from the GPIO pins of the RPi to specific pins on the CCD. First the CCD must be reset after the user selects a system mode on the LCD to ensure a controlled starting point for the data being sent to the ADC, which is essential to the end goal of obtaining a singular spectral image from the spectrometer. A reset command is fairly simple to communicate to the CCD, as the RPi can execute a reset by sending a voltage pulse as an activation signal to the eighteenth pin on the CCD. The RPi has a GPIO python library, so once any CCD pin is defined to its connected GPIO pin the RPi can activate or deactivate the pin with a voltage pulse, written in python as `GPIO.output(NAME_PIN, GPIO.HIGH)` or `GPIO.output(NAME_PIN, GPIO.LOW)`. After the CCD is reset, the next step is ensuring the proper pin configurations before moving on to acquiring the CCD's output. Pins eighteen, seventeen, five, six, twenty-one, and twenty-two should all initially be set to low (Figure 7.2.2).

Circuit Diagram

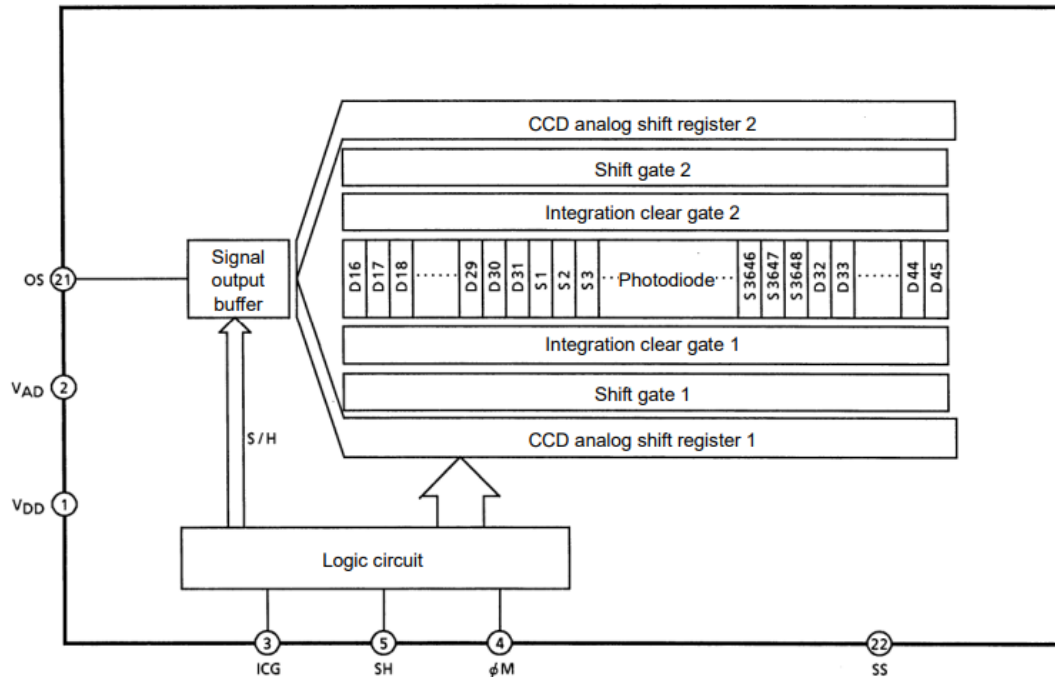


Figure 7.2.2: TCD1304DG Circuit Diagram

The first pin activated after the reset is the shift gate, which lies between the photodiode layer above and the output layer beneath. The photodiode layer contains a row of two hundred and forty-eight semiconductor diodes, each only fifteen by fifteen micrometers in size, and each carrying an electrical charge that represents the intensity of light at its respective pixel within the captured image. When the twenty-second pin is activated the shift gate will transfer these charges into an analog shift register so that the data can then be sent out to the ADC as an analog output signal. After the shift gate is activated and a timer for the integration time has finished, the shift pin is then set back to low and the next step of transferring the shifted electrical data into the output signal begins. The TCD1304DG has three transfer clock pins, located at pins five, six, and seventeen, which control this data transfer from the shift register towards the output signal. After the shift gate has finished the first transfer clock at pin five is set to high, initiating the first phase of the data transfer. At the same time the clamp gate, at pin twenty-one, is set to high, this is in order to keep the output buffer closed until the output signal is prepared. Both the transfer clock and clamp gate are then set back to low before activating the second transfer clock, which starts the second and final phase of the data transfer. The second transfer clock is activated with both pins six and seventeen, pin six corresponding to the second phase of transfer from the shift register to the output buffer, and pin seventeen moving the data finally to the output buffer to prepare the analog output signal for the ADC. At this point the second transfer clock pins are set to low and the data transfer process is repeated

in a loop until every photodiode inside the CCD is accounted for, ensuring that all pixel data is transferred to the ADC. This loop begins with the first transfer clock and clamp gate being set to high, and ends with the second transfer clock pins being set to low.

Inside the internal data transfer loop for the CCD there is one more step, which does not pertain to the CCD specifically, this is the reading of data from the ADC by the RPi controller. This is done after the second transfer clock pins are set to high but before the end of the loop. First a read command is sent to the ADC using the bus communication pathway set up prior to the loop sequence, then the RPi reads the received ADC output before converting the response into an integer. This integer is appended into an array with all other collected ADC output before setting the second transfer clock pins to low and looping back to the beginning of the image acquisition sequence. Once the loop sequence reaches completion, all pixel data values will have been added to the integer array, and the RPi will have what it needs to generate a spectral signature for the user.

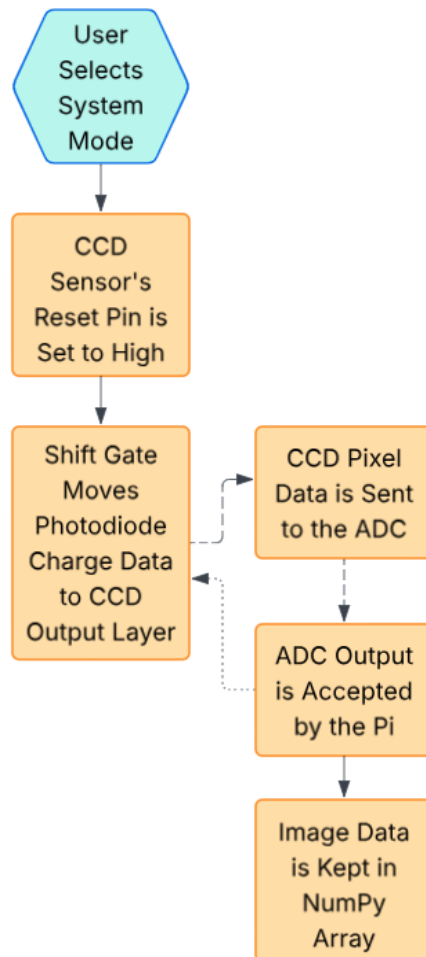


Figure 7.2.3: Spectrum Image Data Extraction Diagram

The sample's spectral signature is generated first by converting the collected integer array into a numpy array for easier analysis, then, just as noise interference is removed in signal

processing, the background will be removed from the image of the spectrum. This is done by finding the minimum value inside the integer array and subtracting it from the data set to better calibrate the soon-to-be generated spectral signature. The dataset can be further improved with polynomial filtering, specifically a third-degree Savitzky-Golay filter. The filter will work to smooth the data inside of the intensity value array to reduce possible noise distortion. This is done through a form of convolution, taking consecutive segments of a custom size from the array, and comparing each data point to a third-order polynomial that approximates each segment, creating a middle ground between the array and the polynomials, which will be a smoothed version of the original data set. Creating the graph used to display the sample's generated signature begins with establishing an x-axis based on wavelength using nanometers as the unit of measurement. This axis will encompass the entire visible light spectrum being sampled by the optical spectrometer, a spectrum that spans three hundred and seventy nanometers, starting with the end of ultraviolet light at three hundred and eighty nanometers and ending with the start of infrared light located at seven hundred and fifty nanometers. The y-axis will use the values collected from the ADC, held inside the numpy integer array, to display the intensity of the spectrum at each corresponding wavelength. This data will be graphed with the pyplot submodule from the MATLAB plotting python library. The resulting graph of the sample's spectral signature will first be displayed to the user on the LCD before being analyzed to determine the textile material of the sample, or if the sample item has already been scanned, depending on which mode the system is currently in.

At this point we reach the final phase of the project, analyzing the generated spectral signature. In both system modes this analysis will be done against prior signatures. First, there is material analysis, this mode works to sort the generated signature into its corresponding group based on identified material. This process is done using a numpy integer array that holds the data that the most recent signature was generated from, comparing it against prior scans to find which fabric group is most similar. Group in this case meaning another numpy integer array containing the data of previously identified signatures, with each subgrouping being the data from an individual prior signature. The data is in chronological order from when each signature was generated. The current signature data will be compared with each previous signature through a process called Dynamic Time Warping (DTW). DTW is a comparison algorithm built to score the similarity of different time series. Time series being any graph of data points arranged in order of time. The algorithm compares the two line graphs by scanning through the first line, going one by one through each data point, and finding a point of comparison in the second line for each one (Figure 7.2.3).

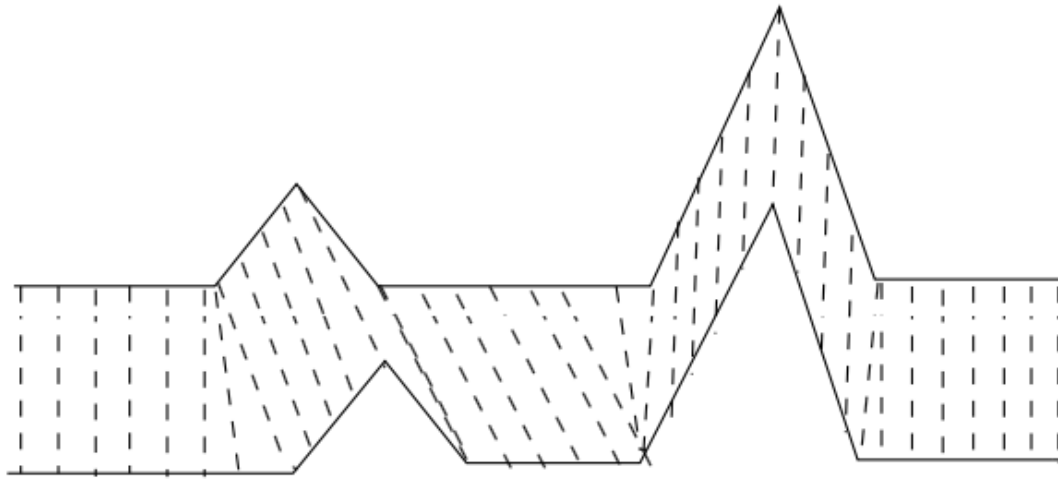


Figure 7.2.4: Points of Comparison in Dynamic Time Warping

The goal of DTW is to limit the effect of time in calculations by choosing points of comparison across the x-axis. The alternative distance calculations to DTW use the difference in corresponding amplitude values at each index on the x-axis to create a total sum of difference between the two lines, but in using this method for comparisons such as audio, movement, or handwriting analysis, time becomes the largest determining factor. In audio a possible match of phrase or words spoken could be missed due to differences in the speed of two speakers, as a direct comparison would be comparing different syllables and miss the fact that the word itself is the same. Similarly analysis of movement could fail to detect that two individuals are both walking because their speeds are not the same, so the position of the one person's body would not resemble the others at a given point despite their movements being the same. The issue is not limited to time series either, as horizontal variations in handwriting could create very similar errors during signature authentication. DTW's points of comparison counteracts this problem. Matches are determined from a cost matrix created using the distance values of every index in the second line from every given index in the first. Distance values can be calculated through a number of methods, in this project it will be euclidean distance used. A path of lowest cost is found through this matrix and from it points of comparison are mapped. When finding the path of lowest cost there are three conditions. First, the earliest and latest point of each line must be matched with its counterpart. Next, every point in both lines must have at least one point of comparison. Finally, a point in one line cannot be matched with a point in the other line that precedes a point in the line that has already been matched, to explain visually this means the lines denoting points of comparison cannot cross over each other. This means that while points 1, 2, and 3 in line A can all match with point 2 in line B, points 2 and 3 in line A cannot match with point 1 in line B. The total cost of the path chosen also functions as the calculated similarity of the two lines, as the end result of DTW is the sum of distances at every point of comparison.

A lightweight version of the DTW algorithm can be installed using the command of “pip install fastdtw” allowing for use of the `fastdtw()` function, which can take in two integer arrays along with a listed distance metric and calculate the DTW similarity score. The array for the current sample will be compared with each prior scan using this function. Three function calls will be made, each with the array of current data and one of the arrays of previously classified data passed as arguments. Inside the function is a for loop that will repeat for the length of the array of previous signatures (`arr2`), calculating the similarity score of each array inside `arr2` and appending it to a results array before looping again. The function finishes by returning the results array. After these three function calls all comparisons will have been made, and the current sample can now be classified based on the results. This is done through one-dimensional clustering of the results array returned by the DTW function. The three arrays of DTW similarity results are combined into one array with a label attached to each entry to list where it was added from. This array is split using KMeans into a set of clusters, and the group most represented in the cluster with the smallest centroid value is chosen as the identified material. This label is displayed on the LCD as a final result for the user (Figure 7.2.4).

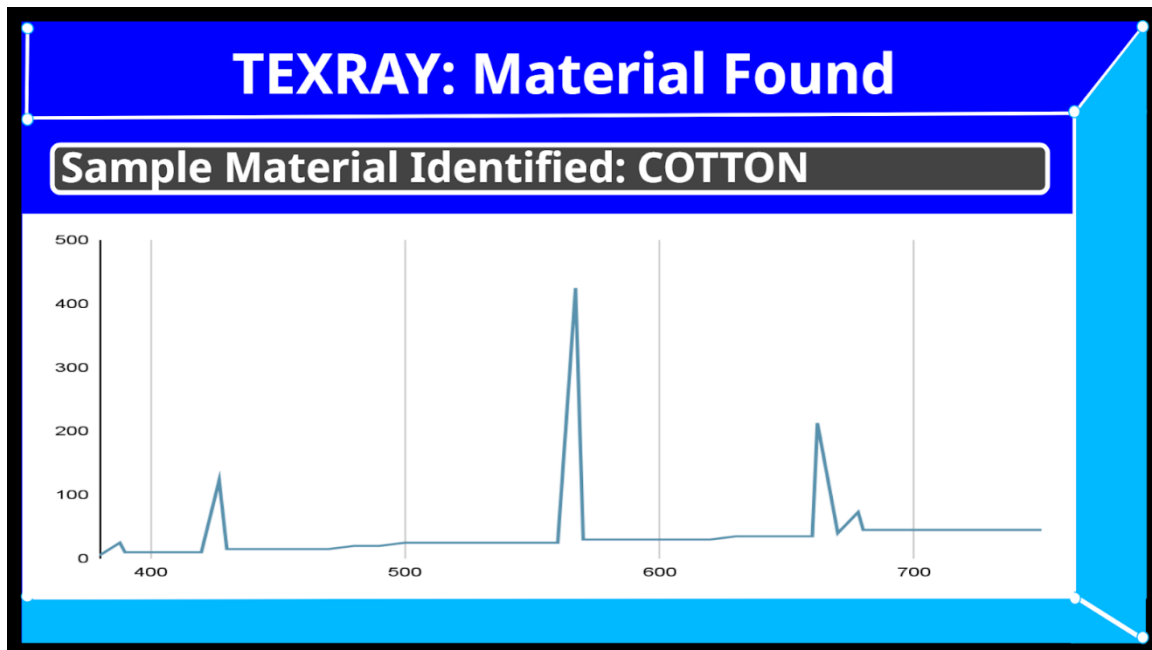


Figure 7.2.5: Signature Results LCD Screen Layout (Mode One)

In the case of the system’s second mode, product comparison, the process is very similar. The raspberry pi messages both the CCD sensor and ADC to obtain the spectrum image data, generating a spectral signature and a corresponding integer array. This array is compared with signature data of previous scans using DTW like in material analysis, but at this point the process is slightly different. When the DTW comparison function is called for the array of previous signatures, each comparison value is returned with the label of the item it was compared to. The comparison results are collected into a common array and analyzed to determine if any item clears the similarity threshold to be determined a match. If it does, the label is displayed to the user as a final result (Figure 7.2.5), and if no item

clears the threshold the user is prompted to enter a label for the item so that it can be added to the array of prior signatures.

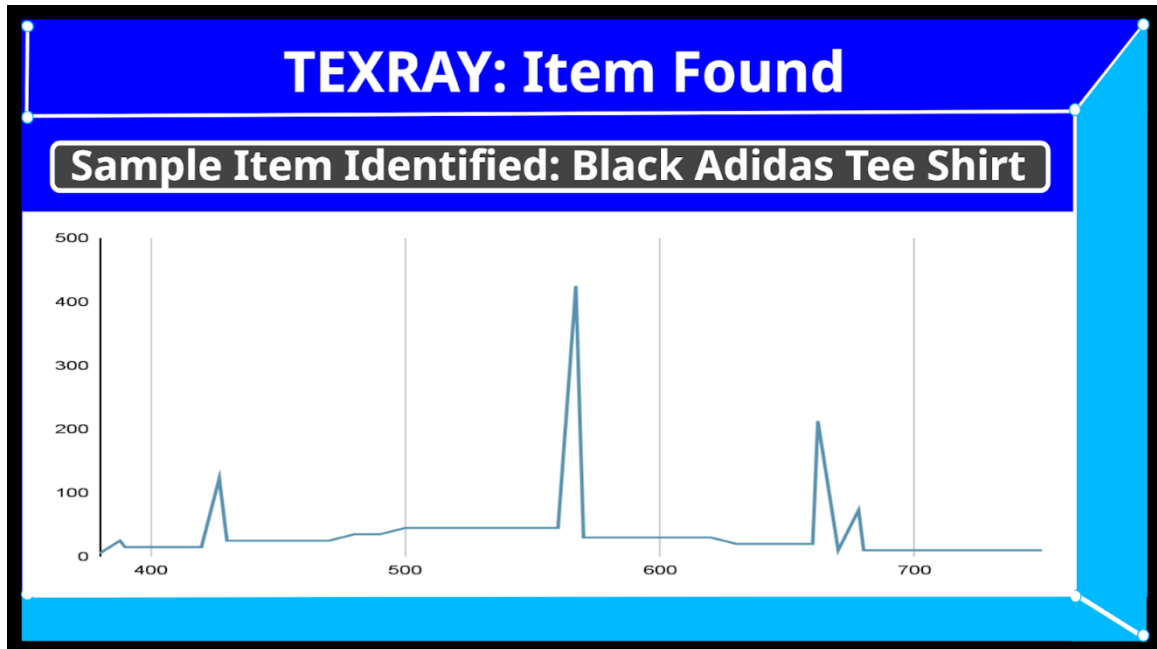


Figure 7.2.6: Signature Results LCD Screen Layout (Mode Two)

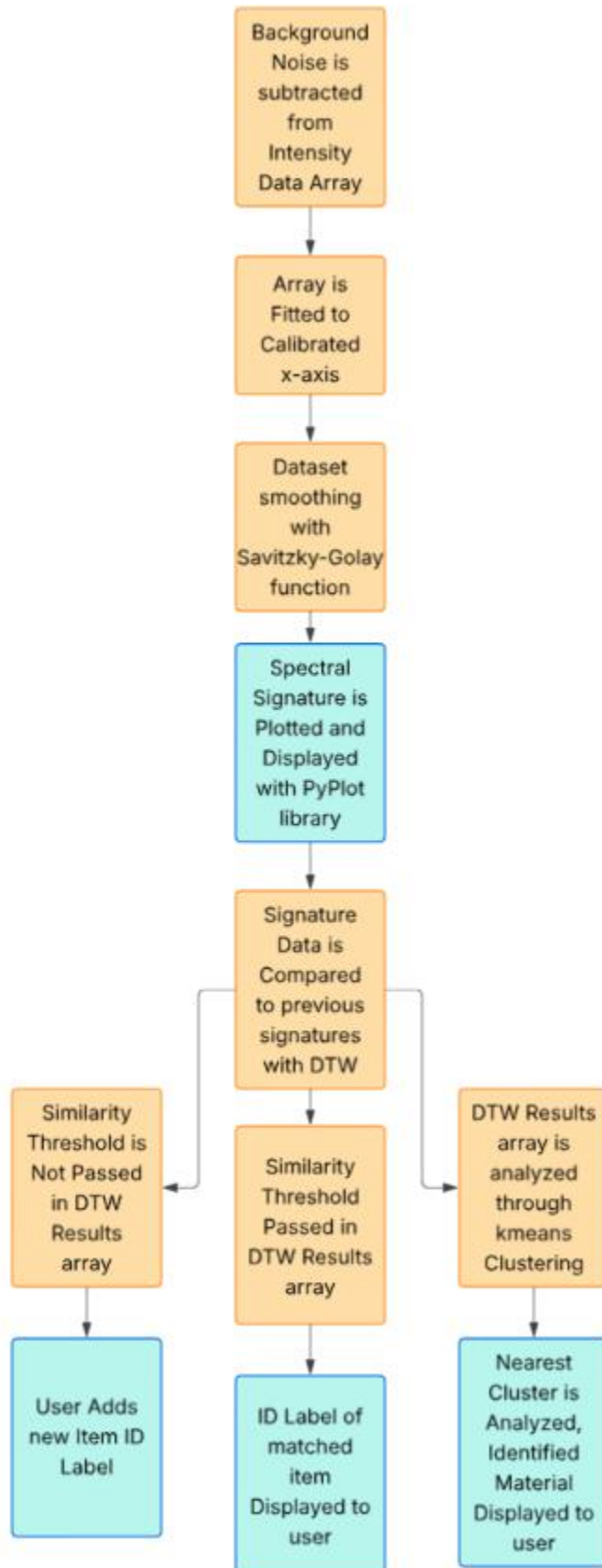


Figure 7.2.7: Spectral Signature Generation & Identification Diagram

8 Chapter 8

9 Chapter 9

10 Administrative Content

10.1 Budget and Financing

This Senior Design project does not currently have an external sponsor, and will be funded entirely by the 4 members of the team. We will be actively searching for a sponsor throughout the documentation and production of our system.

Table 10.1.1 Budget breakdown

Table 10.1.2 Budget breakdown			
Item	Cost	Quantity	Total Cost
Laser diode (520 nm)	\$46	1	\$46
Laser diode driver	\$30	1	\$30
Dichroic mirror	\$250	1	\$250
Long Pass Filter	\$365	1	\$365
Plano-convex lens	\$40	3	\$120
Multimode Fiber	\$15	1	\$15
Slit	\$200	1	\$200
Mirror	\$40	2	\$80
Diffraction grating	\$100	1	\$100
CCD	\$100	1	\$100
PCB	\$70	1	\$70
LCD display	\$67	1	\$32.99

Raspberry Pi	\$35	1	\$69.49
Switch	\$3	1	\$3
Battery power supply	\$15	1	\$15
Switch	\$0.80	1	\$0.80
LEDs	\$0.42	4	\$0.42
Fabric Samples	\$10	1	\$10
Total Cost			\$1,458.94

10.2 Project Milestones

Table 10.2.1 Senior Design I Project Documentation Milestones

Table 10.2.1 Senior Design I Project Documentation Milestones - Spring 2025			
Task	Time Period	Dates	Responsibility
Brainstorming	1 week	1/11	All
Finalize Project Idea	1 week	1/17	All
Divide and Conquer Document	1 week	1/17 - 1/24	All
30-Page Milestone	~1 month	2/24	All
60-Page Milestone	~1 month	3/23 Due 3/24 @ 12	All
90-Page Milestone	~2 weeks	4/2	All
120-Page Milestone	~2 weeks	4/15	All
Final Draft	5-7 days	4/20 Due 4/22 @ 12	All

Table 10.2.2 Senior Design I Project Design Milestones

Senior Design I Project Design Milestones - Spring 2025			
Task	Time Period	Dates	Responsibility

Optics Midterm Demo	~4 weeks	2/25 (9-11:30)	Ariana & Danielle
Electronics Prototyping	~2 months	3/24	Cameron & Austin
PCB Ordering	~2 weeks	4/26	Cameron & Austin
Optics Final Demo	~1 week	4/15	Ariana & Danielle
Upload Mini Demo	5-7 days	4/22	All

Table 10.2.3 Senior Design II Project Design Milestones

Senior Design II Project Design Milestones - Summer 2025			
Task	Time Period	Dates	Responsibility
PCB Testing	~3 weeks	5/31	Austin & Cameron
Optical Systems Integration	1 month	6/9	Ariana & Danielle
Total Systems Integration	~1.5 months	6/30	All
Short-form Report	TBD	TBD	All
Practice Final Presentation	~2 weeks	TBD	All
Final Presentation	TBD	TBD	All

11 Optoelectronics Feasibility Study and Testing

The optoelectronic feasibility of a Raman spectrometer is a relevant consideration, especially considering the low intensity nature of the received Raman signal. Extensive research on Raman spectrometers and their application for fabric identification was the first step in validating the basis of our project. We explored commercial Raman systems and homemade Raman systems for reassurance that one could be built by students within a reasonable budget. We additionally consulted with various faculty members of CREOL for approval on our project motives. The propelling experience in validating our project was our visitation to the NanoScience Technology center. As previously mentioned in Chapter 3, we got to test for respective fabric Raman shifts using the Horiba LabRAM HR Evolution Nano Confocal Raman Microscope. We tested our samples with various

wavelengths, excitation powers, and acquisition times. From this point forward we had a general sense of the feasibility of our project.

The first tests that we completed with the Horiba LabRAM prompted our excitation source selection. Our visitation to the NanoScience center was not only a validation of general proof of concept for our project. We were specifically noting the Raman spectra of cotton, polyester, leather, and wool, given various wavelengths. We tested various fabric samples with different excitation sources and correlated their Raman shifts to those seen in research. Our most notable concern regarded excitation sources that would cause fluorescence of our sample. These findings along with other research on the subject was discussed extensively in Chapter 3. These observations further prompted the basis of our Senior Design midterm demo, which assessed the selection of our laser source that would avoid the presence of fluorescence. We held a 405 nm and 532 nm, 1 mW, laser pointer incident upon a pure, undyed cotton and polyester sample. Using the available StellarNet spectrometers, we held the fiber probe up to the scattered portion of the laser on the sample and assessed their respective spectra. We observed the presence of fluorescence with the 405 nm laser pointer and no fluorescence with the 532 nm laser pointer.

The next iteration of tests involve assessing the Raman spectrometer's illumination optics and spectrometer. Simulation and research will serve as the basis for this testing. Testing the illumination optics can involve taking power measurements at different points of the system to ensure that a readable optical signal is being transmitted. We could advance this testing by connecting our illumination optics with the StellarNet spectrometer in Raman mode. This can help reassure us that we are receiving a discernible Raman spectrum. Testing our spectrometer can involve performing baseline spectral readings of known samples. We would use light sources that produce distinct emission lines, including our laser source, the 520 nm laser diode. A plan of actions towards calibrating our system and ensuring the proper receipt of our Raman signal involves testing a Graphene sample. Graphene has a distinct Raman shift at around 1580 cm^{-1} . This wavenumber lies within the range of our system's operating spectral range. Further, Graphene has a FWHM of 30 cm^{-1} , which is also compatible with our spectrometer's spectral resolution. The completion of these tests requires a significant portion of our spectrometer's design to be completed.

12 References

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13 Appendix A - ChatGPT Prompts and Outputs

Prompt 1:

Provide me with a longpass filter that will effectively block out 520 nm light, has greater than 90% transmission at 530 nm, and has an optical density of at least 4.

Output 1:

To effectively block 520 nm light, achieve greater than 90% transmission at 530 nm, and maintain an optical density (OD) of at least 4, a longpass filter with a cut-on wavelength around 530 nm is ideal. Here are some suitable options:

1. Edmund Optics TECHSPEC® High Performance OD 4 Longpass Filters
 - **Cut-on Wavelength:** [530 nm](#)

- **Optical Density:** [OD 4 \(providing high blocking efficiency\)](#)
- **Transmission:** >90% at wavelengths longer than the cut-on
- **Features:** [High blocking with superior transmission, suitable for applications requiring precise wavelength separation](#)

Note: These filters are designed to offer high blocking with superior transmission, making them suitable for applications requiring precise wavelength separation.

2. Schneider-Kreuznach Longpass Filters

- **Cut-on Wavelength:** Customizable around 530 nm
- **Optical Density:** [High blocking efficiency \(specific OD values can be requested\)](#)
- **Transmission:** [High transmission at wavelengths longer than the cut-on](#)
- **Features:** Steep slopes and high transmission at stable cut-on wavelengths, ideal for high-end machine vision systems

Note: [Schneider-Kreuznach](#) offers customizable longpass filters with steep slopes and high transmission at stable cut-on wavelengths. Specific optical density values can be requested to meet your requirements.

3. SyronOptics LP520 Longpass Filter

- **Cut-on Wavelength:** [520 nm](#)
- **Optical Density:** OD 2 at 200 nm to 500 nm
- **Transmission:** >90% from 530 nm to 1100 nm
- **Features:** Provides high transmission just above 520 nm, ensuring effective blocking at 520 nm and excellent transmission at 530 nm

Note: While this filter offers excellent transmission above 530 nm, its optical density is OD 2 in the blocking range, which may not meet the OD 4 requirement. However, it provides high transmission just above 520 nm, ensuring effective blocking at 520 nm and excellent transmission at 530 nm.

When selecting a filter, ensure that the specified optical density meets your application's requirements. Filters with an OD of 4 will attenuate the blocked wavelengths by a factor of 10,000, providing effective suppression of unwanted light at 520 nm. Additionally, consider the filter's physical dimensions and compatibility with your optical setup.

Prompt 2:

Given a 520 nm laser excitation source. Convert the 1000 cm⁻¹ Raman shift from wavenumbers to wavelengths.

Output 2:

To convert a Raman shift from wavenumbers (cm^{-1}) to wavelengths (nm), follow these steps:

Step 1: Calculate the wavenumber of the excitation laser.

$$\nu_0 = \frac{10^7}{\text{Excitation Wavelength (nm)}}$$

$$\nu_0 = \frac{10^7}{520 \text{ nm}} = 19230.77 \text{ cm}^{-1}$$

Step 2: Find the scattered wavenumber by subtracting the Raman shift.

$$\nu_{\text{scattered}} = \nu_0 - \text{Raman Shift}$$

$$\nu_{\text{scattered}} = 19230.77 - 1000 = 18230.77 \text{ cm}^{-1}$$

Step 3: Convert the scattered wavenumber to wavelength using:

$$\lambda_{\text{scattered}} = \frac{10^7}{\nu_{\text{scattered}}}$$

$$\lambda_{\text{scattered}} = \frac{10^7}{18230.77} \approx 548.8 \text{ nm}$$

✓ Final Answer:

A Raman shift of 1000 cm^{-1} corresponds to a scattered wavelength of approximately 548.8 nm.

Prompt 3

Provide a MATLAB code that will tabulate the spectral dispersion of a Raman signal at 100 cm^{-1} , 1500 cm^{-1} , and 3000 cm^{-1} . Consider a an excitation wavelength of 520 nm, 4 different groove densities: 300, 600, 1200, and 1800 grooves/mm, 4 different focal lengths: 100, 250, 500, and 1000 mm. The equation for reciprocal linear dispersion of a spectrometer for Raman scattering is, $d\nu/dl (\text{cm}^{-1}/\text{mm}) = (d\cos(\theta)(\nu_0 - \nu_j)^2) / (mF)$. Where d is the spacing between grooves, $\cos(\theta) = 1$. ν_0 is the absolute wavenumber of the laser, ν_j is the lowest Raman shift to be observed

Output 3:

To implement a MATLAB code that calculates the **spectral dispersion** of a Raman signal at different Raman shifts (100 cm^{-1} , 1500 cm^{-1} , and 3000 cm^{-1}) based on your provided equation, let's break down the steps and then translate them into code.

Given Equation:

$$\frac{dv}{dl} = \frac{d \cdot \cos(\theta) \cdot (v_0 - v_j)^2}{mF}$$

Where:

- d is the **groove spacing** (inverse of grating density).
- $\cos(\theta) = 1$ simplifies the formula.
- v_0 is the **laser wavenumber** (the absolute wavenumber of the laser in cm^{-1}).
- v_j is the **Raman shift** being observed (in cm^{-1}).
- m is the **diffraction order**, typically $m = 1$.
- F is the **focal length** of the spectrometer in mm.

Steps:

1. **Calculate Groove Spacing d** from the grating density.
 - The groove spacing d is the inverse of the grating density.
 - If the grating density is 300 gr/mm , $d = 1/(300\text{ gr/mm}) = 3.33 \times 10^{-3}\text{ mm}$.
2. **Calculate the Spectral Dispersion $\frac{dv}{dl}$** for each combination of focal length and grating density, and at each Raman shift of interest (100 cm^{-1} , 1500 cm^{-1} , 3000 cm^{-1}).
3. **Output the Results** in a table format.

MATLAB Code:

```

1. % Constants
2. excitation_wavelength = 520; % Excitation wavelength in nm
3. v0 = 1 / (excitation_wavelength * 1e-7); % Wavenumber of the excitation light (cm^-1)
4. m = 1; % Diffraction order
5. raman_shifts = [100, 1500, 3000]; % Raman shifts in cm^-1
6. groove_densities = [300, 600, 1200, 1800]; % Groove densities in gr/mm
7. focal_lengths = [100, 250, 500, 1000]; % Focal lengths in mm
8.
9. % Prepare matrix to store results
10. results = zeros(length(raman_shifts), length(groove_densities), length(focal_lengths));
11.
12. % Loop through each combination of groove density and focal length
13. for i = 1:length(groove_densities)
14.     for j = 1:length(focal_lengths)
15.         % Calculate groove spacing (d) in mm
16.         d = 1 / (groove_densities(i) * 1e3); % Convert gr/mm to mm
17.
18.         for k = 1:length(raman_shifts)
19.             % Calculate the spectral dispersion using the given equation
20.             vj = raman_shifts(k); % Raman shift (in cm^-1)
21.
22.             % Calculate the reciprocal linear dispersion (dv/dl) in cm^-1/mm
23.             dispersion = (d * (v0 - vj)^2) / (m * focal_lengths(j));
24.
25.             % Store the result
26.             results(k, i, j) = dispersion;
27.         end

```

```

28.     end
29. end
30.
31. % Convert results to a table for better readability
32. % Each row of the table corresponds to a Raman shift value
33. disp_table = table;
34.     disp_table.Raman_Shift = repmat(raman_shifts',
length(groove_densities)*length(focal_lengths), 1);
35.
36. % Create column names for Groove Densities and Focal Lengths
37. colnames = {};
38. for i = 1:length(groove_densities)
39.     for j = 1:length(focal_lengths)
40.         colnames{end+1} = sprintf('Grating_%d_Focal_%d', groove_densities(i),
focal_lengths(j));
41.     end
42. end
43.
44. % Flatten the results matrix into a table format
45. flattened_results = reshape(results, [], 1);
46. disp_table(:, colnames) = array2table(flattened_results);
47.
48. % Display the table
49. disp(disp_table);
50.

```

Explanation of the Code:

1. Initialization:

- `excitation_wavelength` is the wavelength of the excitation light in nm. This is converted into wavenumber ν_0 (in cm^{-1}).
- `raman_shifts` represents the Raman shifts we are interested in: 100 cm^{-1} , 1500 cm^{-1} , and 3000 cm^{-1} .
- `groove_densities` are the different grating densities: 300, 600, 1200, and 1800 gr/mm.
- `focal_lengths` are the different focal lengths: 100, 250, 500, and 1000 mm.

2. Result Calculation:

- A loop iterates over all combinations of grating densities and focal lengths.
- For each combination, the groove spacing d is calculated as the inverse of the grating density.
- Then, the reciprocal linear dispersion $\frac{d\nu}{d\lambda}$ is computed for each Raman shift using the provided equation.

3. Result Storage:

- The results are stored in a 3D matrix (`results`), where the dimensions represent Raman shifts, grating densities, and focal lengths.

4. Table Output:

- The results are then converted into a table for easy reading, where each row corresponds to a Raman shift, and columns are combinations of grating density and focal length.

Output:

The output will be a table with the **reciprocal linear dispersion** for each combination of Raman shift, grating density, and focal length. Each row will correspond to a specific Raman shift (100 cm^{-1} , 1500 cm^{-1} , 3000 cm^{-1}), and each column will correspond to the combination of groove density and focal length.

Let me know if you need further modifications or explanations!

Prompt 4:

Carefully consider the units in the dispersion calculations and provide a new MATLAB script

Output 4:

You're right to be cautious about the units in the dispersion calculation. The units of the reciprocal linear dispersion need to be consistent, especially when working with wavenumbers and lengths. Let's go through the corrected MATLAB script, ensuring that the units are consistent.

Corrected MATLAB Script

The formula for reciprocal linear dispersion that you provided is:

$$\frac{dv}{dl} = \frac{d \cdot (v_0 - v_j)^2}{m \cdot F}$$

Where:

- $\frac{dv}{dl}$ is the dispersion in units of cm^{-1}/mm (the change in wavenumber per unit length on the detector).
- d is the groove spacing in mm (calculated from groove density).
- v_0 is the wavenumber of the excitation light in cm^{-1} .
- v_j is the wavenumber of the Raman shift in cm^{-1} .
- m is the diffraction order (set to 1 for first order).
- F is the focal length of the spectrometer in mm.

Units Consideration:

1. **Excitation Wavelength:** The excitation wavelength is given in nm, but we need the wavenumber in cm^{-1} , which is the inverse of the wavelength in cm.

$$v_0 = \frac{1}{\lambda} \quad (\text{in } \text{cm}^{-1})$$

Where λ is the wavelength in cm (so, $\lambda = \text{excitation wavelength (nm)} \times 10^{-7}$).

2. **Groove Spacing:** The groove density is given in lines per mm, but the groove spacing d should be in mm.

$$d = \frac{1}{\text{groove density (lines/mm)}}$$

3. **Spectral Dispersion:** The resulting dispersion $\frac{dv}{dl}$ will be in cm^{-1}/mm .

```
1. % Constants
2. excitation_wavelength = 520; % Excitation wavelength in nm
3. v0 = 1 / (excitation_wavelength * 1e-7); % Wavenumber of the excitation light (cm^-1)
4. m = 1; % Diffraction order (first order)
5. raman_shifts = [100, 1500, 3000]; % Raman shifts in cm^-1
6. groove_densities = [300, 600, 1200, 1800]; % Groove densities in gr/mm
7. focal_lengths = [100, 250, 500, 1000]; % Focal lengths in mm
```

```

8.
9. % Loop through each combination of groove density and focal length
10. for i = 1:length(groove_densities)
11.     for j = 1:length(focal_lengths)
12.         % Calculate groove spacing (d) in mm
13.         d = 1 / (groove_densities(i) * 1e3); % Convert gr/mm to mm
14.
15.         % Display grating density and focal length for clarity
16.         fprintf('Groove Density: %d gr/mm, Focal Length: %d mm\n', groove_densities(i),
focal_lengths(j));
17.
18.         for k = 1:length(raman_shifts)
19.             % Calculate the spectral dispersion using the given equation
20.             vj = raman_shifts(k); % Raman shift (in cm^-1)
21.
22.             % Calculate the reciprocal linear dispersion (dv/dl) in cm^-1/mm
23.             dispersion = (d * (v0 - vj)^2) / (m * focal_lengths(j));
24.
25.             % Display the calculated dispersion for this configuration
26.             fprintf('Raman Shift: %d cm^-1 -> Dispersion: %.5f cm^-1/mm\n', vj, dispersion);
27.         end
28.         fprintf('\n'); % Extra newline for clarity between different focal lengths
29.     end
30. end
31.

```

Explanation of Changes:

1. **Excitation Wavelength Conversion:** The excitation wavelength is in nm, but we need it in cm^{-1} , so we convert it to wavenumber in cm^{-1} using:

$$v_0 = \frac{1}{\lambda} = \frac{1}{\text{excitation wavelength (in cm)}}$$

Where $\lambda = \text{excitation wavelength (in nm)} \times 10^{-7}$.

2. **Groove Spacing:** The groove density is given in lines per mm. To convert this to the groove spacing d in mm, we use:

$$d = \frac{1}{\text{groove density (lines/mm)}}$$

3. **Raman Shifts:** The Raman shifts are already provided in cm^{-1} , so they can be directly used in the calculation.
4. **Reciprocal Linear Dispersion Calculation:** The equation used to calculate the spectral dispersion (in cm^{-1}/mm) for each combination of groove density, focal length, and Raman shift is:

$$\frac{dv}{dl} = \frac{d \cdot (v_0 - v_j)^2}{m \cdot F}$$

Where the units are consistent:

- d is in mm (groove spacing),
- v_0 and v_j are in cm^{-1} (wavenumbers),
- F is in mm (focal length),
- The result $\frac{dv}{dl}$ is in cm^{-1}/mm .

```

1. Groove Density: 300 gr/mm, Focal Length: 100 mm
2. Raman Shift: 100 cm^-1 -> Dispersion: 0.00003 cm^-1/mm

```

```
3. Raman Shift: 1500 cm-1 -> Dispersion: 0.00044 cm-1/mm
4. Raman Shift: 3000 cm-1 -> Dispersion: 0.00088 cm-1/mm
5.
6. Groove Density: 300 gr/mm, Focal Length: 250 mm
7. Raman Shift: 100 cm-1 -> Dispersion: 0.00012 cm-1/mm
8. Raman Shift: 1500 cm-1 -> Dispersion: 0.00110 cm-1/mm
9. Raman Shift: 3000 cm-1 -> Dispersion: 0.00221 cm-1/mm
```

...

14 Appendix B - Supplemental Information

CC stretch	1762 cm ⁻¹	
CCC deform	339 cm ⁻¹	
C=O stretch	1742 cm ⁻¹	
Coo		