

TEXRAY: Textile Identification via Raman Spectroscopy

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1 Executive Summary

In this paper, the concept of Raman spectroscopy is explored in relation to its applications in the textile industry and the modern consumer landscape. Many modern consumers are becoming increasingly conscious about not only the quality, but also the origins of the clothes they buy, and are making a deliberate choice to steer clear of synthetic fabrics for a variety of reasons. Some consumers make this choice for environmental reasons, hoping to cut down on the spread of microplastics. Others stick to natural fibers simply because they feel that they are more comfortable. Whatever their reason, consumers deserve the confidence that the materials in the products they purchase genuinely reflect what was advertised. However, this confidence can be difficult to maintain when counterfeit products are becoming increasingly difficult to distinguish, and as consumers continue to lack convenient ways of verifying their textiles.

A unique solution to this issue can be offered through the use of Raman spectroscopy. Raman spectroscopy operates on the principle of Raman scattering, a rare event that only happens to 1 in 10 million photons. Raman scattering occurs when the electromagnetic field of a photon incident on a molecule excites the molecule's electrons to a virtual state. Due to the instability of this virtual state, the electron relaxes to a different energy level almost immediately, re-emitting the photon as a different wavelength than the incident light. Particularly, in this project we focus on Stokes-scattered light, in which the molecule's electrons are excited to a higher energy virtual state and then relax down to a vibrational state that is at a higher energy level than the initial ground state. This means that the emitted photon is at a higher wavelength (lower energy) than the incident photon. The energy difference between the incident and scattered photons corresponds to specific vibrational and rotational modes within the molecule, allowing the resulting Raman spectrum to serve as a unique molecular fingerprint identifiable only to that molecule. This is particularly useful with regards to textile identification, as fabrics' spectra can be clearly identified and separated based on composition, dye, manufacturer, and a variety of other characteristics via the method of Raman spectroscopy.

Though some commercial textile identification devices do exist on the market, they are often quite expensive for the average consumer, with the cheapest devices still going for \$2,500. Because these devices typically utilize infrared spectroscopy, their price floor is limited by the cost of an expensive InGaAs sensor, driving up consumer costs. Raman spectroscopy is often similarly thought to be an extremely expensive technology, as professional Raman spectrometers can cost upwards of \$20,000. However, because Raman spectroscopy most frequently utilizes the visible light region, relatively cheap optics and sensors can be utilized to still create a workable homemade device. With this method, our team aims to create a cheaper alternative to commercial fabric identifiers with a previously underutilized identification method.

Our team created a tabletop Raman spectrometer that enables the user to easily present a fabric sample and quickly identify the textile type on the spot. Upon placing the fabric in the designated area, a laser is powered on and incident onto the sample, exciting the molecules on the fabric and generating some Raman signal. This Raman signal is collected

by a series of collection optics and directed towards a homemade spectrometer built by our team, upon which the spectrum of the sample will be analyzed by our own software. The results of this spectrum analysis is displayed to the user via an LCD screen, enabling them to determine whether the composition of their sample aligns with their expectations, or if they had been misled by the clothing's manufacturer. The rest of this paper details the research, planning, testing, and prototyping that our team dedicated towards creating this system.

2 Project Description

2.1 Motivation and Background

As the 21st century consumers are 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.

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 [3]. 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 [4]. 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" 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 created 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 [5].

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 [6].

2.2.3 trinimaX: 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 [7].

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 [8], [9].

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 [10].

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 [11].

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 [12].

2.3 Objective and Goals

The main goal of our Senior Design project was 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 intended to avoid NIR spectrometry as a technique and instead rely on Raman spectrometry to achieve material identification.

We intended 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 honed in on a few particular fabrics that we aimed to identify as well as separately conducting a product comparison for a few clothing items.

2.3.1 Goals

Basic goals

- The material analysis function will be able to classify two types of textile samples based on their spectral signature. The three textile types will be cotton 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 that will 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 and 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 have to be undyed, unblended, or one of the two 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 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
- Store reference spectral signatures of cotton and polyester for comparison during material analysis
- Utilize dynamic time warping as well as further classification methods 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 wool.
- 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 that can accurately determine the level of correlation between a sample clothing product and a stored reference item to find a match.

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

2.4.1 Optical System

The system includes 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, including 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.

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 numpy 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

Parameter	Specification	Units
Material Analysis Accuracy	>90%	Percent
Total Response Time	<15	Seconds
Product Comparison Accuracy	>90%	Percent
Spectral Resolution	<12	cm ⁻¹
Spectral Range	800 – 3100	cm ⁻¹
Signal Strength	>1	pW
Battery Life	>5	Hours
Regulated Voltage	3.3 - 5	Volts
Power Consumption	<30	W
Battery Energy	>=72	Wh
Regulated Current	1	Amps
Unit Size	<24’’x18’’	Inches
Unit Weight	<10	lbs
Cost	<\$2,500	USD

Table 2.5.2 Component Specifications

Component	Parameter	Specification	Units
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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
Achromatic Doublet Coupling Lens	a) EFL b) BFL c) Diameter d) NA e) Thickness	a) 75 b) 70.39 c) 25 d) .17 e) 7	a) mm b) mm c) mm d) N/A e) mm
Dichroic Mirror Chroma T550lpxr	a) Cut-on wavelength b) Transmission wavelength c) Reflection wavelength d) Diameter e) Transmittance f) Reflectance g) Thickness	a) 550 b) 550-1000 c) 390-540 d) 25 e) >96 f) >97 g) 1	a) nm b) nm c) nm d) mm e) % f) % g) mm
Q-Baihe 532 nm laser diode module	a) Wavelength b) Output power (typ.) c) Current (typ.) e) Voltage (typ.) f) Spectral bandwidth g) Parallel beam divergence h) Perpendicular beam divergence	a) 532 b) 40 c) 500 e) 12 f) 1 g) <1 h) <1	a) nm b) mW c) mA e) V f) nm g) mrad h) mrad
Longpass Filter Chroma ET542lp	a) Cut-on wavelength b) Transmission wavelength c) Rejection wavelength d) Diameter e) Optical density f) Transmittance g) Thickness	a) 540 b) 555-1000 c) 300-540 d) 25 e) 6 f) >98 g) 3.5	a) nm b) nm c) nm d) mm e) OD f) % g) mm
Bandpass filter Edmund Optics #26-981	a) Center wavelength b) Diameter c) Thickness d) FWHM e) Optical density	a) 532 b) 12.45 c) .4 d) 10 e) 2	a) nm b) mm c) mm d) nm e) N/A
Thorlabs LC2969 Plano-concave lens	a) EFL b) BFL c) Diameter	a) -6 b) -6.8 c) 6	a) mm b) mm c) mm

	d) Thickness e) Radius of curvature	d) 2.6 e) -4.7	d) mm e) mm
Thorlabs LA1509 Plano-convex lens	a) EFL b) BFL c) Diameter d) Thickness e) Radius of curvature	a) 99.7 b) 97.3 c) 25.4 d) 3.6 e) 51.5	a) mm b) mm c) mm d) mm e) mm
Edmund Optics #36-043	a) Diameter b) Thickness c) Coating d) Reflectivity	a) 25.4 b) 3 c) Protected Silver d) >98	a) mm b) mm c) N/A d) %
Entrance slit DIY-Optics	a) Width b) Height c) Thickness	a) 50 b) 12 c) 0.2	a) μm b) mm c) mm
Collimating Mirror Edmund Optics #43-471	a) Focal length b) Radius of curvature c) Diameter	a) 100 b) 200 c) 2	a) mm b) mm c) inches
Ruled Reflection Diffraction Grating Thorlabs GR25-1205	a) Groove density b) Blaze wavelength c) Blaze angle d) Size	a) 1200 b) 500 c) 17 d) 25 x 25	Grooves/mm mm Degrees mm
Focusing Mirror Edmund Optics #43-471	a) Focal length b) Radius of curvature c) Diameter	a) 100 b) 200 c) 2	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	a) Resolution b) Screen Size c) Color	a) 800 x 480 b) 5.6 x 6	a) Pixels b) Inches c) Bits

	d) Supply Voltage	c) 18 (262,144 total colors) d) 3.3	d) Volts
Battery Lithium Iron Phosphate Power Bank	a) Voltage b) Current c) Capacity	a) 12 b) 2 c) 6000	a) Volts b) Amps c) mAh
Raspberry Pi	a) RAM b) Processing Speed	a) 4 b) 2.4	a) Gigabytes b) Gigahertz

2.6 Hardware Block Diagram

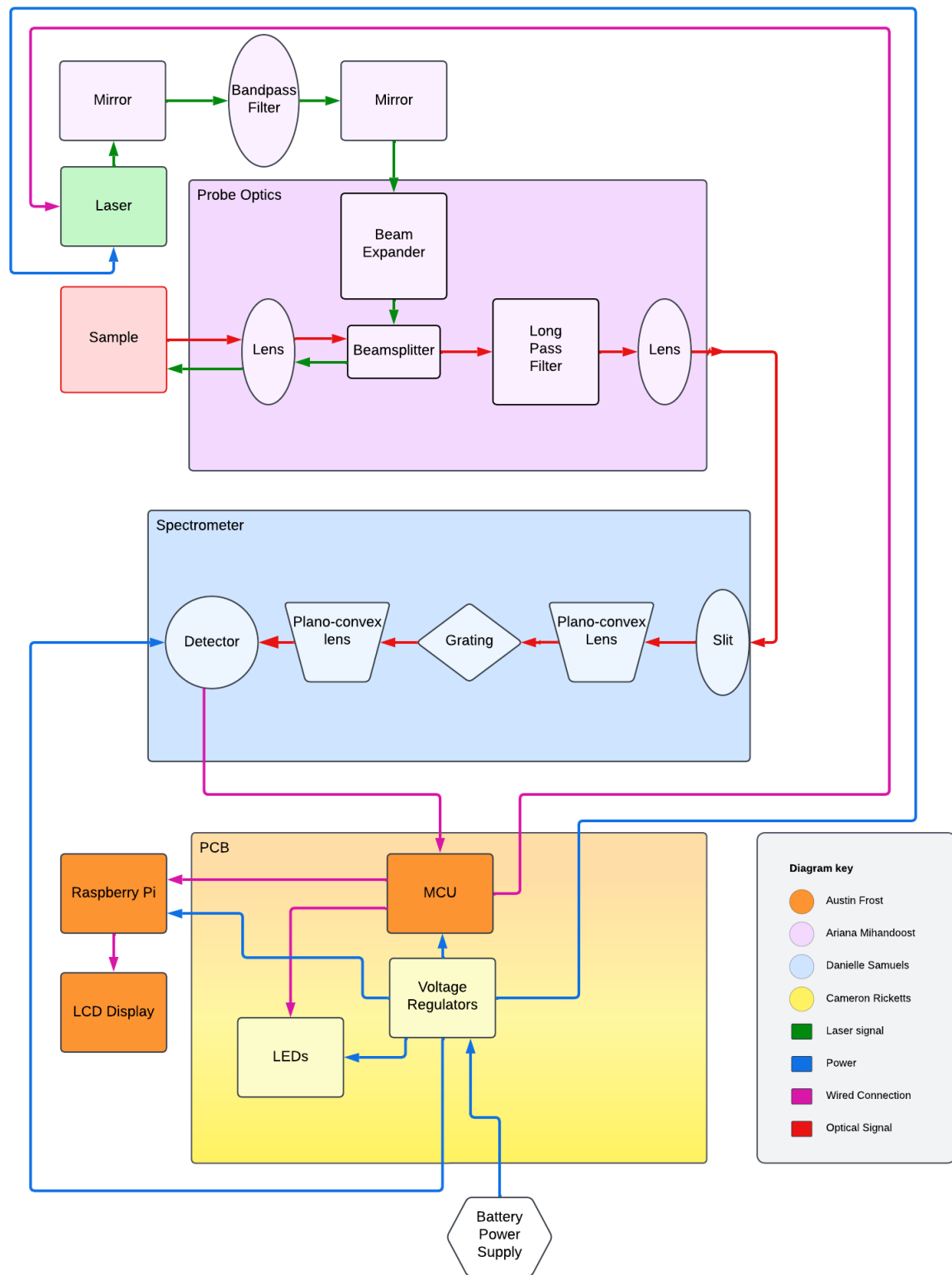


Figure 2.6.1 Hardware Block Diagram

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	13	12	13	13
Engineering Requirements	Maximum Cost	Material Analysis Accuracy	Total Response Time	Product Comparison Accuracy	Spectral Resolution	Signal Strength	Unit Size	Unit Weight	Battery Life	Regulated Voltage	Regulated Current	Signal to Noise Ratio	Spectral Range	Power Consumption	Battery Energy
Customer Requirements (Explicit and Implicit)															
Direction of Improvement	▲	▲	▼	▲	▲	◇	▼	▼	▲	◇	▲	▼	▲	▼	▼
Accuracy	▲	↓	↑↑	↑↑	↑	↑						↑↑	↑↑	↑↑	
Speed	▲	↓↓	↑	↓↓	↑	↑						↑			
Performance	▲	↓↓	↑↑	↓↓	↑↑	↑↑			↑	↑	↑	↑	↑	↑	↑
Safety	▲									↑	↑			↑	↑
Portability	▲						↑↑	↑↑	↑↑	↑	↑		↑		
Cost	▼	↑↑	↓↓	↓	↓↓	↓↓	↓↓	↓↓	↓↓	↓	↓↓	↓	↓↓	↓	↓
Target	<\$2500	>90%	<10 sec	>90%	<12 cm ⁻¹	>1 pW	Approx. 24" x 18"	<10 lbs	>5 hours	3.3 V < x < 5 V	1 Amp	> 50	600 - 3000 cm ⁻¹	<7 W	>=72 Wh

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.

3.1 Raman Background

3.1.1 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 [13].

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.

3.1.2 Stokes 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, v_1 , rather than returning to its initial ground state, v_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, v_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, v_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. [13]

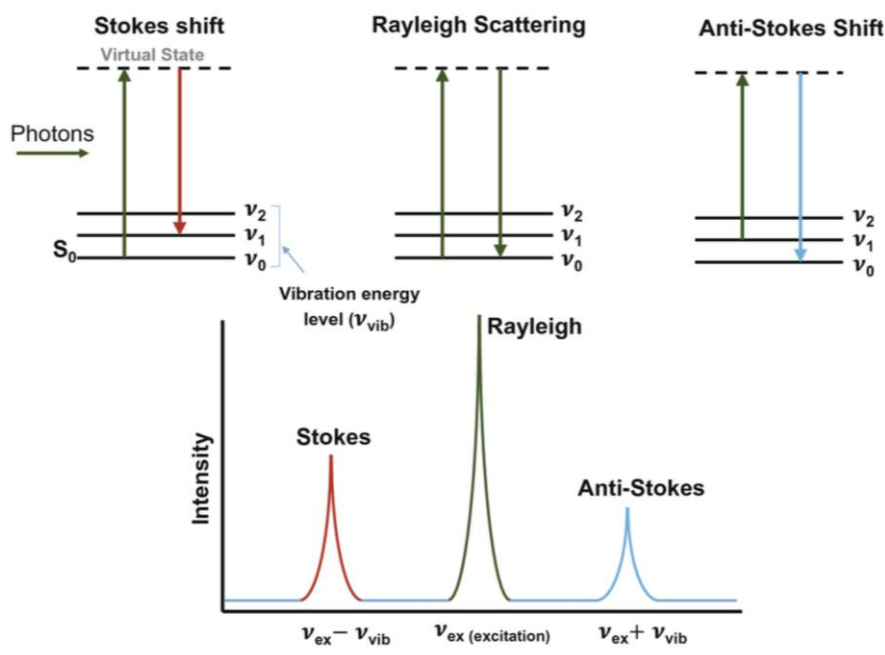


Figure 3.1.1 Demonstration of Stokes Scattering, anti-Stokes scattering, and Rayleigh Scattering

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.

3.1.3 Raman Spectroscopy

Raman spectroscopy is a primary analytical technique to assess the vibrational and rotational modes of a material through Raman scattering [14]. 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" [14]. 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 leverages 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.

3.1.4 Raman Scattering

In 1928, physicist Sir Chandrasekhara Venkata Raman and his student Sir Kariamanikkam Srinivasa Krishnan observed the first Raman scattering event from liquids [15]. 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, he 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 [16]. 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 [17]. 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 [18]. 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.

3.1.5 Raman Spectroscopy Methods

Raman spectroscopy comes in over 25 variations [14]. 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 [19].

Raman Microscopy

Raman microspectroscopy uses the same techniques as a typical dispersive Raman spectrometer. However, it not only provides 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 can 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 [20].

3.1.6 Spectrometer Configurations and Comparison

Most Raman Spectrometers are designed under the Czerny-Turner arrangement. They are all marked by their use of reflective gratings, which advantageously avoids chromatic aberrations. However, their tedious alignments and optical components make them more complex and sensitive to misalignments. Therefore, as we originally were going to proceed with a Czerny-Turner spectrometer configuration, we ultimately moved forward with a lens-grating-lens reflective spectrometer. This configuration still takes advantage of the efficiency of reflective gratings, while being more robust to alignment errors. The design of the system is further discussed in Section 6.2. Using an appropriate spectrometer arrangement for our system determines our capacity to receive a high enough Raman signal off 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 [21].

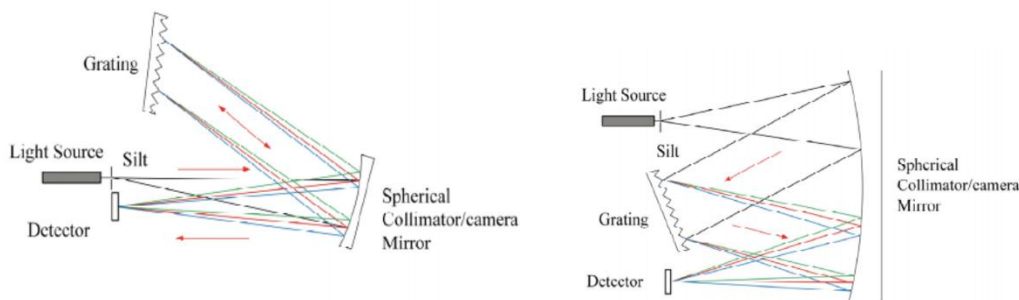


Figure 3.1.2 (Left) Littrow spectrometer. (Right) Ebert-Fastie spectrometer.

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 realignment, 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 minimize 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 [22]. 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 the second concave mirror. This second concave mirror focuses the light onto the detector.

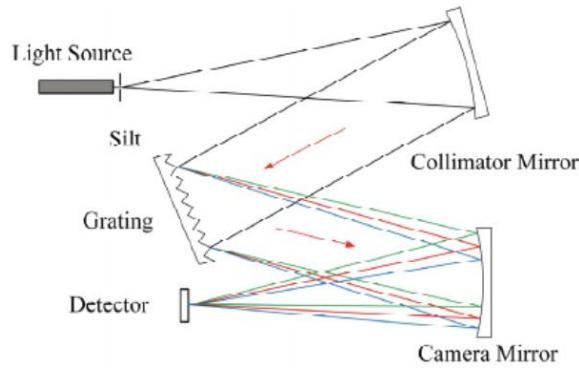


Figure 3.1.3 Czerny-Turner Spectrometer configuration.

Despite the advantages of the Czerny-Turner configuration, there are 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 [23]. A very precise alignment of the gratings, mirror, and detectors is required to attain a highly resolved spectrum. Raman signal by default is of a reduced intensity, and one may be faced with a limited light throughput of our signal.

3.1.7 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 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 [24]:

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 guided 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.

3.2 Electrical Hardware

3.2.1 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, both 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.

3.2.2 LCD Selection

The system output will be shown to the user on a liquid crystal display. The LCD will allow the user to select from the system's setting options 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 match. These functions require the LCD in question to be small enough to fit the scale of the system but also large enough for interaction with the user, providing space for easy touchscreen selection 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 portable system LCD model. It is the same model used in UCF classes such as Embedded Systems, Real Time Systems, or 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 [25]. Without touchscreen functionality, it is unable to take any form of direct input from the user, and with a dot matrix display, 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 to the previously mentioned LCD (\$32.99 vs \$6.99), but is far better in terms of functionality. The Hosityond 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 [26]. The downside of the Hosityond is that, given its dependency on the Raspberry Pi, if another controller is selected, then the display will be impossible to implement, as the display serial interface used by the Hosityond for communication only works with a Raspberry Pi.

The third option is an LCD with a similar level of functionality as the Hosityond but developed for common microcontroller units. The LCD would still have 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 most often more expensive than development for an MCU like the ESP32. As a result, all directly connected components like the LCD should be lower cost than the alternative Raspberry Pi product. The chosen LCD model for this option is the Adafruit ILI9341 ESP32 development board smart display. The display is a touchscreen, 4.7 x 3.2 inches in dimension, has a 240 x 320 pixel display, and has a price tag of \$17.99, fulfilling all four previously stated requirements [27].

Table 3.2.1 Liquid Crystal Display Product Comparison

	Dot-Matrix	Hosityond Touchscreen	ESP32 Display
Cost	\$6.99	\$32.99	\$17.99
Touchscreen Functionality	No	Yes	Yes
Size	1.4 x 3.1 inches	5.6 x 6 inches	3.2 x 4.7 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 is 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 Honyond is the clear choice, otherwise, the Adafruit 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 Honyond was chosen.

3.2.3 System Controller Technology Comparison

All actions done in the software end of the project will be done through a 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.

On the opposite end, a microcontroller, while small enough to accomplish the goal of system portability, is not sufficient for all project goals. While a microcontroller can have the support necessary to accomplish each aspect of the project, namely the extraction of CCD frame data, data preprocessing, signature generation, dynamic time warping, and clustering calculations, as all are feasible for more robust microcontrollers, the technical specifications of even an ESP32 would be lacking when implementing all previously mentioned parts of the project together, and the result would be unacceptable performance for the system. With only an integrated circuit MCU, it would take far too long to deliver the user an output, even if the end results are found to be accurate. Early testing of dynamic time warping using Google Colab, the Raspberry Pi, and an ESP32 development kit showed that the function call of standard DTW on the ESP32 alone would be roughly the total allotted time for the entire system response, and while there would still be significant room for improvement through lightweight DTW implementations and further algorithm optimization, the processing problem remains when considering this is only one feature in the full role that the MCU fills. For this reason, a single-board controller was chosen to provide a preferable middle ground that allows for all goals of the project to be achieved. An MCU will still be used for data frame acquisition from the CCD sensor to satisfy PCB design requirements, but further data analysis will be done using a separate single-board controller.

3.2.4 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, \$69.49, \$89.99, and \$129.99, respectively. The board has forty general-purpose input and output pins and is compatible with the Hosyond 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 [28].

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 [29]. The board has quality library support, especially for Python libraries, which is a notable upside for this project [30]. 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 [31]. 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 3.2.2 System Controller Product Comparison

	Raspberry Pi 5	NVIDIA Jetson Nano	Coral Development Board
Price	\$69.49	\$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 is also capable of closing all performance gaps while maintaining an advantage in cost and support. The RPi 5 has additional first-party commercial devices that expand the board's memory and processor performance. SD card add-ons increase the internal eMMC storage from thirty-two or sixty-four gigabytes for \$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.

3.2.5 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[32]. 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) [33]. 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[34]. 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 [33]. 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.

3.2.6 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 3.2.3 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 PCB tools	Dedicated PCB tools	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
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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 it has 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, 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.

3.2.7 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 [35]. 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[36]. 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 [37]. Instead, digital signals encode information using discrete binary values, typically represented as a series of ones and zeros[37],[38]. 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 [39]. 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 3.2.4 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

3.2.8 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[40]. 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[41],[42],[43].

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[43]. 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.

3.2.9 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 3.2.5 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.

3.2.10 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[44],[45],[46].

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[47].

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[48].

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 their features to isolate the best choice.

Table 3.2.6 Battery Comparison

Feature	Lithium-Ion (Li-ion)	Lithium Iron Phosphate (LiFePO ₄)	Sealed Lead Acid (SLA)
Chemical Composition	Lithium-ion (Li-ion)	Lithium Iron Phosphate (LiFePO ₄)	Lead and sulfuric acid

Energy Density	High (compact & lightweight)	Moderate	Low (bulkier & heavier)
Portability	Excellent	Good	Poor (heavy & large)
Charge Cycle Lifespan	2,000 - 5,000 cycles	2,000 - 5,000 cycles	300 - 500 cycles
Charge Retention	1-2% loss per month	2-3% loss per month	Excellent (long shelf life)
Voltage Output	11.1V (12.6V peak)	12V	12V
Capacity	3.5Ah (3500mAh)	6Ah (6000mAh)	7Ah
Max Discharge Current	4.2A	12A	70A
Max Power Output	46.6W	144W	840W
Size (L × W × H)	2.75" × 2.17" × 0.8"	4.4" × 2.6" × 2.8"	5.95" × 2.56" × 3.7"
Weight	5.3 oz (0.15 kg)	0.7 kg	1.91 kg
Safety	Moderate (risk of overheating, must be recycled properly)	High (stable, low fire risk)	High (sealed to prevent leaks)
Environmental Impact	Requires recycling due to lithium content	Eco-friendly, no toxic metals	Can cause lead/sulfuric acid contamination if not disposed of properly
Cost	~\$89.99	~\$79.00	~\$16.00
Applications	Portable electronics, EVs, solar storage	Renewable energy, stable power supply	Backup power, emergency lighting

After comparison, the conclusive battery selected is the Lithium Iron Phosphate. This battery ensures stability and safety reducing risk of explosions and fires. It remains a safe option while also providing reliable voltage with a high capacity and long lifespan.

3.2.11 Voltage Regulators

This section will explore voltage regulators, which are crucial components in electronic devices responsible for maintaining stable voltage levels. Their primary function is to ensure that electrical components receive a consistent voltage supply, regardless of fluctuations in the input voltage. This stability is essential, particularly for sensitive components that require precise voltage levels to function properly without disruption. Voltage regulators not only maintain steady power delivery but also offer control over both voltage and current levels, allowing for increases or decreases as needed. They achieve this by accepting an input voltage and adjusting it to a fixed output voltage determined by the regulator's design. Additionally, regulators act as a protective buffer between power

sources and components, preventing damage caused by voltage spikes or drops. Another key advantage of voltage regulators is their ability to enable a single power source to supply multiple components requiring different voltage levels, though in such cases, multiple regulators may be necessary.

Types of Regulators

There are two primary types of voltage regulators: linear regulators and switching regulators. The key difference between the two lies in their efficiency and power handling. Linear regulators are simple and cost-effective but tend to be inefficient as they dissipate excess power as heat, making them unsuitable for applications where power conservation is a priority. They are best suited for stepping down an input voltage to produce a lower output voltage, functioning similarly to a voltage divider. However, their inefficiency often necessitates additional cooling solutions such as heat sinks. Switching regulators, on the other hand, are more efficient and versatile. They not only reduce voltage but can also increase it, making them more adaptable. Unlike linear regulators, which continuously dissipate excess energy, switching regulators operate by rapidly turning the input voltage on and off, significantly reducing power loss. While they tend to generate more electrical noise, they offer better performance and power conservation, making them ideal for many modern applications[49],[50].

For the PCB design of TEXRAY, a switching regulator will be the primary choice due to its ability to efficiently handle different voltage requirements. The system will be powered by a 12-volt battery pack, but various components will require different voltage levels, such as 3.3V and 5V. To achieve this, a Step-Down (Buck) regulator will be used to reduce the voltage from 9V to the necessary lower levels. On the opposite end Step-Up (Boost) will be used to raise the 9V input to 12V. While a linear regulator could technically achieve the same result, its inefficiency makes it a less favorable option for this project. Additionally, in scenarios where certain components require a higher voltage than the battery provides, a Step-Up (Boost) regulator will be implemented. This type of switching regulator increases the voltage to meet the required specifications. By incorporating these regulators, the TEXRAY system will achieve reliable and efficient power distribution, ensuring stable operation across all its components.

3.2.12 Communication Protocols

Devices within a system communicate following a set of predefined rules known as communication protocols. These protocols enable seamless data sharing between components while ensuring that the transmission is structured, accurate, and reliable. Since the data being exchanged is often critical, error protection methods are incorporated to maintain precision and prevent miscommunication. Communication protocols play an essential role when sending commands to a device or retrieving stored information, making them a crucial aspect of TEXRAY. For instance, the data collected by the analog-to-digital converter (ADC) needs to be transmitted to the microcontroller for processing, making an efficient communication protocol necessary. The selection of a protocol depends on

various factors, such as speed, power consumption, complexity, number of devices involved, and the capabilities of the system itself.

Types of Communication Protocols

Communication protocols are broadly classified into two main types: serial communication and parallel communication. Serial communication transmits data one bit at a time, making it ideal for long-distance or low-pin-count connections due to its simplicity and efficiency. Parallel communication, on the other hand, transfers multiple bits simultaneously, allowing for faster data exchange but requiring more physical connections and increasing the risk of signal interference over longer distances.

SPI

Among the different serial communication protocols available, SPI (Serial Peripheral Interface) is one of the fastest. It utilizes four dedicated lines—MOSI (Master Out Slave In), MISO (Master In Slave Out), SCLK (Serial Clock), and SS (Slave Select)—to facilitate full-duplex data exchange between master and slave devices. The clock signal synchronizes data transfer, ensuring precise timing. Due to its high speed, SPI is ideal for applications requiring rapid communication, such as display modules, sensors, and memory chips. However, its requirement for multiple physical connections can be a drawback in systems with numerous devices.

UART

Another widely used serial communication protocol is UART (Universal Asynchronous Receiver-Transmitter). Unlike SPI, UART does not rely on a clock signal to synchronize communication. Instead, it transmits data in packets containing start bits, data bits, parity bits (optional), and stop bits to ensure accurate transmission. This method helps minimize errors, making UART highly reliable for point-to-point communication. It is commonly used in debugging, wireless modules (such as Bluetooth and GPS), and simple microcontroller-to-microcontroller communication. Although slower than SPI, its simplicity and error-checking features make it a popular choice for embedded systems.

USB

USB (Universal Serial Bus) is another well-known communication protocol, widely used for interfacing microcontrollers with external peripherals. It supports plug-and-play functionality, meaning devices can be connected and recognized without manual configuration. USB allows for high-speed data transfer, making it ideal for applications such as external storage, input devices (keyboards and mice), and debugging tools. Unlike SPI and UART, USB supports multiple device types and allows for both power delivery and data transmission over a single cable, increasing its versatility.

I2C

An Inter-Integrated Circuit (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.

Communication Selection

Each communication protocol offers distinct advantages and is chosen based on the system's needs regarding speed, reliability, and complexity. In many cases, embedded systems utilize a combination of protocols to optimize performance. However, for TEXRAY, I2C (Inter-Integrated Circuit) will be implemented, as it offers the most efficient data transfer between the ESP32 and the RPi. I2C allows multiple devices to communicate over just two wires (SDA for data and SCL for clock), making it an efficient solution when working with multiple sensors or peripherals while minimizing wiring complexity.

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 3700-200 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 [51]. 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. 3.3.1, 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 [52]. 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.

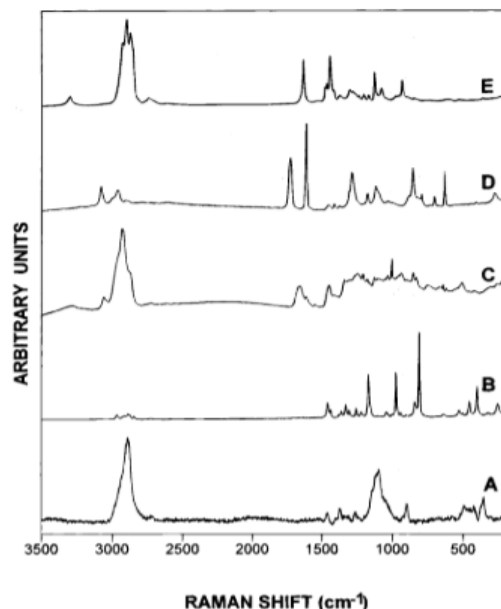


Figure 3.3.1 Raman microprobe spectra of (A) rayon; (B) polypropylene; (C) wool; (D) polyester; (E) nylon.

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 [53], 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. 3.3.2. 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.

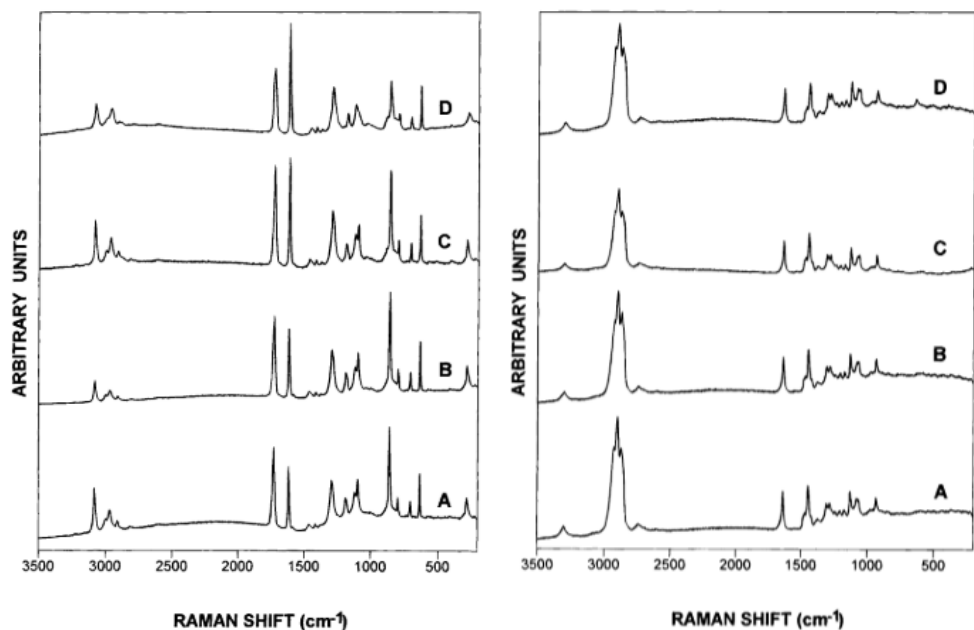


Figure 3.3.2 Raman microprobe spectra of polyester samples from four manufacturers (left). Raman microprobe spectra of nylon samples from four manufacturers (right).

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 [54].

Polyethylene terephthalate (PET), most commonly referred to as polyester when in fiber or textile form [55], is a synthetic fiber produced through the polymerization of ethylene glycol and terephthalic acid [56]. 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[54]. 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 [54], [57], [58]

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% [59]. 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[60]

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 C=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 [54]

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 3.4.1. 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 were applied towards guiding the optical hardware we should integrate, specifically the excitation wavelength we implemented into our system. Since fluorescence is far more likely to occur than Raman scattering, and thus can effectively swamp any meaningful Raman signal, it was in our best interest to choose an excitation wavelength which offers low fluorescence while maintaining high Raman intensity [61].

Table 3.4.1 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 μ m, 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 3.3.2. 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 [62].

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 [63]. 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 [64].

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 [61]. 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 maximize Raman signal strength.

3.4.3 Laser Comparison and Selection

Though testing and literature point towards the 473 nm laser potentially being the best option for our samples, we must consider our system 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 comparison between laser choices [65]. Table 3.4.2 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 3.4.2 Comparison of various single transverse mode lasers.

Specification		Thorlabs DJ532-40	ams-OSRAM PL 520B	Q- BAIHE 532nm module	Thorlabs L473P10 0	Thorlab s L450G3	Civil Laser GH0458 0A2G
Peak Wavelength		532	520	532	473	450	450
Output Power (mW)		40	80	40	100	100	80
Operating Current (mA)		330	200	500	120	80	110
Threshold Current (mA)		160	40	N/A	20	12	22
Operating Voltage (V)		1.9	6	12	5.7	5.2	5.3
Beam Divergence	Parallel	.69°	6.3°	<1 mrad	10°	8.4°	10°
	Perp.	.69°	22.5°	<1 mrad	24°	21.5°	24°
Spectral Linewidth		.0283 pm	1 nm	1 nm	1.25 nm	1.25 nm	N/A
Price		\$212.64	\$46.00	\$43.98	\$3,032.68	\$138.57	\$9 (min. 10 purchase)

After sorting through various sites and listings of lasers, these options seemed the most suited to our project. Just by looking at the table it is clear that finding laser diodes or laser modules at the particular wavelength of 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 [65]. 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 [66], [67].

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 were 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 520 nm ams-OSRAM PL 520B is significantly cheaper than the DJ532-40, while also having a lower threshold current, and having the highest output power of 80 mW, which will ensure high Raman signal generation. On the other hand, the Q-Baihe 532 nm laser has the advantage of being a laser module, meaning it is already collimated and thus we would not need to pay for additional focusing optics. This module is also the cheapest of all the green laser options. Though it has less power than the ams-OSRAM diode, 40 mW would still be plenty of power to generate a strong Raman signal. For these reasons, we believe the Q-Baihe 532 nm laser diode module would be the best choice for the excitation source of our system. In the case that this option did not pan out somehow, we considered the ams-OSRAM 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 [68]. 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 [69]. 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 [70].

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 [71], 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 [72], [73]. 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 allows 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 only reflects light in a narrow band around 532 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 [67]. 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 [74], and thus the system still requires a secondary optical filter in the system to further reduce noise [75].

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 [76], 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 [77]. 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 was 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 [78], [79]. For our purposes, we will need to block out the 532 nm source by reflection while allowing the higher wavelength Stokes scattered light to pass through. Since 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 was to maintain a continuous-wave laser power at or 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 [80]. The goal for our system was to have an exposure time of 15 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. Though, the beam diameter at the sample surface is a factor that can be influenced by optics used to collimate or expand the beam. All of these factors must be considered when determining if the damage threshold of the proposed longpass dichroic mirrors are sufficient for our application [80], [81].

Our system to implemented 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 3.5.1 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

	MKS Newport DCM13	Chroma T550lpxr	Chroma RT532rdc	Edmund Optics #86- 393 / #86-386	Thorlabs DMLP550 / DMLP550T
Cut-on wavelength (nm)	552	550	536	552	550
Transmission wavelength (nm)	561.4 - 790	550 - 1000	536 - 1000	561.4 - 790	565 - 800
Reflection Wavelength (nm)	514.5-543.5	390 - 540	390 - 532	514.5- 543.5	380 - 533

Diameter (mm)	25	25	25	25 / 12.5	25.4 / 12.7
Thickness (mm)	3.5	1	3	3.5	3
Reflectance	>98%	>97%	>97%	>98%	>90%
Transmittance	>95%	>96%	95.97%	>95%	>85%
Angle of Incidence	45°	45°	45°	45°	45°
Clear aperture diameter (mm)	22	22.5	22.5	21.33 / 8.8	>22.9 / > 11.4
Damage threshold (J/cm ²)	N/A	N/A	N/A	N/A	.5
Cost	\$359	\$250	\$600	\$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 RT532rdc being the best option, as this filter is specifically built for Raman spectroscopy at our excitation source of 532 nm, and would effectively block out the laser photons without reflecting 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 532 nm source corresponds to a Raman shift of 615 cm⁻¹. This means that any peaks below 615 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. The 532 nm cut-on mirror is a significantly better option than the 550 nm cut-on wavelength mirrors in terms of performance, however, this mirror costs much more than the other options at a price of \$600.

Unfortunately, the Chroma dichroic mirrors did not have a very comprehensive datasheet, and thus lacked some 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 [79], [82]. Upon reaching out to a Chroma representative, however, we were able to confirm that all Chroma optics have an AR

coating on their reverse surface. Notably, both the Thorlabs and Edmund Optics dichroic mirrors were also stated to have anti-reflection coatings, meaning that all of these filters demonstrate high quality manufacturing and would contribute to a high system SNR.

Through further discussion with a Chroma representative, we were assured that though not all of their optics are damage-threshold tested, the parts that have been tested are able to comfortably withstand megawatts of power, and thus there should be no concern of damaging the optics within our system. Only one of the presented options provided the dichroic mirror's damage threshold on the actual datasheet, 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 of our system which we previously described, but Idex provides a laser damage threshold calculator on their website compatible with Semrock's line of optical components [83]. This calculator indicates that a 532 nm CW laser with a 100 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 [79], 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 was the Chroma T550lpxr. Though the RT532rdc had the best performance of all the presented filters at our excitation wavelength, the price is too steep compared to the other choices, and would be counter-intuitive to our goal of creating a "cheaper" spectrometer build. It could have also created issues with staying under our \$2500 goal down the line. The T550lpxr is shown to achieve full transmission at 556 nm, corresponding to a Raman shift of 811 cm^{-1} . This means an unfortunate loss of Raman signal prior to this wavelength, but this signal loss cannot be further minimized without sacrificing more of our budget. We believed we could still achieve accurate textile identification even with this decreased spectral range, and thus thought the T550lpxr would be a fine choice. This filter also has a higher transmittance than the other options,

minimizing Raman signal loss as it passes through the dichroic. The T550lpxr dichroic mirror has a large diameter of 25 mm, having comparable collection efficiency to the other three provided options, as well as having very high reflectance at the respective bands. For these reasons, we plan to implement the Chroma T550lpxr into our system, and we thank Chroma for loaning us this component for the duration of Senior Design II.

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,

$$\lambda = 2n_{eff}\Lambda \quad (1)$$

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 [84]. 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 [85]. 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 [86]. 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 [87]. 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 [88]. 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 [87].

Considering the potential filter options, we believed a longpass filter would 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 3.5.2 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 3.5.2 Comparison of prospective longpass filters

	Semrock BLP01-532R-25	Chroma ET542lp	Chroma RET537lp	Edmund Optics #29-191	MKS Newport 10CGA-530
Cut-on wavelength (nm)	541	542	537	550 ± 1	550 ± 5

Rejection wavelength (nm)	270 - 532	300 - 540	300 - 536	200 - 539	N/A
Transmission wavelength (nm)	546.9 - 900	555 - 1000	540 - 1100	560 -1650	N/A
Transmission (%)	> 93	> 98	> 98	> 91	> 90
Optical density OD (average)	> 6	6	> 6	> 4	> 5
Thickness (mm)	3.5 ± .1	N/A	N/A	2 ± .1	1.1 ± .1
Diameter (mm)	25	25	25	12.5 ± .2	25.4
Clear Aperture (mm)	>22	22.5	22.5	> 10	> 22.86
Cost	\$409.00	\$365.00	\$600.00	\$199.28	\$47.00

The most important factors when choosing a longpass filter for our system is the rejection and transmission wavelengths. Ideally, the longpass filter implemented should enable near 100% rejection of light at and below 532 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, all of them meet these conditions, but some of them have larger rejection bandwidths than others. At a glance, it would seem that the Semrock filter is the best choice for our system, as the rejection bandwidth only extends to 532 nm. Though the cut-on wavelength is at 541 nm, if this is the 50% transmission point then there would still be some transmission of Raman signal between 532 – 541 nm. This filter also has a transition width of 13 nm, which is relatively steep, as well as a large diameter indicating high light collection efficiency and making it seem like the best choice.

However, inspecting the raw data for this filter shows that it fully blocks all wavelengths up until 538 nm. This means that the Semrock filter is comparable to the Chroma RET537lp in terms of rejection wavelength. With the RET537lp having full blocking up until 536 nm, this Chroma filter actually reduces light loss more than the Semrock filter. The RET537lp also has greater than 98% transmission, whereas the Semrock filter has only 93% transmission. Though, these minor improvements come at a price of the RET537lp costing over \$200 more than the Semrock filter.

When considering the specifications of these filters, is it important to remember that the dichroic mirror we chose has a cut-on wavelength of 550 nm, and only reached full transmission at 556 nm. Meaning, any light below this wavelength will already experience some loss independent of it passing through the longpass filter. As a result, paying more money for higher quality longpass filters with cut-on wavelengths close to 532 nm will have diminishing returns as the price of these high-performance filters increases. It could be more efficient to buy a filter with a higher cut-on wavelength that more closely aligns with our dichroic beamsplitter, while still trying to recover as much Raman shifted light as possible within our budget. The Chroma ET542lp has a lower price than the Semrock filter, but has a cut-on wavelength of 542 nm. According to the transmission curve on the Chroma website, it blocks all wavelengths up until 539 nm, and reaches near full transmission at about 544 nm, meaning it has a very steep edge transition. This filter has a comparable rejection band to both the Semrock filter and RET537lp for a cheaper price. It also achieves 98% transmission in the pass-band, making it higher performing compared to the Semrock filter. Additionally, because full transmission occurs at 544 nm, it would still be able to recover any light between 544 - 556 nm that managed to pass through the dichroic mirror.

The Edmund Optics filter and the MKS Newport filter both have even higher cut-on wavelengths of 550 nm, with the Edmund Optics filter having full blocking up until 539 nm according to the datasheet. However, both options have the lowest transmission of all the prospective filters, which would result in more Raman signal being lost as it passes through the longpass filter when compared to other selections. Additionally, the Edmund Optics filter seemingly does not achieve full transmission until 560 nm, which is even greater than the full-transmission point of our dichroic mirror, causing even greater signal loss. The MKS Newport filter did not have a thorough datasheet, and information regarding the specific rejection and pass bands were not available. This makes it difficult to determine exactly what wavelengths of light will be able to make it through the filter, and how much the Raman signal will be diminished.

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 [89], [90]. 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 [91]. Of the filters presented in the table, only the Semrock and Chroma filters have optical densities of 6 or greater. The Edmund Optics filter has an average optical density of 4, indicating it may not be the best choice for Raman spectroscopy applications. The MKS Newport having an OD of 5 may be passable, but is still not ideal.

Taking all of these factors into consideration, it seemed that the best choice of longpass filter for our system was the Chroma ET542lp. This selection minimized cost while still being comparable to the Semrock and RET537lp filters in performance. It also had OD6 blocking at our laser line and has the highest transmission in the passband of all the

selections. This ensured that as little of our Raman signal is lost as possible before reaching the spectrometer, and a high signal-to-noise ratio was maintained in 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 [92]. 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 wavelength precision since we're observing small wavelength shifts from the excitation wavelength. 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 peaks which correspond to various vibrational modes. We can understand this as the separation of relevant peaks, which could range from as little as 10 cm^{-1} to 30 cm^{-1} . A general rule of thumb when designing a spectrometer, 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 [93]. 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 of the 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, 5 cm^{-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, which 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 desired spectral range of the fingerprint region of 300 cm^{-1} to 1800 cm^{-1} defined in wavenumbers into wavelengths to guide our filter, grating, detector selections.

$$\Delta\nu = \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_s} \right) \times 10^7 \quad (2)$$

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 3.6.1 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 component selections for the illumination optics and the spectrometer, we must take this, our primary desired spectral range in wavelengths is 540 nm to 588 nm. As we make c quantity into consideration. Generally, a greater spectral range comes at the expense of our spectral resolution.

3.6.3 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

The first characteristic of the diffraction grating to consider is whether it is ruled or holographic. 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 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 [94], [95]. However, we see more usage of ruled gratings in commercially available spectrometers [95]. 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 [96]. Transmission gratings are subject to low alignment sensitivity, which can help eliminate alignment errors in our spectrometer. In reflection gratings, diffracted orders reflect off the grating at different angles. 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 [97]. 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 limit 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 improved efficiencies under increased groove densities.

3.6.4 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 3.6.1. 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

	Thorlabs GR25-1205	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)	25 x 25	12.5 x 12.5	12.7 x 12.7	12.5 x 12.5
Price	\$128	\$94	\$81	\$155

As specified previously, the ideal spectral range contains the Raman shifts from 800 cm⁻¹ to 3000 cm⁻¹. This corresponds in wavelength to 540.6 nm to 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 allows us to lean into higher groove density gratings to focus on 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 diffracted by a grating can be specified with Equation 3.6.2.

$$m\lambda = d(\sin\alpha + \sin\beta) \quad (3)$$

Equation 3.6.2 Grating equation

Where m is an integer value describing the order of diffraction, 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. Considering an incident angle of 0°, which was chosen based upon testing in Section 9.5, we can determine the diffraction angle for each wavelength given a respective groove density using Equation 3.6.2. This would ensure

that the groove density can compensate for the dispersion in our desired spectral range. We see that 1,200 lines/mm diffracts the first order 550 nm at 41.3° and diffracts 640 nm at 50.2°. A 900 lines/mm grating diffracts 540 nm first order at 29.7° and diffracts 640 nm at 35.2°. 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.

The resolving power of a diffraction grating is provided by the Rayleigh criteria and defined by Equation 3.6.3.

$$R = \frac{\lambda}{\Delta\lambda} = nN \quad (4)$$

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). Considering illuminating the full 12.5 mm width of commercially available gratings, the resolving power is 15,000. Let's consider our desired spectral resolution of 4 cm^{-1} . Converting this quantity to wavelength using Equation 3.6.3 corresponds to a resolution of 0.11 nm. Using Equation 3.6.2, 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 a full 12.5 mm width provides a resolving power of 11,250. Therefore, in even lighting a portion of a 1,200 lines/mm or 900 lines/mm groove density grating, our desired spectral resolution can be met. In considering the next biggest commonly available size of gratings, 25 mm x 25 mm, we see that we could achieve an even higher resolving power with larger available coverage.

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 efficiency is relatively maintained across our desired spectral range.

Overall, selecting the Thorlabs GR25-1205 diffraction grating is the most appropriate choice. It's high groove density enables greater spectral dispersion, which improves our resolution. Further, it is available in a larger size at a comparable price to the competing options. It is a performance and cost-effective match for our system.

3.6.5 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 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. [98]

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. [99]

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. [100]

3.6.6 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 [101].

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 passing through 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 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,

$$I = \sqrt{\text{shot}^2 + \text{dark}^2 + \text{readout}^2} \quad (5)$$

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.

Spectral Resolution

As discussed in Section 2.3.2, our desired spectral range is 540 nm to 633 nm. Therefore, our detector must display a high QE within that range. Most commercial CCDs operate well in the visible range. A CCD loses that sensitivity as we shift red. In the beginning of our systems design, avoiding an IR source governed our choice of Raman spectroscopy and the use of a green laser, because detectors that can efficiently detect IR wavelengths InGaAs specifically lie outside of the systems budget. Luckily, a detector should be able to receive 540.6 nm to 588 nm well, conveniently this fingerprint region will have the most prominent bands. However, we must note the accurate detection of such lies in a detectable Raman signal and high enough spectral resolution. We will evaluate detectors based on their sensitivity to incident light and their operational spectral range. Detectors have fundamentally limited spectral range/ resolution due to their material characteristics. As we will be discerning fabric samples of 2 distinct chemical compositions, we must ensure the detector can compensate for both spectral readings.

Assessment of the CCD

CCD format is the number and size of pixels in the two-dimensional photoactive area. The more photons that reach a CCD pixel in each time frame, or the longer the pixels are allowed to impact the pixel, the more charge is built up, resulting in a larger detected signal.

This statement by Richard McCreery describes the complementarity of slit and pixel width on spectral resolution. “As a rule of thumb, the resolution is determined by the larger of the pixel width and the slit image width, multiplied by $d\tilde{\nu}/dl$ ”. Weak signals may prompt us to increase our integration time, which consequently increases the noise levels. This makes cooling the CCD ideal. However, to maintain the low power consumption of our portable system, leaving the detector uncooled is ideal. Therefore, the Raman signal must be as high as possible for integration time to be short, and to avoid increased noise from a cooler system.

The pixel size of the detector directly correlates to the received resolution of the spectrometer

$$\text{spectral resolution, } dv = \left(\frac{dv}{dl} \right) * Wp \quad (6)$$

Equation 3.6.5 Spectral resolution for a given pixel width

Where dv is the Raman shift observable across a CCD pixel. Since the selected slit width of 50 μm is larger than the pixel width amongst all the detectors, the spectral resolution is primarily limited by the slit size. According to the Nyquist Criterion, 2-3 pixels are needed to resolve a spectral feature. The spectral feature is defined by the slit in this instance. Therefore, all of the pixel widths allow for sufficient sampling of the slit image and dispersed spectrum.

With a finite number of pixels on a given detector, we must consider the resulting spectral range as well. The number of pixels and the resulting width of the detector determines received spectral range of our spectrometer. Having a detector width smaller than the linear distance of our highest and lowest Raman shifts after dispersion, would mean some of our spectrum would be cut off. Of course, the actual received amount of the spectrum is limited by the wavelength of the light source and detector capabilities, however it is important to ensure our detector width can compensate for our desired range. To determine an appropriate size of the detector, we can use the following equation

$$\text{spectral range } (cm^{-1}) = v_0 - v_j - \left[(v_0 - v_j)^{-1} + \frac{d(Wd)}{mL_F} \right]^{-1} \quad (7)$$

Equation 3.6.6 Spectral range

Where, v_j is the lowest observable Raman shift. v_0 is the absolute wavenumber of the laser. The focal length of the focusing lens, L_F is 50 mm for setting a general metric to compare CCD types against each other. However, please reference Section 6.2 for a more comprehensive spectrometer design.

$$v_0 = \frac{10^7}{532 \text{ (nm)}} = 18797 \text{ (cm}^{-1}\text{)}$$

$$v_j = 800 \text{ cm}^{-1}$$

$$d = \frac{1}{1200 \left(\frac{\text{lines}}{\text{mm}} \right)} = 8.33 * 10^{-4} \text{ mm}$$

Using these values in Equation 3.6.6, the Sony IXL511, and Toshiba 1209DG 28.6 mm detector width allows for a received spectral range of 8308 cm^{-1} . The spectral coverage with the Toshiba 1304DG CCD with a detector width of 29.1 mm offers a spectral coverage of 8385 cm^{-1} . The Toshiba TCD2717 53.3 mm detector width allows for a spectral coverage of 11069 cm^{-1} , and the Hamatsu S14660-1024 14.3 mm detector has a spectral coverage of 5400 cm^{-1} .

Having a detector the size of the Toshiba TCD2717 would allow for a larger received spectral range, however, we are only looking to detect Raman shift up to 2200 cm^{-1} . It would use more power than necessary. The Hamatsu S14660-1024 has too small of a detector width to compensate for our desired spectral range. While the Toshiba TCD1209DG can compensate for our desired spectral range and resolution, as well had high a high dynamic range, which contributes to higher variation in the received brightness of the image, it unfortunately requires 12 V power supply, which is higher than our portable system can compensate for.

The dynamic range of a CCD refers to the ratio of the full-well capacity over the readout noise. In this context it will determine the brightness contrast of the received Raman signals. Each dispersed Raman shift will be of a varying intensity level. Dark noise was a major consideration in the detection capabilities. Cooling the CCD suppresses the dark noise that could consequently overcome the Raman signal. The specified operating temperature as well as the Efficiency vs. Temperature graph gives useful insight into the workability of the CCD. However, the specifications of the TCD1304DG prove proper operations of the CCD even under room temperature conditions. The data rate of the CCD refers to how quickly it can read a charge and convert it into an electron, and a quicker speed is more desired to capture low signals. In comparing the TCD1304DG against the other detectors, it provides adequate electrical capabilities for its low power consumption. Specifically, between the Sony IXL511 and the Toshiba TCD1304DG, the Toshiba offers a higher spectral coverage, resolution, and dynamic range. Therefore, this is CCD that was implemented into our Raman spectrometer. Chapter 9 discussed some of the early testing phases of linear Array CCDs in receiving low intensity signals. We specifically noted a comparison of the CCD chosen for our system and the one implemented in commercial portable spectrometer.

Table 3.6.2 CCD comparison and selection

	SONY CCD IXL511	TOSHIBA CCD TCD1304DG	TOSHIBA CCD TCD2717B FG	TOSHIBA TCD1209D G	HAMATSU S14660-1024
Pixels	2048	3648	7500	2048	1024
Pixel size (μm)	14 x 200	8 $\times$ 200	4.7 x 4.7	14 x 14	14 x 14
Total Detector Width (mm)	28.6	29.1	53.3	28.6	14.3
Spectral Response (QE)	70-90%	~100%	90-100%	N/A	~75%
Package/ Case	22 pin DP	22 pin Cerdip	32 pin CLCC	22 pin Cerdip	24 pin ceramic DIP
Operating temperature	-10 to 60°C	-25 to 60°C	0 to 60°C	-25 to 60°C	-50 to 50°C
Dark Current	3 to 6 mV	2 to 5 mV	1 to 6 mV	1 to 2.5 mV	50 - 500 (e-/ pixel/s)
Dynamic Range	267	300	N/A	2000	3330 - 6660
Data Rate (MHz)	2 (Max)	0.2 to 1	0.5 to 1 (35 Max)	1	0.5
Power Supply Voltage (V)	5	3 (min)	10	12	5

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 was developed by the same company that developed the Raspberry Pi and is the official operating system for the device. Raspbian is also the OS with the highest level of support of all the available options, as it is the most commonly used OS for the RPi and the easiest option for when troubleshooting or looking for terminal command examples, with the large 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 work the same when transferring between the two, and in fact, it is very common that they do not [102]. Given the fairly controllable size of the base Raspbian OS, this flaw represents a significant drawback of DietPi, and in the circumstances of this project, restricts it to a backup option for potential sRAM 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 related open-source projects, Ubuntu has the largest support of any available OS option when considering non-RPi systems running on the 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 project is. However, given its development for web-based projects, it is not the best option given the technical constraints of the RPi 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 outway 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

A caveat of this choice is that, given the lack of true implementations of Python on microcontroller units, another language would have to be chosen when programming the microcontroller unit embedded into the PCB. Since an ESP32 Devkit V1 was already owned and Arduino is fully capable of accomplishing all required tasks, this was the language chosen. Arduino's programming language is a variant of C, developed specifically for embedded programming, and functions well in acquiring frame data from the CCD sensor.

3.7.3 Python Packages

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 consider when designing our system.

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 [103]. 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 [104]. They are thus exempt from any control operation and do not require particular safety measures to be taken [105].

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 eyeglasses 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 [105]. 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 the 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 [104].

Our system utilizes 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 [106].

This standard is important to our system as it helped 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 allowed 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 ensured our system is of the highest quality performance and build for our budget.

4.1.3 Communication Standards

Inter-Integrated Circuit

An Inter-Integrated Circuit (I2C) is one of the two 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 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 data transmission rates, 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, 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 [107].

Display Serial Interface

The system's liquid crystal display (LCD) module is attached to the Raspberry Pi controller through a display serial interface (DSI) connection. This connection is established using a one hundred and sixty millimeter DSI flat printed circuit (FPC) cable, which has each end latched into place inside DSI connection ports on the LCD module and the RPi. FPC cables are often confused with flexible flat cables (FFCs), as both are connection cables thinner than ribbon wire and used for electrical systems. The distinction is that an FPC cable describes actual circuits that are printed onto flexible material, while FFCs function as standard connection cables, usually without additional embedded components beyond conduction layers [108]. DSI is an industry standard developed by the Mobile Industry Processor Interface (MIPI) Alliance, an industry body founded in 2003 with the goal of creating standards for mobile devices and components. The group is the same organization that developed the Improved Inter-Integrated Circuit (I³C) bus, also called SenseWire, the System Power Management Interface (SPMI), the Display Pixel Interface (DPI), and the Camera Serial Interface (CSI). Today, DSI is one of the most common methods of communication between processors and display devices. Originally released in 2005, the interface is still regularly updated today. Its widespread adoption is largely due to the lack of additional stress put on the processor during data transmission, which comes from how lightweight the communication protocol is. This is especially true when the interface is connecting a processor to a liquid crystal display, as the interface itself was originally designed with LCDs in mind. In the commercial industry, the protocol is most often seen inside smart tablets, smartphones, and display boards, as the thinness of the cable makes the interface ideal for display communication within a device. While DSI is a closed-source standard, there is still extensive documentation on the interface dating back nearly twenty years, so the communication method and protocol itself are well understood. The interface uses serial bus communication, with clock and data lanes, all carrying differential signals from the host processor device to the display. Due to the use of differential signaling, every lane is comprised of two wires, each sending signals identical to their pair in magnitude but inverted in polarity. The connection is most often built with two modes, low and high power. In high power mode, the first lane is used for a high-speed clock, unlike in low power mode, where in-baud signaling is used, storing control data such as clocking information within the outgoing signal [109].

Analog to Digital Conversion

While not an independent communication method, analog-to-digital conversion is crucial to the project and is specifically an integral part of the communication systems mentioned previously. The ESP32 development board and microcontroller unit both contain two embedded successive approximation register (SAR) type analog-to-digital converters (ADCs) [110]. These ADCs are used to process the output signal of the TCD1304DG CCD sensor and allow the analog data to be viewed and analyzed as digital integer values by

both the MCU and the Raspberry Pi. IEEE 1241 is the widespread standard for ADCs and helps to provide a common set of terminology, specifications, and testing processes for all ADC devices. This includes specifying the model number, power requirements, package type, and physical dimensions of any ADC, as well as a listing of the conducted system testing in the form of results such as gain error, offset error, total harmonic distortion, signal-to-noise and distortion ratio, or effective number of bits [111]. This information creates a universal system of comparison between ADC devices and ensures the quality of commercial products.

4.1.4 Textile Standards

For the textile identification portion of our system, we designated pure, homogenous samples to be tested upon. A pure textile sample is made exclusively from one type of fiber, and contains no additives, dyes, finishers, softeners, blending, or contaminants [112]. Scientific grade textiles are backed by standards which designate the specifications and test methods for the physical, mechanical, and chemical properties of textiles, fabrics, and cloths, as well as the natural and artificial fibers that constitute them. As the American Society for Testing and Materials (ASTM) expressed, “standards are specified to help fabric and cloth designers and manufacturers in testing textiles to ensure acceptable characteristics towards proper end use. [113]” In having the Raman spectrometer conduct material identification, using a standardized test material provides a proper baseline of what the Raman spectra should resemble. The ability to accurately compare unknown samples against known standardized references will overall improve the reliability and reproducibility of our system.

Consumer-Grade “pure” samples from suppliers such as JOANN Fabric and Crafts, Walmart, Micheals, etc., generally display a deceptive purity. Most available fabrics are blended, or treated with dyes, finishers, or softeners. Production and handling may introduce contaminants such as oils, starches, or sizing agents [114]. These factors can distort the Raman signal. Further, these samples are not traceable or reproducible. Unlike standardized fabric samples, consumer-grade textiles are not specifically mindful of compositional uniformity. The use of uniform samples is especially important in the early stages of calibrating our Raman spectrometer to detect the cotton and polyester characteristic bands. Variability amongst the consumer grade batches may introduce uncontrolled variables. Consumer-Grade “pure” samples from suppliers such as JOANN Fabric and Crafts, Walmart, Micheals, etc., generally display a deceptive purity. Most available fabrics are blended, or treated with dyes, finishers, or softeners.

There are internationally recognized textile standards which govern textile material properties, as well as the methods of analysis. The International Organization for Standardization, specifically, ISO 1833 outlines specific standards to guide the production of quality, reliable textiles. Standardizing production in this context is specifically important when considering the numerous steps that bring textiles from their raw form into a finished good. ISO/TC 38/SC 23 regards the method of tests, terminology, and definition of fibers as well as the auxiliaries and chemical products required for processing and testing. The American Association of Textile Chemists and Colorists (AATCC) further

defines various fabric standards. AATCC TM20 and AATTM20A describe the qualitative and quantitative means of fiber analysis, respectively. AATCC TM94 defines the identification of finishes in textiles. Further standards are placed by the American Society for Testing and Materials, where the ASTM D7139-20 outlines the standard terminology for cotton fibers and the ASTM D5430-13 describes the standard test methods for visually inspecting and grading fibers. By determining the signature Raman bands for cotton and polyester, we must ensure our sample is produced under these standardized conditions to truly ensure the reliability of our system.

We will source our scientific grade textile by Testfabrics, Inc., which produces textiles in close accordance with ISO fabric standards. Most of the documentation describing ISO adjacent fabrics in 105 F 1-10 was taken from production data supplies by Testfabrics, Inc. Ultimately, the use of standardized materials, especially in the testing and calibration phase of the Raman spectrometer, directly impacts the integrity of TEXRAY for material identification. [115]

4.1.5 Standardized Characteristic Raman Spectra

Standardized Raman databases assess and describe the characteristic Raman bands of specific molecules under rigorous scientific and controlled conditions. Section 3.2.3 referenced the experiment results that amounted to the Raman shifts which correspond to the molecular activity within cotton and polyester. Across various studies, the measured Raman shifts from the molecular vibrations vary within 5 cm^{-1} . Where small changes in Raman shifts are scientifically informative, the unfortunate variations result from instrumental or random error [101]. Various outlets outline the standard Raman shifts resulting from molecular vibrations and rotations. While there are no explicit standards that pertain to the Raman spectra of textiles, we can reference Raman spectrum databases and standards on Raman shifts that correspond to the primary molecular structures seen in the fabrics.

The Spectral Database for Organic Compounds (SDBS) is compiled by the National Institute of Advanced Industrial Science and Technology (AIST). The measuring conditions of Raman are described as the following, “All of the Raman spectra were observed with a laser- Raman spectrometer in the region of 4000 cm^{-1} to 0 cm^{-1} , with an excitation wavelength of 4800 nm. The slit width was 100-200 micrometers. The states of the samples were liquid, powder, or grain.” [116]

While explicit signatures are not provided for cotton or celluloses, or polyester, one can look deeper in the smaller molecular chains. For instance, AIST provides various Raman spectral information for terephthalic acid. Terephthalic acid is a monomer used in the production of PET, of which they share structural features. Specifically, the compound zinc terephthalate, while chemically different from PET does share the same terephthalate backbone. The active vibrational modes from the aromatic rings and carboxylic acid groups will resemble those seen in polyester fibers. Specifically, the Raman spectrum seen in Figure 4.1.1 shows the aromatic C=C stretching expressed at $\sim 1610\text{ cm}^{-1}$ to 1620 cm^{-1} , this

is a comparable signature of the aromatic stretching seen in Section 3.2.3. As shown in the figure, the most intense characteristic bands are explicitly expressed.

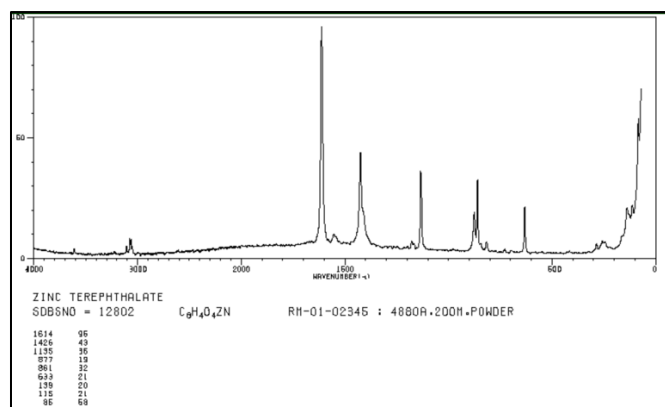


Figure 4.1.1 Raman spectrum of zinc terephthalate

SpectraBase is an online spectral database that hosts a variety of spectral information of organic compounds, inorganic compounds, polymers, and more. The data comes from various academic labs and commercial instruments, which one can expect these institutions to adhere to standard measurement practices. SpectraBase would still be useful to reference the characteristic Raman peaks and confirm the presence of functional groups. For instance, cellulose acetate phthalate, a derivative of cellulose will display comparable characteristic peaks to cellulose in cotton. Polysciences, Inc., Warrington, Pennsylvania, provided its Raman spectrum, Figure 4.1.2 (top). The following additional information is provided on the nature of the spectrum, “instrument name: Bio-Rad FTS 175C with Raman accessory, Raman corrections: Referenced to internal white light source; Baseline subtracted, Raman laser source: Nd:YAG, and technique: FT-Raman”. While peaks corresponding to explicit wavenumber values aren’t provided, interactive spectrums allow for the zoom into a graph and approximation of where the Raman peak lies. Similarly, while explicit PET polyester spectra aren’t provided, Polyester (Polyethylene Terephthalate), 30% glass fiber is (Figure 4.1.2, bottom), and can be used as a general reference for the characteristic activity of PET. [117]

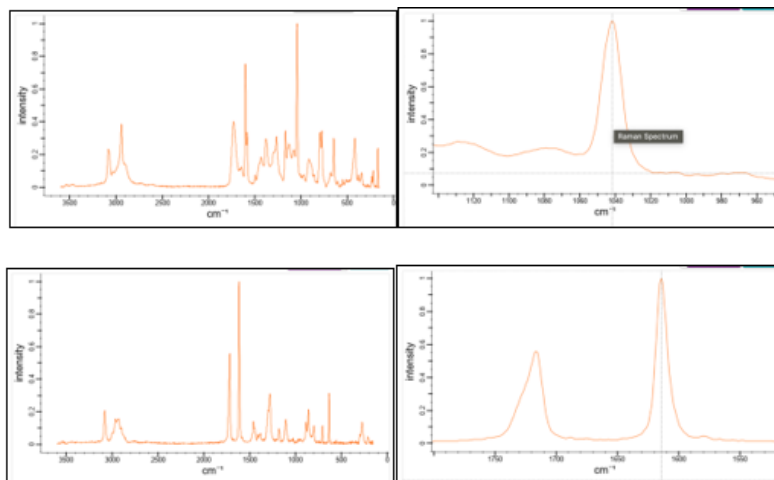


Figure 4.1.2 Top: Spectrum of Cellulose Acetate cellulose acetate phthalate. Bottom: Spectrum of Polyethylene Terephthalate (30% glass fiber)

Similarly, the Raman Open Database (ROD) is an open access collection of Raman spectrum. It was created in conjunction with the SOLSA2020 project and is funded by the European Union's Horizon 2020 Research and Innovation program under grant agreement No. 689868, it is considered an academic project that confirms reports in peer reviewed publications. The database references research papers and includes theoretical and experimental Raman data. The Raman bands of interest outlined in Section 3.3.2 were also determined from peer-reviewed research. However, this database further provides the .CSV files of the spectra, which would allow for supplemental concise Raman shift comparisons. [118]

The ASTM, the American Society for Testing and Materials, selected and analyzed several obtainable materials for Raman shift standards. Materials were assessed from six independent laboratories using a combination of dispersive and FT- Raman spectrometers. The Raman shift values were not preemptively administered, and they proceeded with the standard calibration process they had in place. The committee tabulated and published the results. This information, while not directly advantageous for identifying the Raman bands of fabrics, can be useful for the calibration process of the spectrometer. [101]

Using ASIT, SDBS, the ASTM, and the Raman Open database in conjunction with the research from Section 3.3.2, we will ensure the Raman spectrum corresponding to the material characteristics are as standardized and reliable as possible. Adhering to these practices will allow us to ensure accurate material identification with our Raman system.

4.1.6 PCB Standards

IPC standards are global standards utilized within the electronics manufacturing industry meant to ensure high-yield circuit boards and reduce communication between the designer and manufacturer. These standards outline design, assembly, packaging, interconnection, material, performance, and inspection specifications.

Specifically, IPC-2221 lays the groundwork for effective component placement on circuit boards built using organic PCB materials or a combination of organic and inorganic substrates. The standards set in IPC-2221 are considered generic and should be utilized in conjunction with more detailed standards specific to our PCB design. Such standards differ between rigid, flex, MCM-L and HDI boards. Because our design will implement a rigid circuit, we should consider IPC-2222: sectional standard for rigid boards alongside IPC-2221 to ensure that our circuit is held to as high quality of a manufacturing standard as possible.

One important aspect of IPC-2221 is that it defines the optimum distance between two conductors or nodes in the air, also referred to as clearance. It specifies the clearance required for different components, such as component leads, test probe sites, mounting hardware, and solder masks, among others. Similarly, it defines the recommended creepage, or the distance between conductors or nodes along the surface of the board. IPC-2221 recommends that clearance and creepage should both be maximized as much as possible to ensure there is enough space for the etch compensation of other features on the PCB. The distance between features should also leave room for conductor imperfections and other unpredictable factors. Following these guidelines will ensure that the PCB will still remain functional and high quality despite any unexpected discrepancies that may arise.

IPC-2221 additionally defines the recommended thickness of PCB traces based on the signal characteristics, current carrying capacity, and temperature. The thickness of the trace must be appropriate for the current carried so as to avoid burning the trace as the current travels through it. To similarly avoid damaging the PCB, this standard recommends various insulation tests to ensure that the PCB is properly protected against various factors such as short circuits, overheating, and corrosion [119].

Most importantly, IPC-2221 emphasizes how adhering to these standards is integral for realizing Design for Manufacturing (DFM). DFM rules define a set of guidelines that ensure a circuit board can actually be manufactured; this requires that the PCB design meets the fabricator's capabilities such as trace width, trace to copper, board edge to copper, etc. If a board design is sent to a manufacturer without considering their capabilities, they will simply inform you that there are DFM issues and that they require you to modify your design such that it can be fabricated more easily. This costs additional money and time that is very limited in a Senior Design project. To be certain that as little time is wasted as possible in the PCB acquisition process, it is integral that our design adheres to IPC-2221 and DFM principles [120].

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 objective. 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 most 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 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 dictate 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 532nm 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 532 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

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 [121]. which are the settings that control and optimize how the model generates responses to a user's input [122]. 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 [123]. 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 [124]. 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 [125].

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 [126]. 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 3.5.4. 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. McCeery. 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.

When looking for battery options Chatgpt was a good help in this. I prompted it requesting reliable battery supplies that can power the components needed in the TEXRAY system including the Raspberry Pi, laser diode, LCD, CCD, and ADC. The software responded back with a variety of options to choose from while providing benefits of each one. That allowed for a head start in the research for the power supply being able to narrow down which ones are worth conducting more of my own research on for the betterment of the project. The information provided was accurate when cross-referenced with my own conclusive research and Chatgpt proved to be a viable source.

When creating the schematic, if there was a moment upon confusion when designing and conclusions weren't able to be made from the datasheet, Chatgpt would be of great use. For example, when wiring the TCD1304DG CCD certain pins seemed unclear where they would be connected to. Chatgpt was prompted asking which pins should be connected for the ICG, which was then met with a logical response allowing me to complete the connections recommending that it be connected to the GPIO of the Raspberry Pi.

We discovered that Chatgpt, also has some limitations. When we were first attempted to obtain a 3D model for the TEXRAY, Chatgpt was used for inspiration. The AI software was prompted to design a 3D model for the project and through various attempts was unsuccessful. An image was produced, but evidently had several flaws seeming too complex to process. Nonetheless, that image was useful in giving an idea of what it could look like with the exclusion of the flaws. It also was able to give a layout of how components should be connected.

5.2 Perplexity

Another large language model search engine used on the project was Perplexity AI. What separates Perplexity from more standard search engines like ChatGPT is the use of reference links and source citations inside every text response. In this regard, the search thread feature is in the same category as websites like ChatGPT, but gives responses that are more visually similar to an encyclopedia entry than they are to other LLM search engines. This makes Perplexity a great option in helping find further resources on a given topic, due to the ability to function as both a question-and-answer service, as well as a more sophisticated web crawler. The search engine outputs a formulated answer, but arguably more important for our project, it gives the user every source that was drawn from in the response, allowing for easier verification of the information received and providing a jumping off point for further research. This could be done by compiling more information through asking the search engine further questions on the subject, followed up with digging through the reference links and source citations provided, and using them as the start of a larger list of resources to pull from throughout a project. Whether by researching further within the linked websites, or by looking for similar sources with common search engines. Perplexity also saves any thread, even when not signed in or without creating an account, unlike ChatGPT, where you must be signed in to see previous threads. This means that any prompt can be revisited by returning to the thread's URL (e.g. perplexity.ai/search/this-is-an-example-prompt-R1A2N3D4O5M).

5.2.1 Example

To give an example of Perplexity’s use, when researching effective implementation methods for dynamic time warping, I went to Perplexity to check if there were any options that I had not yet seen. I asked the search engine, “What are the most lightweight or fastest methods of implementing dynamic time warping?” and Perplexity responded with three recommendations. Each recommendation originates from an open-source project and is easily implementable in the form of a Python package or library. While the normal dynamic time warping process has a quadratic computational complexity ($O(n^2)$), each option described in the response has linear time and memory complexity ($O(n)$). The first method described was fastDTW, which, similar to the latter two methods, was created to maintain the accuracy of alignment calculations during the DTW process, but trim down the computational complexity. It does this by finding cost matrix pathways in higher and higher resolution through each iteration. In addition to this information the response also links a pdf of the report from the original project where the algorithm was created, the report is written by the same students who developed the algorithm, Stan Salvador and Philip Chan at the Florida Institute of Technology in 2004. The response also links to a page from PyPi.org, providing a description of a separate project, a Python package implementation of fastDTW by Kazuaki Tanida. The second recommendation is fastDDTW (derivative dynamic time warping), developed based on the same fastDTW algorithm described before. FastDDTW is open source as well, with the entire project available in a public github repository created and developed by Gail Rosen and Zhengqiao Zhao, who were students at Drexel University in 2020, when the project was developed. The project is based on another derivative dynamic time warping project from 2001, developed by Eamonn Keogh and Michael Pazzani at the University of California Irvine, as well as the 2004 fastDTW project mentioned before. The fastDDTW algorithm condenses processing items by eliminating unnecessary alignment calculations through dynamic derivative programming and Sakoe-Chiba band constraints. The github repository this information was pulled from is linked in the response. Finally, Perplexity recommends EDTW (efficient dynamic time warping), which works to eliminate cells unlikely to be part of a chosen pathway, in order to improve the complexity of cost matrix analysis. The source linked is the article the algorithm was first published in, taken from an issue of the Indian Journal of Science and Technology from 2016, written by Kumar Vasimalla, Narasimham Challa, and Manohar Naik. The response selected fastDTW as the best option of the three due to it being the most widespread in its usage, the easiest in its implementation, and the highest in average accuracy of the three [127]. This is the same conclusion that our group came to after testing all three methods and others using Google Colab.

5.3 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 a 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 which will be collimated, cleaned up by a bandpass filter, redirected by kinematic mirrors, and expanded by a beam expander, 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 3 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 4 into a slit, 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 [65]. 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 [128]. 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 [129]. Taking the beam diameter at this point encompasses 87% of the beam's total energy [130], 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:

$$f = \frac{\frac{\emptyset_{\perp}}{2}}{\tan\left(\frac{\theta_{\perp}}{2}\right)} \quad (7)$$

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 [131]. Because the divergence angles of a 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 [129]:

$$d_{\frac{1}{e^2}} \approx 1.7d_{FWHM} \quad (8)$$

$$d_{FWHM} \approx \frac{3 \text{ mm}}{1.7} = 1.76 \text{ mm} \quad (9)$$

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:

$$f = \frac{\frac{1.76 \text{ mm}}{2}}{\tan\left(\frac{22.5^{\circ}}{2}\right)} = 4.435 \text{ mm} \quad (10)$$

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:

$$NA_{diode} = \sin\left(\frac{\theta_{\perp}}{2}\right) = \sin\left(\frac{22.5^{\circ}}{2}\right) = .195 \quad (11)$$

Equation 6.1.4 NA of laser diode

For this reason, we selected DTR-G-2 as our collimating lens. This aspheric 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:

$$d = (4 \text{ mm}) \times \tan\left(\frac{22.5^{\circ}}{2}\right) \times 2 = 1.591 \quad (12)$$

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

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 would 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°:

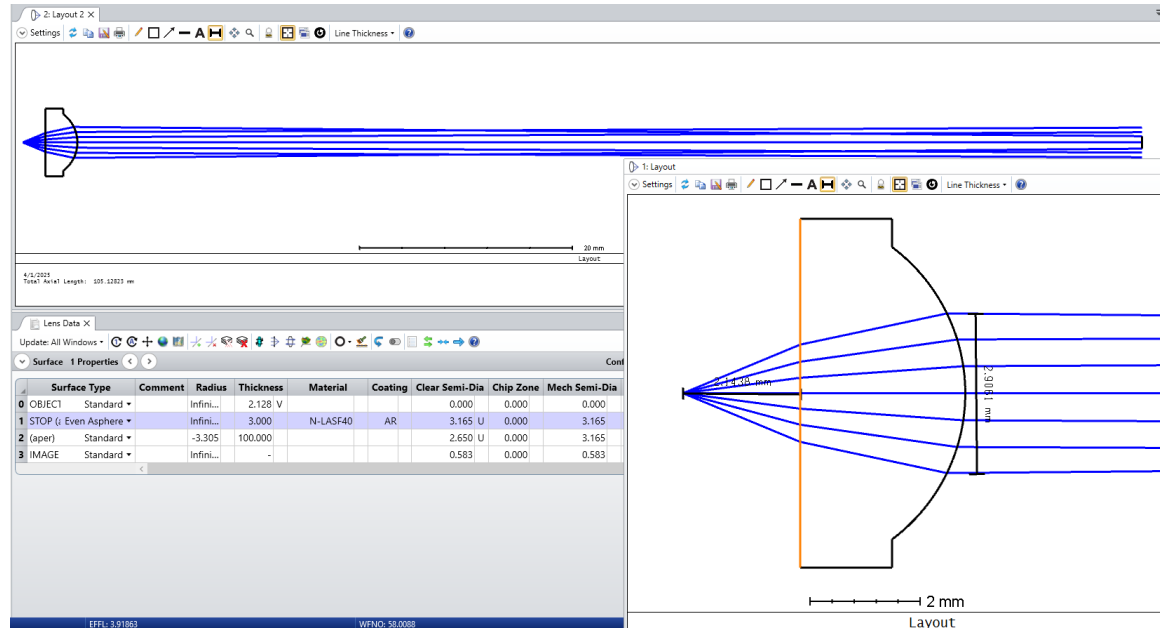


Figure 6.1.1 Zemax simulation of the chosen collimating lens

This simulation indicates that in order to collimate our 532 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.

Though we initially made all of the above considerations anticipating the integration of a highly divergent laser diode into our system, we later decided to integrate the Q-BAIHE DPSS laser module, which already has an integrated collimating lens. Additionally, though we made considerations to achieve a 3 mm beam, the actual collimated beam size of our laser was 1 mm in diameter, affecting following calculations.

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 aimed for a spot size of 5 μm , as the smaller the spot size is, the better. Knowing our ideal spot size, we then used the following equation to estimate the appropriate focal length needed in our focusing lens [132].

$$f = \frac{2\omega_0\pi D}{4M^2\lambda} \quad (13)$$

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 [133]. 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 would be approximately 2.9 mm with a laser diode, we solve for the focal length:

$$f = \frac{2(2.5 \mu\text{m})\pi(2.9 \text{ mm})}{4(1.2)(520 \text{ nm})} = 18.25 \text{ mm} \quad (14)$$

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 chose 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 the calculated value, meaning our spot size would ideally be able to focus to even smaller than 5 μm . After having chosen this lens, we calculate our new anticipated spot size:

$$2\omega_0 = \frac{4M^2\lambda f}{\pi D} = \frac{4(1.2)(532 \text{ nm})(18 \text{ mm})}{\pi(2.9 \text{ mm})} = 5.05 \mu\text{m} \quad (15)$$

Equation 6.1.8 Calculation of new spot size

Thus, in a perfect scenario, our focused spot diameter under these conditions would be approximately 5.05 μm , a perfect spot size for Raman spectroscopy. However, all of these considerations were made assuming we had collimated our laser to a 3 mm beam diameter. In reality, because our laser beam diameter was only 1 mm, and we had already purchased the 18 mm focal length lens, the resulting focused spot size would be larger:

$$2\omega_0 = \frac{4M^2\lambda f}{\pi D} = \frac{4(1.2)(532 \text{ nm})(18 \text{ mm})}{\pi(1 \text{ mm})} = 14.63 \mu\text{m} \quad (16)$$

Equation 6.1.9 Actual resulting spot size

Though technically this is still acceptable for Raman spectroscopy, in practice it was difficult for us to achieve any results with this spot size. Thus, to achieve the tightest spot possible and maximize Raman signal generation, a beam expander was implemented into the illumination optics.

6.1.3 Beam Expander and New Focused Spot

As previously mentioned, larger beam diameters will be able to focus to tighter spots than small beam diameters when passed through a focusing lens. This is because when light is contained in a small area, it will diffract or diverge. Though, because a perfectly collimated beam should be diffraction limited, a laser beam confined to a small collimated diameter will only experience divergence based on said diameter. Thus, increasing the diameter of this collimated beam would increase the area to which the light is confined, decreasing the beam divergence. This means that upon incidence to a focusing lens, the beam can be concentrated into a smaller area [134].

The smallest optic in our setup when making these considerations was the 18 mm diameter focusing lens. Thus, to achieve the tightest spot possible while avoiding wasted laser power, we decided to expand the beam to as close to 18 mm in diameter as possible. In hindsight, this is something we should have done differently and chosen a smaller diameter, as overfilling a lens can lead to aberrations, which will be seen later on. To achieve the 16 mm diameter, we implemented a Galilean beam expander as opposed to a Keplerian beam expander. The Galilean configuration utilizes a negative lens to diverge a collimated beam and a positive lens to re-collimate the diverging beam, with the distance between the lenses equaling the difference of their focal lengths. On the other hand, the Keplerian configuration utilizes two positive lenses separated by the sum of their focal lengths [135]. The Keplerian design has an intermediate focus between the lenses while the Galilean does not. We decided to implement the Galilean configuration as it is more compact. Keeping in mind limitations on the sizes of optics available, we selected a -6 mm focal length bi-concave lens and a 100 mm focal length bi-convex lens, enabling a distance between them of 94 mm. The beam expansion ratio equals the focal length of the output lens divided by the focal length of the input lens, resulting in an expanded beam diameter of 16 mm. A quick Zemax simulation demonstrates this configuration with our chosen lenses:

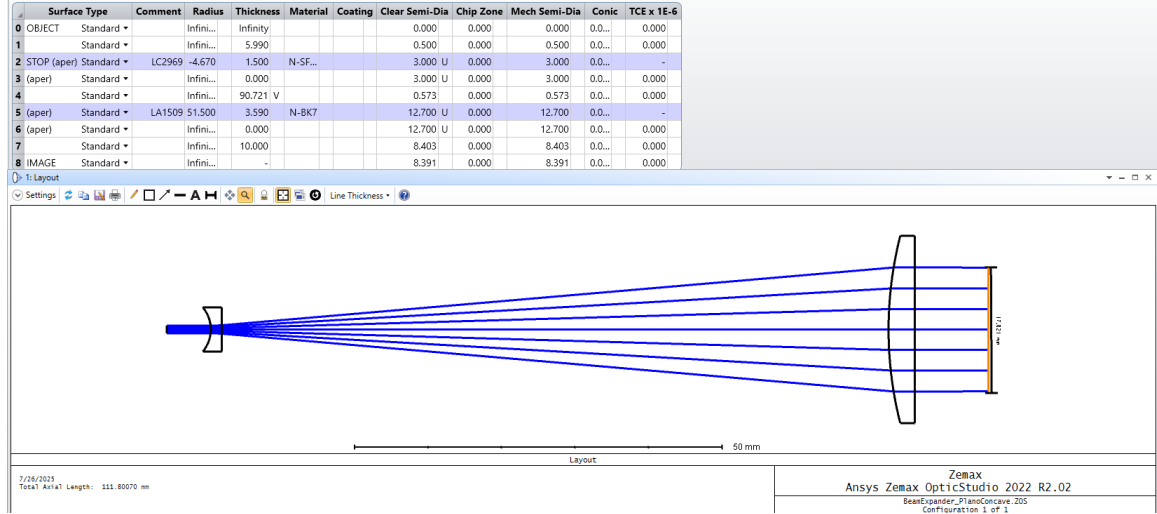


Figure 6.1.2 Beam expander simulation

The Zemax simulation indicated a collimated beam diameter of 16 mm. However, after measuring the beam diameter in our physical system, it was closer to 13 mm. This is likely because, though we roughly measured the laser beam's original diameter to be approximately 1 mm, it was likely smaller than this as we did not use a very precise method of measurement. We can determine the new spot size after focusing the 13 mm beam with an 18 mm focal length lens onto the sample:

$$2\omega_0 = \frac{4M^2\lambda f}{\pi D} = \frac{4(1.2)(532 \text{ nm})(18 \text{ mm})}{\pi(13 \text{ mm})} = 1.13 \mu\text{m} \quad (17)$$

Equation 6.1.10 New focused spot size after beam expander

Thus, assuming perfect conditions, our focused spot diameter would be approximately 1.13 μm . However, as was mentioned when discussing collimating lenses, the 18 mm focal length lens is designed for a different wavelength of 587.6 nm, and thus the focal length is similarly designed for the specific wavelength of this lens. Because our laser line is 532 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 spot diameter differing from 1 μm as calculated. 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 13 mm:

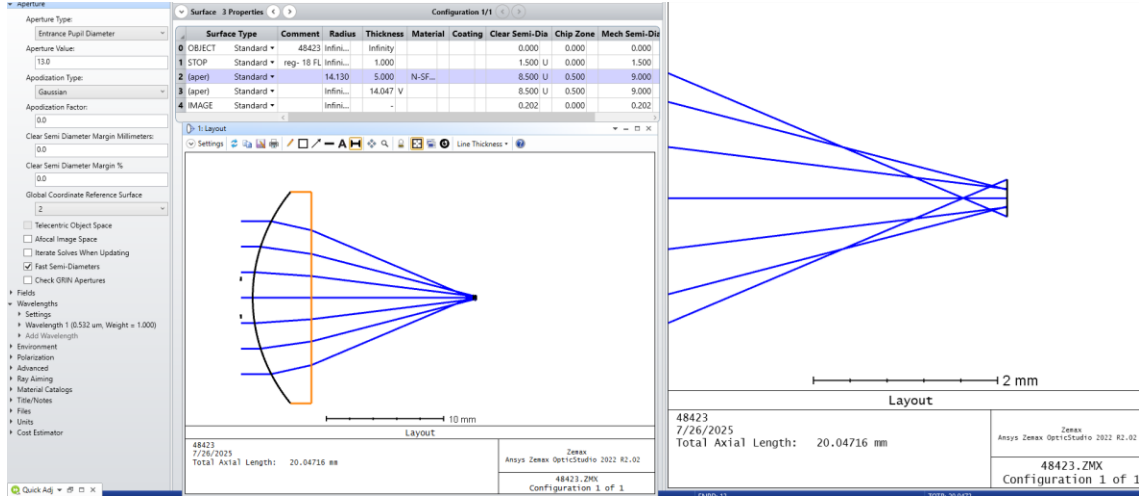


Figure 6.1.3 Focusing the expanded beam to a point

As mentioned earlier, in hindsight we should have expanded the beam to a smaller diameter than the intended 16 mm. This is because it is generally recommended to avoid a beam diameter larger than 80% of the lens diameter, as this can lead to overfilling and aberrations, as shown by the spherical aberration present in the Zemax simulation. This means that though we did achieve a tight spot size, the amount of laser power focused at that tighter spot is reduced, because light passing through the lens at different distances from the axis focus at different lengths. Ultimately, our system can still function in this manner, but for future optimization these factors should be considered.

6.1.4 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 was planned to be used to couple our Raman signal into a multimode fiber which would 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:

$$EFL_{lens} = \frac{\phi_{beam}}{2 \times NA_{fiber}} \quad (16)$$

Equation 6.1.11 EFL for coupling light from lens into fiber

where $\varnothing_{beam}$ 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 3, 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 chose for our system was 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 had a core diameter of 200 μm , and a numerical aperture of .22. Now knowing this information, we used equation 6.1.12 to determine the ideal effective focal length of our coupling lens:

$$EFL_{lens} = \frac{18 \text{ mm}}{2 \times .22} = 40.91 \text{ mm} \quad (17)$$

Equation 6.1.12 Calculation of EFL for coupling lens

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

The lens we had 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 3 (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 μm). 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.

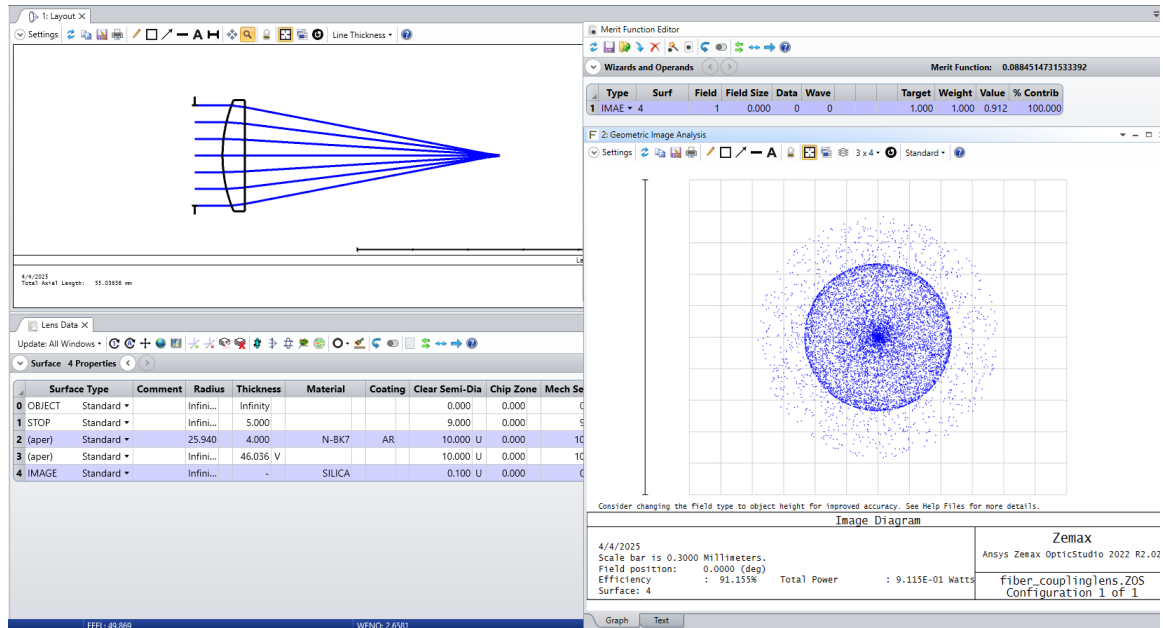


Figure 6.1.4 Simulation of coupling light into fiber via lens

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.

However, ultimately our team decided to remove the fiber from our design and did not implement these choices, opting to instead focus light directly from a focusing lens onto the spectrometer slit to avoid power loss from the fiber and simplify our design.

6.2 Spectrometer Design

This section will be a discussion on the hardware components and design that were implemented into the spectrometer portion of TEX-RAY. In original design considerations, a Czerny-Turner spectrometer configuration was going to be implemented. Though this is a traditional spectrometer configuration, we ultimately moved forward with the lens-grating-lens configuration which provides simpler system integration and sufficient throughput. The lens-grating-lens spectrometer configurations consists of a focusing 50 mm achromatic lens, a planar reflective-ruled diffraction grating, and another 50 mm achromatic collimating lens. With careful selection of the optical components and design constraints, the two achromatic lenses paired with the reflective grating allowed for the detection of our desired spectral range with the highest possible spectral resolution, aberrations provided.

The fundamental working principle begins with the focused Raman signal from the probe optics being coupled onto the slit. This initial slit determines how much light will enter the

spectrometer. The first achromatic lens collimates the light onto the grating. The Raman light is dispersed into its constituent wavelength components and is reflected off the diffraction grating onto the second achromatic lens. This second achromatic lens will focus the light onto the CCD. The pixels of the CCD will be illuminated by the separated wavelength range. Figure 6.2.1 is a preliminary Zemax simulation of the spectrometer, which helped guide design choices.

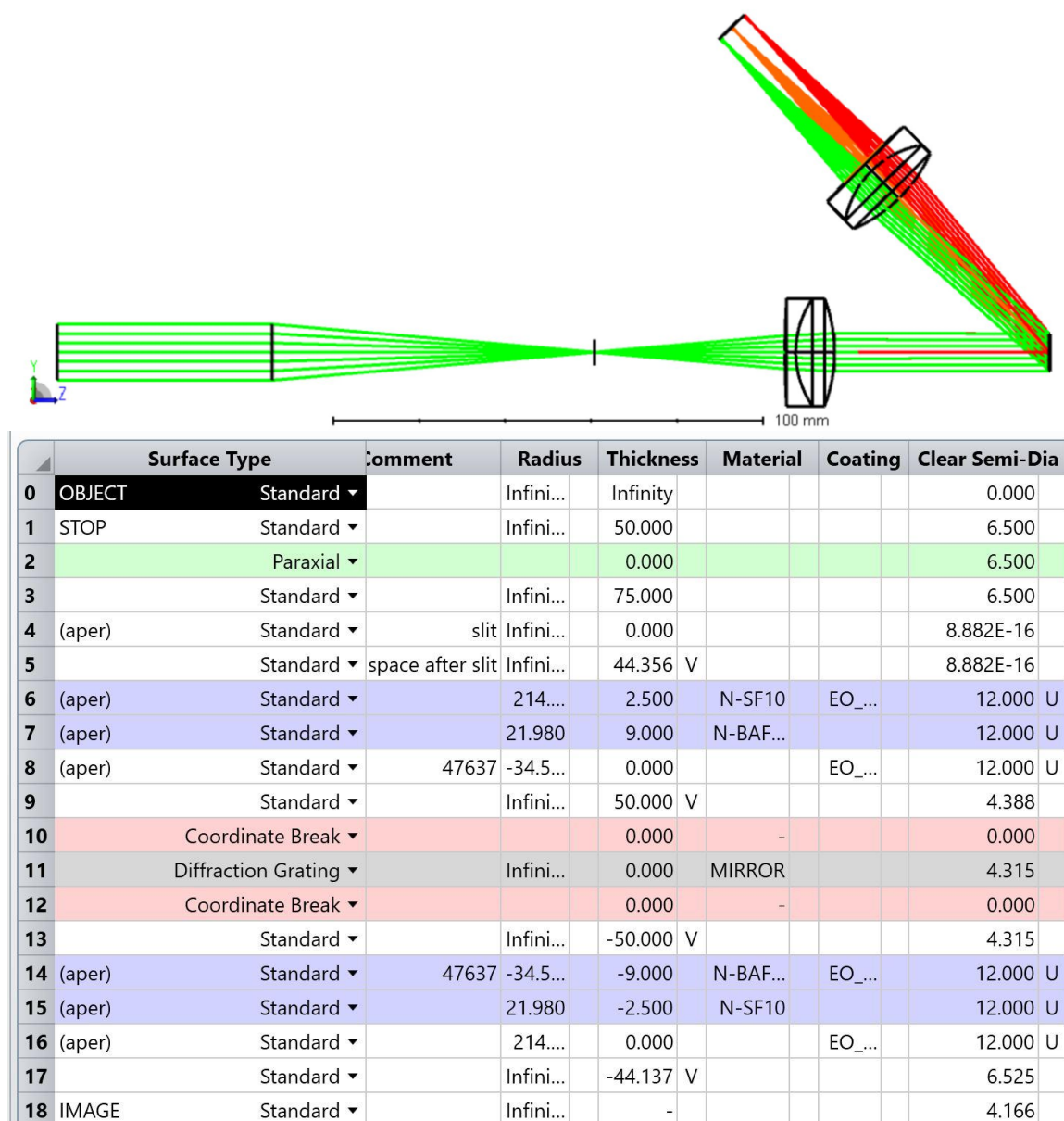


Figure 6.2.1 Zemax simulation of spectrometer configuration

6.2.1 Coupling Into the Spectrometer

The F/# is regarded as the ratio of the focal length of the lens to the diameter of the aperture. The F/# in this context helps defines the spectrometer's light collection capabilities and therefore the magnitude of the Raman signal. The general goal is to keep the F/# minimized while retaining dispersion and flat field performance. Lowering the F/# of our system increases light collection at the sample, and overall sensitivity of our system—this results in a shorter focal length system or larger optics. These quantities can increase aberrations and stray light. [101]. With this being said, there are two forms of optimization of the spectrometer which regard the F/# that could impact the spectral resolution or spectral range of the spectrometer. The focal length of the condenser lens, the lens that couples the light onto the entrance slit of the spectrometer, should be matched to the focal length of the collimating lens within the spectrometer. This will contribute to a properly collimated beam incident onto the grating and ensure throughput of the light. Another optimization involves matching the F/# of the illumination optics to the spectrometer. Matching the F/# of the illumination optical system to the spectrometer can increase the illumination of the grating therefore increasing the resolvability of the spectrometer. In this system, we focused on the latter approach of matching the F/# of the probe optics and spectrometer system. This allowed us to customize the condenser lens choice that could be compatible with various focal length lenses in the spectrometer system. Equation 6.2.1 [136] provides the respective F/# equations, and how they relate to NA, the numerical aperture, f , the focal length, D , the diameter of entrance pupil, and θ the half angle of the focused light.

$$F \text{ number} = \frac{f}{D} = \frac{1}{2 \sin(\theta)} = \frac{1}{2 * NA} \quad (18)$$

Equation 6.2.1 F/#

To ensure optimal coupling between the probe optics and the spectrometer, we calculated the F/# on both sides of the system using the focal length of the lenses and the beam size diameters using Equation 6.2.1. The 75 mm condenser lens focuses a 13 mm beam onto the entrance slit, resulting in an F/# of 5.769. After the slit, the diverging beam is collimated by a 50 mm lens, the resulting approximate beam diameter at the focal length is 8.776 mm as specified through Zemax in figure 6.2.1, resulting in an F/# of 5.69. Overall, the calculated F/#s theoretically confirm sufficient coupling of the probe optics to the spectrometer system.

6.2.2 The Slit

The entrance slit of the spectrometer controls how much light enters the spectrometer system and 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. The appropriate slit width can be determined with Equation 6.2.2 [137]. Using a 50 mm collimating lens (L_c), a 0° grating incident angle (α), and a target resolution ($\Delta\lambda$) of 0.6 nm results in a calculated slit width of 36 μm . There are no precision slits commercially available at that size. There are

variable slits, however, at a cost. We can reasonably choose the next commercially available slit width option at 50 μm , which results in a theoretical resolution of 0.83 nm.

We initially aimed to implement a 25 μm slit to achieve a theoretical spectral resolution of approximately 0.5 nm. However, we completed a feasibility test to assess the power loss of the 25 μm slit versus the 50 μm slit once integrated into the spectrometer system. Using a 0.87 mW green laser pointer as the source, we measured the power of the diffracted first order at the detector plane. With a 25 μm slit the resulting power was 73 μW and through the 50 μm slit the resulting power was 208 μW . We decided using the 25 μm slit for increased resolution was not worth the power loss.

$$w_{slit} = \frac{G\Delta\lambda L_C}{\cos(\alpha)} \quad (19)$$

Equation 6.2.2 Width of the slit

Given the Raman signal is focused onto the slit, we can assess the divergence from a 50 μm wide slit using Equation 6.2.4 [139]. We will use our longest expected wavelength 633 nm, which corresponds to a Raman shift of 3000 cm^{-1} , which would have the highest divergence. The resulting angular spread, θ , would be 0.01266 radians or 0.75°. Therefore, we can assert that the width of the slit will not impede the divergence on the beam, but only improve the spatial resolution of the beam.

$$\theta = \frac{\lambda}{\omega} \quad (21)$$

Equation 6.2.3 Divergence through a single slit

6.2.3 The Collimating Lens

The collimating and focusing lenses were selected based on Zemax simulations evaluating the spectrometer's performance with various plano-convex and achromatic commercial lenses. We ultimately implemented the Edmund optics #47-637 50 mm achromatic lens, as it produced the most near-diffraction limited spot at the detector plane. As the spectrometer operates over a range of wavelengths, achromatic lenses were critical to suppress chromatic aberrations.

The collimating lens is responsible for taking the diverging light from the slit and sending collimated light towards the reflection diffraction grating. Having a collimated beam incident upon our diffraction grating is important to avoid unwanted dispersion. To collimate the beam in the spectrometer, the focused spot on at the slit must be located at the lens's focal length.

The diameter of the collimated beam before it's incident upon the condenser lens in the probe optics is 13 mm. The newly collimated spot after diverging from the slit is approximated through Zemax as 8.766 mm. Therefore, we know that the 25 mm optic diameter can comfortably compensate for this spot size. The space between the collimating lens and the grating can be changed to optimize our system.

6.2.4 The Diffraction Grating

The collimated light from the 50 mm lens will land incident onto the diffraction grating, and the placement of which determines the resulting dispersion activity. The incident and diffraction angles of the grating were optimized to enable the ideal spectral resolution and spectral range of our spectrometer. While we originally optimized the system in Zemax for a -10° incident angle, we found that we could not fit our 3D printed mounts when the resulting diffracted beam was at the -1^{st} order at 29° . While this configuration would provide the highest efficiency amongst our options as seen in the in Section 9.5, we chose to optimize around our mounts. This led to the implementation of a 0° angle of incidence. Although this is unconventional for a grating configuration, testing demonstrated that keeping the grating perpendicular to the input beam allows for a balance of efficiency and mounting convenience in capturing the first-order diffracted beam.

To determine the linear spread of wavelengths across the detector we can use Equation 3.6.2 paired with Equation 6.2.6 [141]. Equation 6.2.6 describes the linear position of the diffracted beam relative to the optical axis, where β is the angle of diffraction, and x is the focal length of the focusing mirror. This is a relevant assessment metric as we could determine the diffracted wavelengths that will be received by the detector.

With a 0° angle of incidence, the angle of diffraction for 540 nm is 40.3° and for 640 nm is 50.17° .

$$y = x * \tan(\beta) \quad (23)$$

Equation 6.2.4 Linear position of diffracted wavelength

The resulting theoretical linear spread on the detector is 16.2 mm.

6.2.5 The Focusing Lens

To proceed with a symmetrical design of the spectrometer, the focal length of the focusing mirror will be the same 50 achromatic lens. The incident angle onto the focusing mirror will vary depending on wavelength. Therefore, to have proper focusing of the diffracted Raman wavelengths onto the detector, as discusses earlier, we chose to use an achromatic lens.

6.2.6 Theoretical Spectrometer Performance

With the physical design of the spectrometer determined, we estimated its expected spectral resolution and range. The design process was iterative, where initial resolution estimates guided component choices and testing informed changed to performance and calculations.

The reciprocal linear relationship describes how widely a Raman shift increment is spread across a focal plane— where a lower dv/dl corresponds to a higher spectral resolution and

a smaller dv/dl further implies a smaller receivable range of wavenumbers. The reciprocal linear dispersion of a spectrometer is provided by Equation 6.2.7 [101]. Where d is the distance between rulings on the diffraction grating, m is the diffraction order, L_F is the focal length of the focusing lens in the spectrometer, β is the diffraction angle, v_0 is the absolute wavenumber, and v_j is the lowest Raman shift to be observed. Higher density gratings, like one with a groove density of 1200 lines/mm correlates to higher dispersion. Inserting 615 cm^{-1} (550 nm) into v_j , which has a corresponding diffraction angle of 40.3° , results in a reciprocal dispersion value of $435 \text{ cm}^{-1}/\text{mm}$. The reciprocal linear dispersion relationship could then be applied to Equation 6.2.8 [101] to provide an estimated spectral resolution, as it describes the Raman shift increment observable within a given pixel width. Given the $8 \mu\text{m}$ pixel width, Equation 6.2.8 results in an approximate theoretical spectral resolution of 16.464 cm^{-1} or 0.58 nm .

$$\frac{dv}{dl} = \frac{d \cos(\beta) (v_0 - v_j)^2}{m L_F} \quad (24)$$

Equation 6.2.5 Reciprocal linear relationship

$$dv = \left(\frac{dv}{dl} \right) * Wp \quad (25)$$

Equation 6.2.6 Spectral resolution for a given pixel width

There is a finite range of widths observable from the spectrometer limited by the width of the CCD. The Raman shift range observable with a detector width is approximated with Equation 6.2.9 [101]. We previously determined the expected spectral range and explicitly noted that the linear spread of the diffracted Raman wavelengths will not extend to the entire size of the detector. Section 6.2.3 calculated an expected 16.2 mm wavelength spread across the detector.

To further determine the full extent of the expected wavelength range, we can use Equation 6.2.9 [101]. Provided the detector width is 29.1 mm; the resulting spectral range is 8379 cm^{-1} , which translates to receivable wavelengths up to approximately 959 nm. While this is limited by detector capabilities, we know our 90 nm desired spectral range is being captured.

$$\text{spectral range} = v_0 - v_j - \left[(v_0 - v_j)^{-1} + \frac{dWd}{mL_F} \right]^{-1} \quad (26)$$

Equation 6.2.7 Spectral range

Aberrations

Inherently, the Czerny Turner spectrometer design eliminates chromatic aberrations due to its use of mirrors. However, aberrations still pose themselves as a significant threat to the spectral resolution and signal-to-noise ratio of the received signal. Since this is an off-axis design, the aberrations in other optical planes must be considered as well. While the Czerny-Turner was going to be our original configuration, we moved forward with the lens-grating-lens configuration. The use of lenses does introduce chromatic aberrations,

however the use of achromatic lenses works to suppress such. Further, the 0° incident angle can help reduce off-axis aberrations [142]

Stray Light Reduction

Stray light is a considerable detriment within a Raman spectrometer for its tendency to interfere with the Raman scattering. The sources of stray light within the spectrometer are rooted in optical imperfections, dust, and reflections from the internal components. Smaller focal length and F/# spectrometers, like the one designed, are more vulnerable to the detriments of stray light, as scattering and reflections can more efficiently reach the detector. While the primary measure for stray light reduction comes from the illumination optics eliminating the laser line wavelength, additional measures can be implemented in the spectrometer design to further minimize stray light. Beginning with the slit, a precise slit with a blackened coating may be considered. Baffles and beam dumps can be integrated into the off-axis areas and capture the unused orders that dispersed from the reflection grating. The spectrometer will be enclosed with blackened internal structures to further absorb stray light. Careful alignment will be critical in this context as to not cut off the beam and create unwanted reflections. Accounting for stray light in the design process will be critical as to maintain our Raman signal [101].

6.3 PCB Schematic

6.3.1 Voltage Regulators

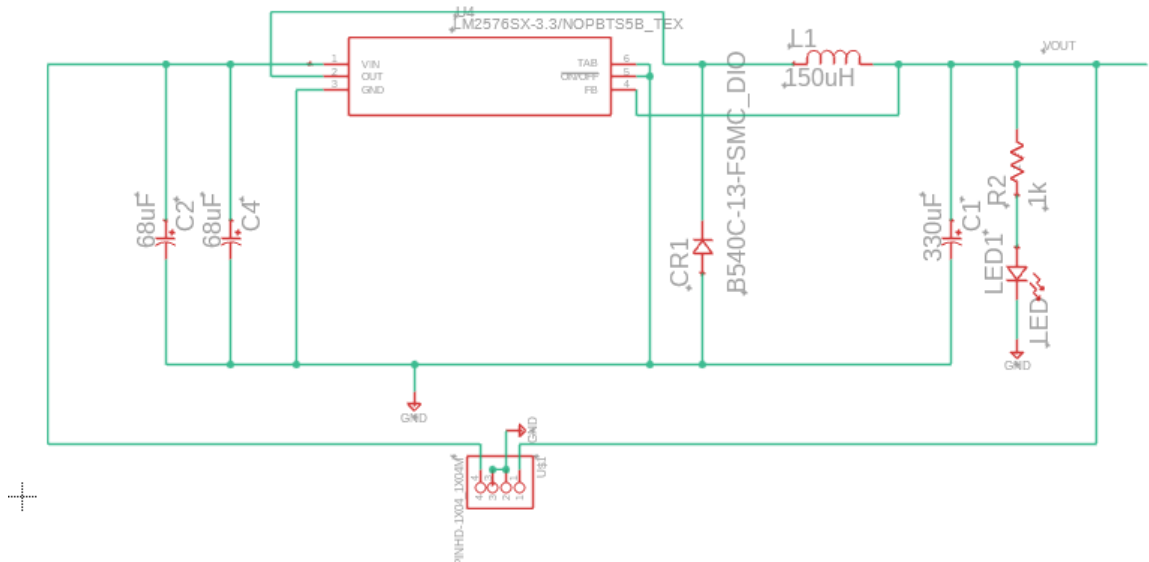


Figure 6.3.1 Voltage Regulator 3.3 Volt

This schematic shows the 3.3 volt regulator. The input voltage will be 9 volts and the purpose of this is to take that voltage and output a regulated 3.3V output. Once the task is

completed the 3.3V output now feeds into the ESP32 input voltage pin allowing for it to receive a proper voltage supply.

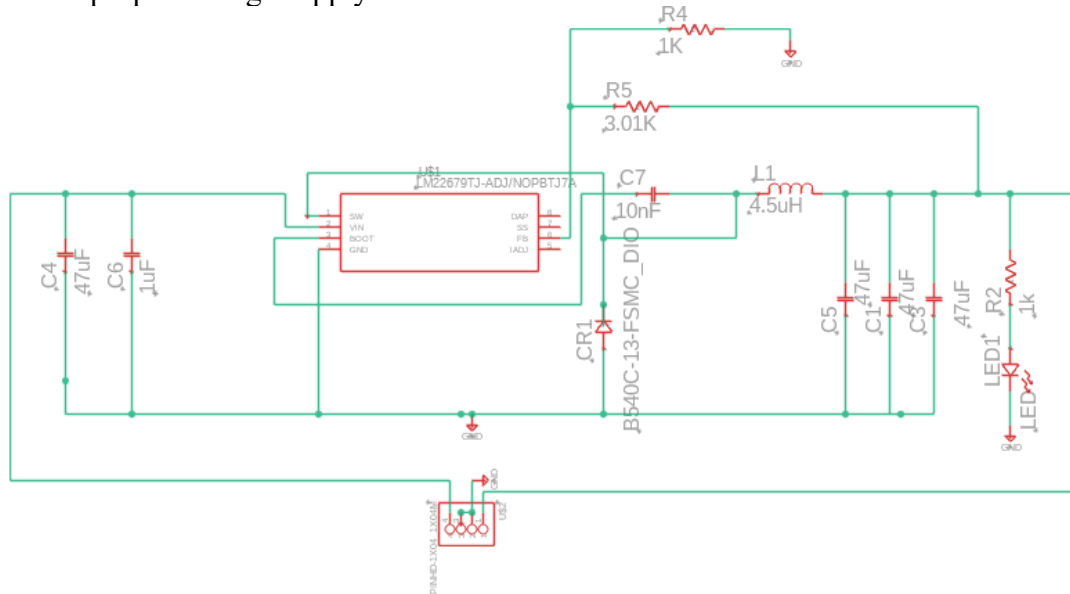


Figure 6.3.2 Voltage Regulator 5 Volt

This circuit uses a LM22679-ADJ voltage regulator to step down the input voltage to a stable adjustable output. The voltage is decided by the feedback resistors, being R4 and R5, and this allows for the output to be controlled for our needs, which would be a 5.4V output. The regulator also allows for a high current output, which is crucial because the objective of this regulator is to power the Raspberry Pi 5 which can draw up to 5A under operation.

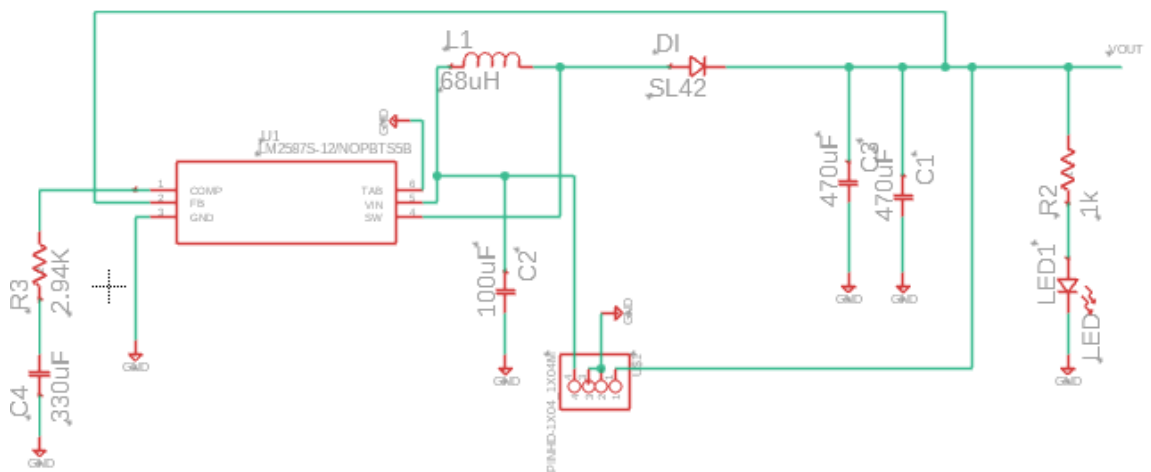


Figure 6.3.3 Voltage Regulator 12 Volt

Here is the schematic of the 12 Volt regulator using the LM2587. Oppose to the other regulators, this will be a boost regulator, taking the 9V input and raising it to 12V. This regulated voltage supply will be routed to the positive terminal of the laser.

6.3.2 Main Board

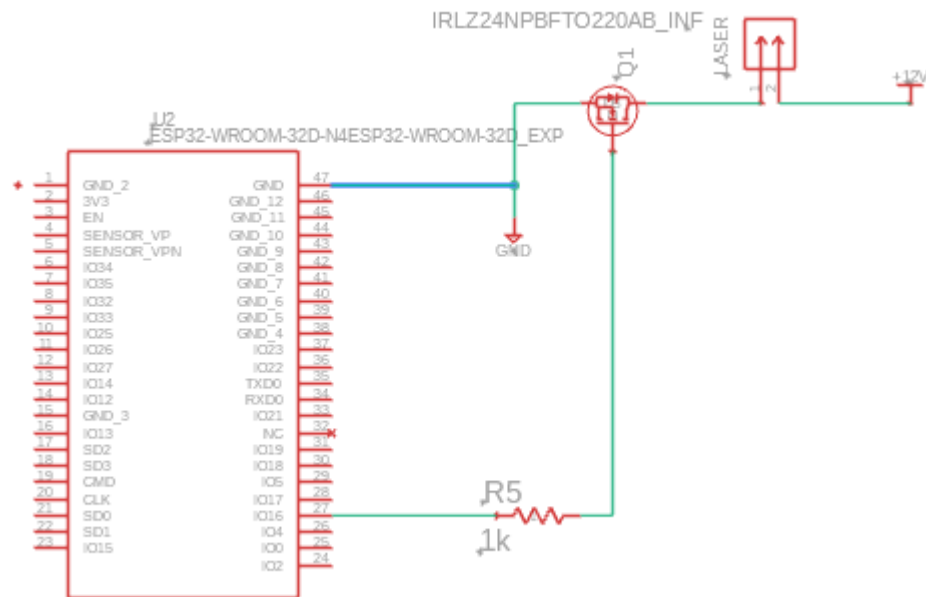


Figure 6.3.4 MCU to Laser Diode

The laser diode will be connected to a transistor which is connected to the ESP32 acting as a switch ensuring allowing the user to dictate when or when not the laser will need to be in use via software. Upon analysis of the spectrum the laser will need to be on. Once the spectrum is collected, the laser no longer needs to be on. The integration of the laser is simple, only having a positive and negative terminal while pin 3 is not connected.

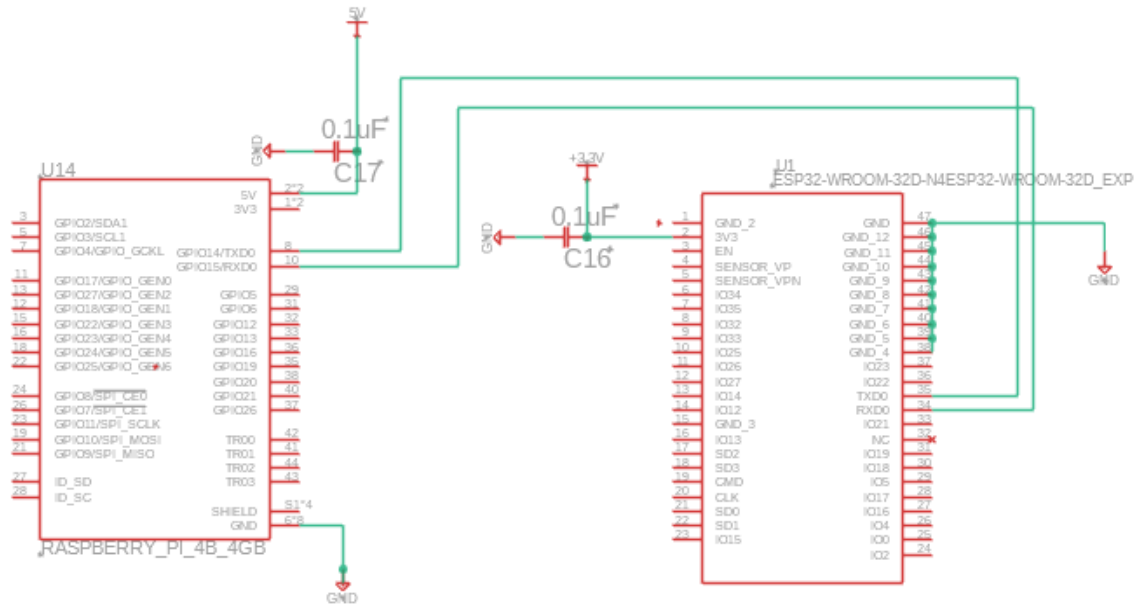


Figure 6.3.5 MCU to Raspberry Pi

In this setup, the Raspberry Pi and the ESP32 are connected to allow communication between each other. The Raspberry Pi receives a regulated 5V input through pin 2, and a regulated 3.3V input is used to power the ESP32 module. A 0.1 μ F capacitor is placed on each power line (C17 and C16) to reduce noise and stabilize the voltage being supplied. For communication, GPIO14 (TXD) and GPIO15 (RXD) from the Raspberry Pi are linked to the RXD and TXD lines of the ESP32, allowing for communication between the two boards. All ground pins are tied together to keep a common reference point, making sure signal integrity is maintained. This connection allows the Raspberry Pi to send commands or receive data from the ESP32, which will have the data received from the CCD.

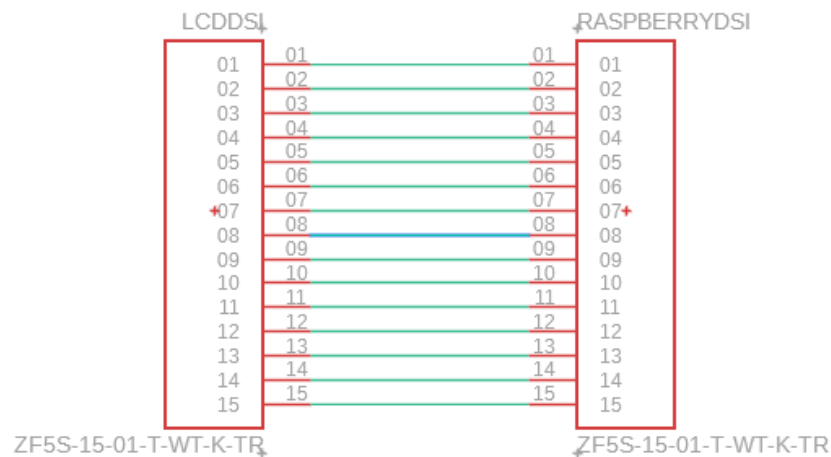


Figure 6.3.6 Raspberry Pi to LCD

This connection demonstrates the connection between the Raspberry Pi and the LCD. The LCD will be an external component from the PCB, however this portion of the schematic

allows for a visual representation of the pin routing. The Raspberry Pi and LCD both use DSI connections making for a seamless and simple connection.

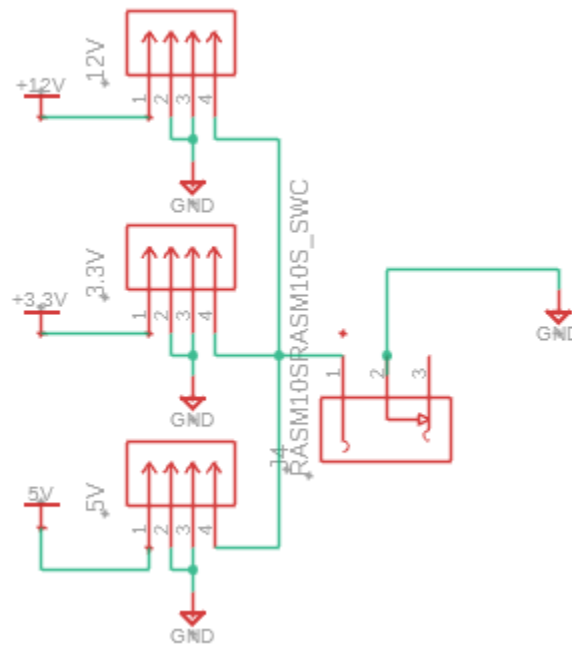


Figure 6.3.7 Battery to Regulators

The 9 volt LiFePO₄ battery source will be connected to a switch as an external component. This will then lead to the necessary 12 volt, 3.3 volt, and 5 volt switching regulators which will adjust the voltage and regulate a 12V, 3.3V, and 5V output to supply to the inner components.

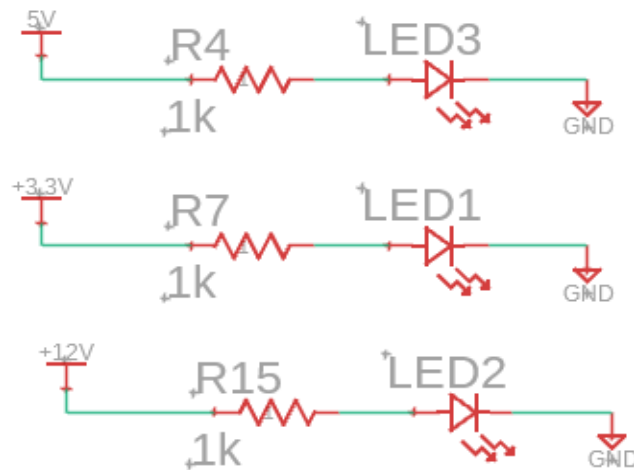


Figure 6.3.8 LED Implementation From 5V

These LEDs will be implemented into the main PCB to show that the board is on and functioning from the power supply and voltage regulators. Each LED receiving different voltages will emit a different color (red for 12V, blue for 3.3V, and green for 5V) indicating

the components that require voltage from their respective supply are being properly powered.

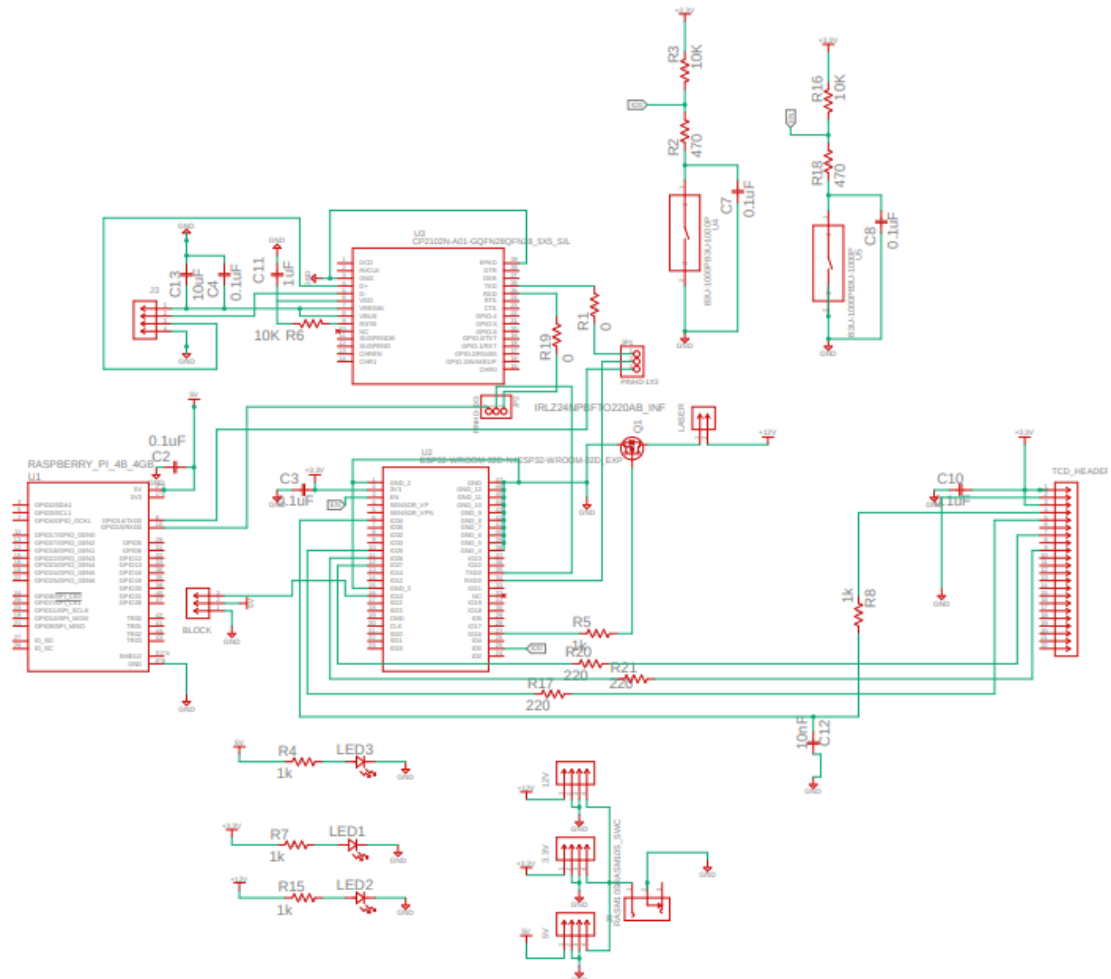


Figure 6.3.9 Complete Main Board Schematic Layout

This displays all the components and connections previously discussed and shows how they will be integrated together. There is also the addition of the CP2102 connections being made which will serve as a USB-to-UART bridge to allow for programming of the ESP32. It should also be noted that although there are connections made at for the TCD1304DG sensor, but on this board they ultimately were left unconnected as the TCD1304dg connections were made elsewhere.



This schematic is the connections made for our STM32. The schematic was created by referencing the STM32 Black Pill development board schematic found online. The purpose was to make this board identical to the Black Pill reference to swap out the development board that has been used during our testing with the newly designed board with ease.

model of our housing is shown in figure 6.4.1, and the eventual real-life result is shown in figure 6.4.2.

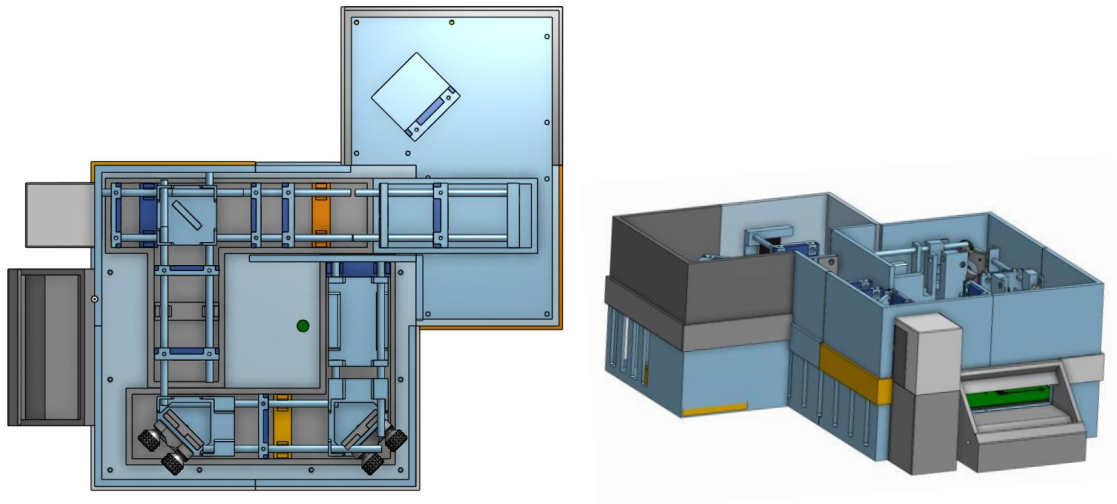


Figure 6.4.1 3D Model of housing design for TEX-RAY

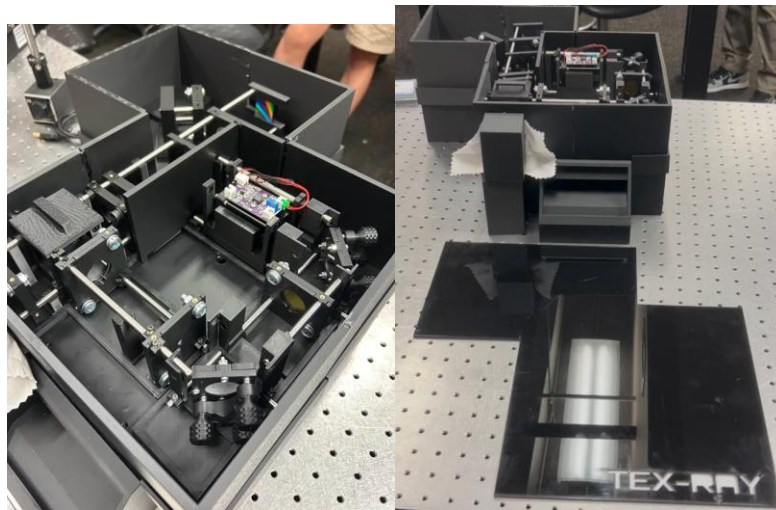


Figure 6.4.2 Implementation of 3D modeled design.

7 Software Design

7.1 Use Case Diagram

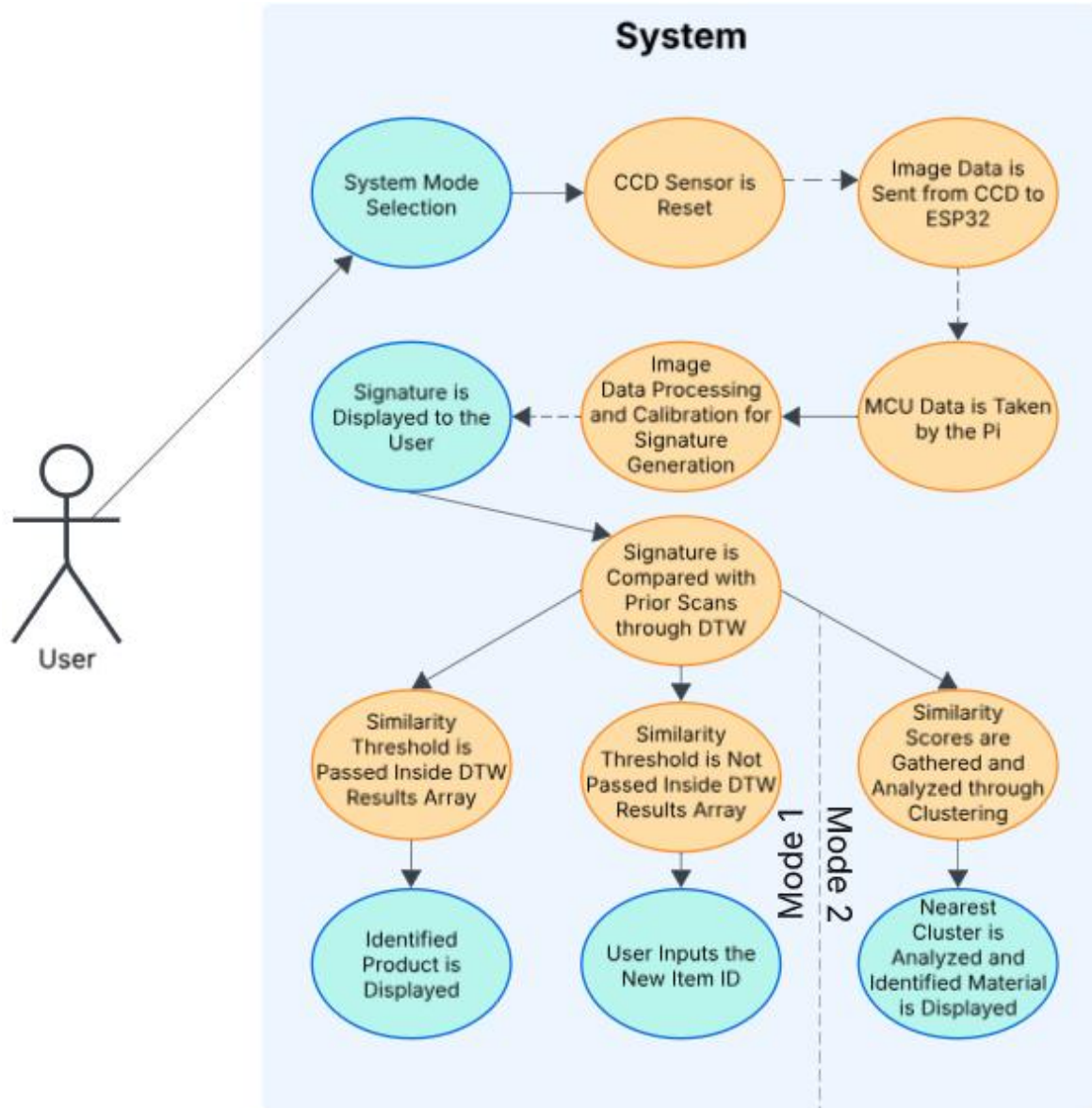


Figure 7.1.1 Use Case Diagram

7.2 Software Summary

The user's interaction with the system begins with a 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 selection is between two options for the mode of the system, choosing between settings of "Material Analysis" and "Product Comparison" (Figure 7.2.5). Once the selection is made, the Raspberry Pi, which is connected directly to the LCD, will communicate with the MCU on the PCB via general-purpose input and output (GPIO) pins, beginning the process of obtaining the spectral data from the CCD detector inside the optical spectrometer. A few 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, but an STM32 can, due to an embedded ADC component. This converter will work to process the incoming analog signal from the CCD into usable data for analysis. The sensor functions by capturing a frame of spectral data as input and sending out a series of analog voltage signals showing the intensity of light for each specific pixel in the sensor. This is done by representing each pixel with a photodiode, a photon-sensitive semiconductor diode 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 STM32 and made readable for the RPi controller. Once the analog signal is converted into a digital format, it is sent to the RPi, where it can 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 generating a steady flow of data from each photodiode. 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 MCU and the CCD is to obtain the data of a singular frame of spectral data 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 by the STM32. This control will ensure that the MCU only accepts the data asked for by the user, taking only the spectral data from one singular frame and cutting off anything else being sent. An analogy for this process would be attempting to grab a specific frame from a live video feed, but instead of this being done with an editing software, the process is done through pins and serial bus communication. The initial steps are done through GPIO pins on the STM32, communicating directly with the CCD detector, sending activation pulses to specific pins on the CCD in order to synchronize the output of the spectrometer and the data taken by the MCU, ensuring that only what is necessary is being received. The first steps taken are to define the pins used by STM32 for communication with the CCD; each of these four pins is defined by its location on the microcontroller and the function it corresponds to on the CCD sensor. These four pins communicate with the shift gate, integration clear gate, master clock, and output signal of the CCD. They are defined at the second, fourth, fifth, and thirty-sixth GPIO pins on the ESP32, respectively. This is because pins two, four, and thirty-six all function as both GPIO pins and ADC inputs. Pin five was chosen as it controls the timing of bus communication for the MCU. An integer array is then created with a size of 3648 items, the total number of pixels within the CCD (3694) minus the forty-two “dummy” pixels included in the CCD output signal in order to help establish frame differentiation. Next, the pin-mode of each of the four communication pins is defined, with the shift gate, clear gate, and master clock pins all being set as output, and the output signal pin set as the sole input taken by the MCU. During testing, this is also the point in the code where a serial data transmission line was started at a specified baud rate. Using this line, the obtained spectral data could be viewed through the COM port established on the Raspberry Pi, with different types and levels of lighting being used on the sensor to verify component

integration. At the other end of the wire connections, the communication pins on the CCD sensor for the integration clear gate, master clock, shift gate, and output signal are located at pins three, four, five, and twenty-one, respectively (Figure 7.2.1). Each pin should be set initially to low.

TCD1304DG

Circuit Diagram

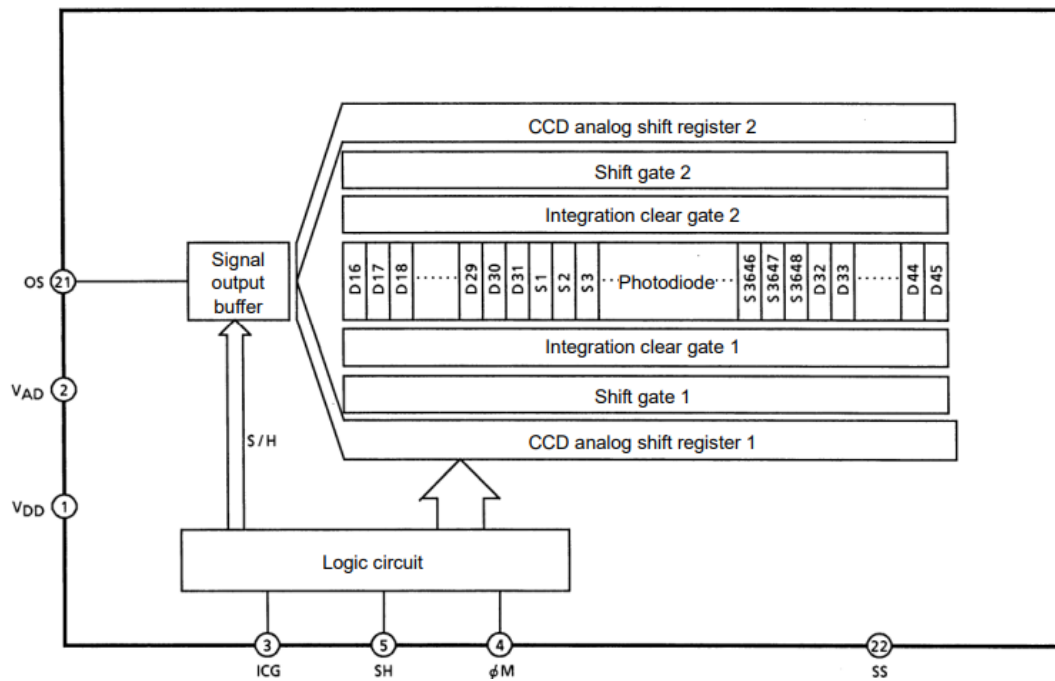


Figure 7.2.1 TCD1304DG Circuit Diagram [143]

The first pin to be activated is the integration clear gate, which resets the CCD sensor's output signal and photodiodes, allowing for more precise control of timing and frame demarcation. The reversed polarity of the clear gate means that its activation leaves it in a low state at the beginning of the CCD's timing. After six-hundred nanoseconds have passed, the shift gate is set to high. Next comes a four-microsecond period to allow for integration, followed by the lowering of the shift gate, which lies between the photodiode layer and the output signal buffer. The photodiode layer contains a row of three thousand and forty-eight semiconductor diodes, each only eight by two hundred micrometers in size, and each carrying an electrical charge that represents the intensity of light at its respective pixel within the spectral frame. When the corresponding 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 MCU as an analog output signal. The clear gate is set back to high at a period synchronized with the readout rate of the CCD, clearing the voltage signal before the device transfers the shifted electrical data through the output signal buffer. The clock pin is switched to high and then low for every incoming pixel value. The STM32's embedded ADC will automatically process the incoming analog signal, as the duty cycle of the signal driving the ADC is synchronized with the master clock frequency setting the readout rate. This means that the ADC will sample once for every pixel readout by the CCD. The ADC

is also connected with the direct memory access writing system on the STM32, ensuring each converted integer value is written into a DMA buffer of a set length. Each time the buffer reaches its capacity the data is transferred through the connected USB-C cable powering the MCU, and the buffer is cleared for further writing. Once all the CCD elements have been processed, the Raspberry Pi will begin signature generation and sample classification.

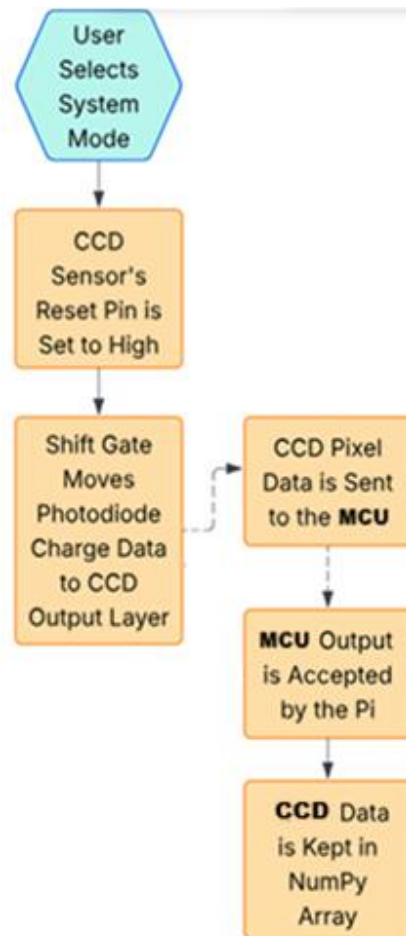


Figure 7.2.2 Spectral Data Extraction Flowchart

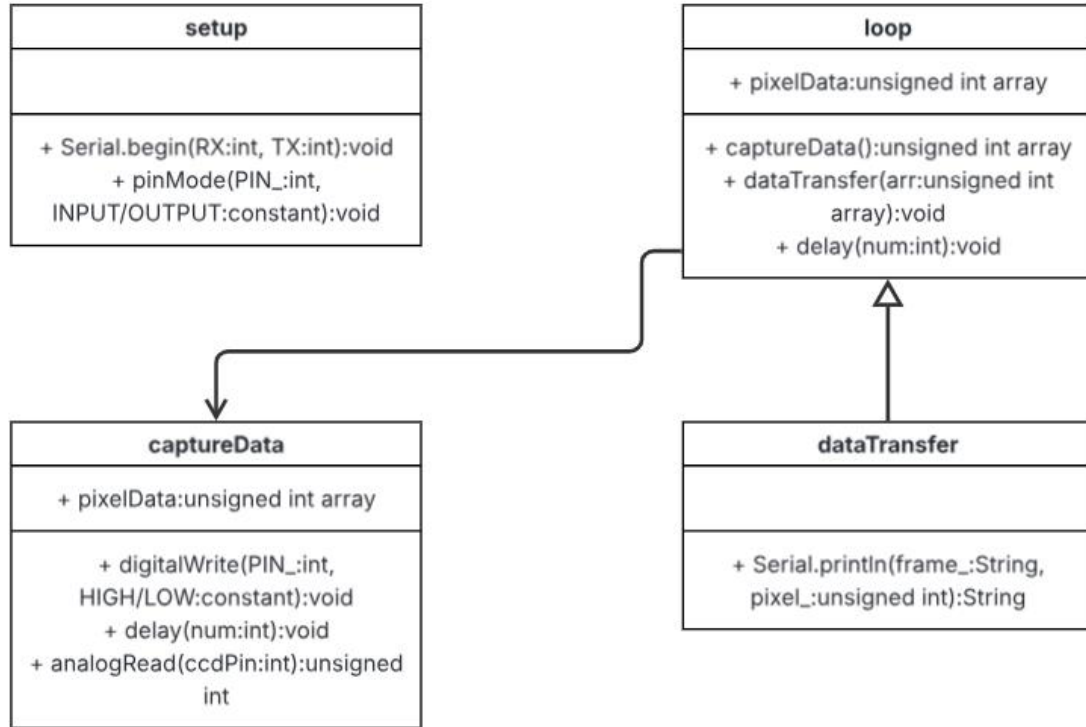


Figure 7.2.3 Spectral Data Extraction Class Diagram

The next goal is to generate a spectral signature for the current sample. To do this, the integer array of collected spectral data must first be converted into a numpy array for easier and faster data analysis. Then, just as noise interference is eliminated during signal processing, the presence of background noise in the data array is removed. This step is straightforward. The integer array is searched through to find the smallest intensity value, and the found value is then subtracted from each index in the dataset through a far loop. The result is a better-calibrated array for the soon-to-be-generated spectral signature. The dataset can be further improved with polynomial fitting, specifically by using a third-degree Savitzky-Golay filter. This filter will work to smooth the data inside of the intensity value array in order 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 within the segment to a third-order polynomial approximation of the section, creating a middle ground between the integer values in the array and the polynomial approximation. The final result of the filter is a smoothed version of the original dataset. Creating the line graph to display the sample's spectral signature to the user begins with establishing an x-axis based on wavelength, which will use nanometers as the unit of measurement. This axis encompasses 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 processed integer values held inside the numpy array to display the intensity of the spectrum at each corresponding wavelength, and normalize the data array to avoid

any impact of excess fluorescence on the sorting results. This data will be graphed using the pyplot submodule from the MATLAB plotting Python library. The resulting line graph of the sample's spectral signature will then be displayed to the user via the LCD module before being further analyzed with comparison against the data of previous signatures through algorithm functions to determine either the textile material of the sample or if the sample item has already been scanned, depending on whether the system mode selected was material analysis or product comparison.

At this point, we reach the final phase of the project, analyzing the generated spectral signature. Regardless of the system mode, all signature analysis will be done first against prior spectral signatures. In the case of material analysis, the goal is to sort the generated signature into its corresponding group based on the identified textile material, whereas in product comparison, the goal is to test whether the most recently created signature passes a similarity threshold when compared to any given stored signature. This process is done using the numpy integer array that holds all the data that the most recent signature was generated from, comparing it against prior scans in order to select the most similar subgrouping. Group, in this case, meaning another numpy integer array containing the data of previously sorted spectral signatures, with the subdivisions being the data from individual prior signatures. 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 calculate the similarity of different time series. A time series being any line graph of data points arranged in order of time. The DTW algorithm calculates a similarity score of the two line graphs by scanning through the first line, going one by one through each data point, and finding a comparable point in the second line for each one (Figure 7.2.4). These points of comparison are the basis for the similarity score, with the distance of each comparison being one part of the calculated sum that the resulting score is taken from.

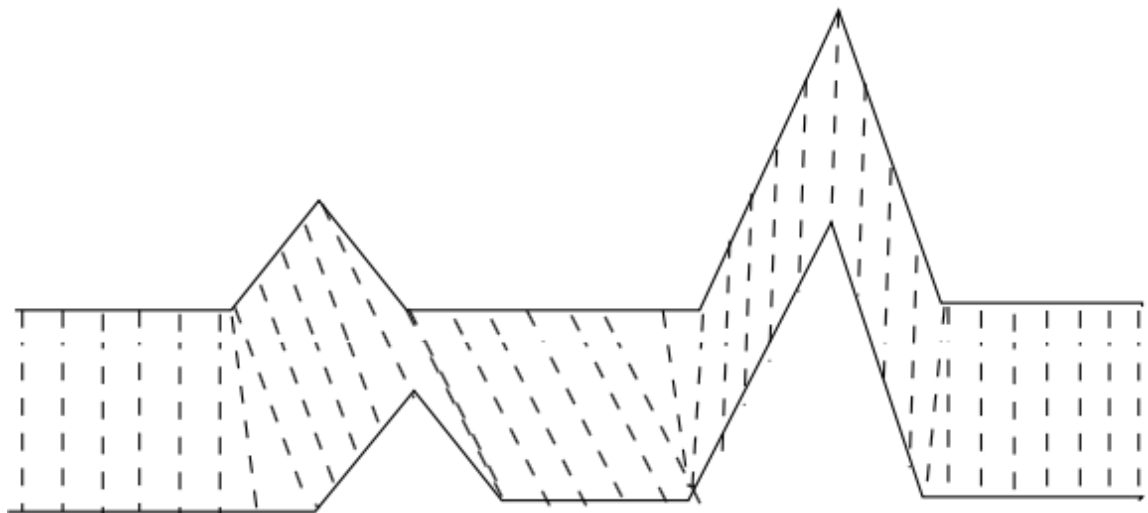


Figure 7.2.4 Points of Comparison in Dynamic Time Warping

The goal of DTW is to limit the effect to which time factors into similarity calculations, doing so by making comparisons at differing points across the time-axis. The alternative distance calculations to DTW use the difference in corresponding amplitude values at each

index on the x-axis to create total sums of difference between the two lines, but when using this method for comparisons such as audio, physical movement, or handwriting analysis, time becomes the single largest determining factor in the results. 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 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 focus on points of comparison counteracts this problem. Matches along the x-axis, or time axis, are determined from a cost matrix that is created using the value of distance from every index in the second line to every given index in the first. Distance values can be calculated through several different standard formulas; in this project, Euclidean distance will be used due to the simplicity of the calculation and the availability level of the function in software. A path of lowest cost is charted through the matrix, and from it, every point of comparison is mapped. When finding the path of lowest cost, there are three additional conditions. First, the earliest and latest point on both lines must be matched with their counterpart, meaning index one in line one is required to have a point of comparison with index one in line two, and the same goes for the final indexes of each line. Next, every point on both lines must have at least one point of comparison, there cannot be a single index in either line that is not involved in at least one distance calculation. Third, and finally, a point in one line cannot be matched with a point in the other line if that point in the second line precedes any already selected index for any previous point of comparison. To put the final rule in other words, this means the lines denoting points of comparison cannot ever cross over with one another. An example would be that while points 1A, 2A, and 3A in the first line can all be matched with the point 2B in the second line, in doing so, points 2A and 3A in the first line then cannot be matched with the point 1B in the second line. This is because a line between points 1A and 2B will have already been placed as a point of comparison. To make a visual comparison, dynamic time warping is similar to rope or wire connections between notches on two boards length-wise, like a sewing string surface or a musical instrument such as a harp or lyre. In these examples, the third rule would mean that you cannot place a string underneath or over another string to connect to a point. The end cost of the path chosen through the matrix also functions as the resulting similarity score for the two lines, as the end result of dynamic time warping is the summation of all calculated distances for every point of comparison [145].

A lightweight version of the DTW algorithm can be installed using the terminal command “pip install fastdtw” on the Raspberry Pi, allowing the fastdtw Python function to be used, which will take in two integer arrays along with a selected distance metric and provide the resulting DTW similarity score. The fastdtw function has linear complexity for both time and space, compared to the standard DTW process, which is quadratic, meaning that while standard DTW is not a possible option for this project, lightweight implementations like fastdtw are much more realistic [146]. The array obtained from the current sample will be compared with each prior scan using the fastdtw function. In the code, three function calls will be made to find DTW results, each passing the array of data for the current spectral

signature in tandem with one of the arrays containing previously classified data as arguments. Inside the called function is a for loop that will repeat for the length of the array containing the previous signatures, in the function it is passed as “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 is now able to be classified based on these returned arrays. This is done through one-dimensional clustering of the results arrays. The three returned arrays of DTW similarity results are first combined into one array, with a label being attached to each entry so that it can be traced back where each similarity value was added from, i.e. a “Cotton” label for values from array one, “Polyester” for array two, and “Silk” for array three. This array is segmented using the KMeans algorithm into a set of clusters, and the group found to be most represented in the cluster with the smallest centroid value will then be chosen as the identified material of the user’s sample. The label of this group is displayed to user on the LCD screen as a final result for the system. There will be a catch case that is triggered by a lack of similarity scores within an expected range for all groups by a given sample, meaning that no group had comparison results within this range, in which case the material will be determined as unknown, and the fact that no match was found will be displayed to the user on the LCD screen (Figure 7.2.5).

When the system’s second mode, product comparison, is selected, the spectral signature analysis and classification process will still be very similar to that of material analysis. The Raspberry Pi communicates with both the CCD sensor and the STM32 to obtain the necessary spectral data to generate the sample’s spectral signature and corresponding integer array. This array is then compared with the signature data of previous scans using dynamic time warping, the same as in material analysis, but after this point, the process is slightly different. When the DTW comparison function is called with an array of previous signatures, each comparison value will be returned with the label of the item it was compared to, as the array in this case is two-dimensional, not three. The comparison results are then collected into a common array and analyzed to determine if any item is found to have cleared a specified similarity threshold, in which case the item will be selected as a match. In the case that a match is found, the matched array will have its label displayed to the user as the final result of the system (Figure 7.2.5), and in the case that no item clears the similarity threshold, the user will be told that there is no match and will then be prompted to enter a name-tag for the new item using a pop-up touchscreen keyboard, so that this new product can be added to the array of prior signatures.



Figure 7.2.5 Graphical User Interface Flowchart

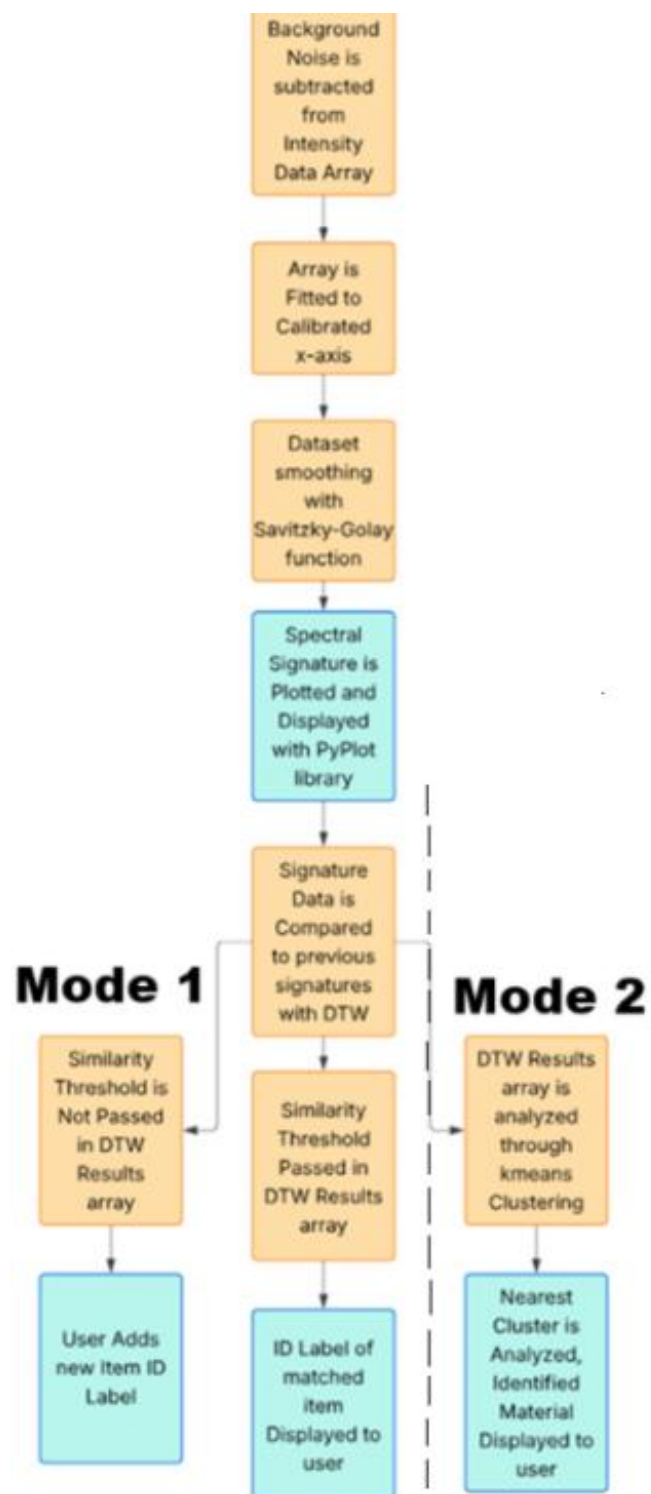


Figure 7.2.6 Spectral Signature Generation & Identification Flowchart

8 PCB Fabrication

8.1 Design

To create the PCB, the first step is to identify all the components that are needed for the system based on the functionality and design goals. This includes microcontrollers, sensors, voltage regulators, connectors, and any passive components like resistors and capacitors. Once the complete list of components is finalized, the next task is to gather the proper footprints for each part. The footprint acts as the physical representation of the component in the PCB layout, and it includes the pin spacing, dimensions, and pads that will be soldered on the board. It's critical that the correct footprint is chosen, otherwise there could be major issues during fabrication or assembly. These footprints are often downloaded from online libraries like *Ultralibrarian*, *SnapEDA*, or from the manufacturer's site, and it's important to make sure they are compatible with the design software being used. In this case, *Autodesk Fusion 360* with the *Electronics* workspace is being used, so the *Fusion-compatible* library format must be selected.

After collecting the footprints, a new project is created within *Fusion*, and all of the downloaded components are imported into the *Fusion* library so they can be easily accessed during the schematic and layout process. Once everything is imported, the schematic design can begin. In the schematic editor, each component is added and their pins are connected to one another based on the circuit design. This is where all of the logic of the system comes together, such as defining how the power rails connect, how data flows between the microcontroller and peripherals, and where each signal goes. It's important to double check all of the connections and make sure each pin is defined exactly as needed. Only after confirming the schematic is correct can the PCB layout process actually begin.

Switching to the PCB layout screen shows a blank workspace with all of the components listed below it in a default arrangement. These components are initially unplaced, and they are still connected by airwires which are yellow lines that indicate logical connections between pins as defined in the schematic, but they are not real traces yet. These airwires act as a guide for how everything should be wired, showing which pins need to be connected together. The first step in the process is to drag all the components onto the PCB workspace. At this point, exact placement and orientation don't matter much, the focus is just on getting everything onto the board.

Next comes arranging the components in a way that makes sense for the design, while trying to keep the layout clean and efficient. It's helpful to try to reduce the number of overlapping airwires, which can get very messy and make routing difficult. Components are rotated and moved around to minimize crossovers and keep signal paths as short as possible. Once satisfied with the layout, the actual wiring can begin. This is done using the routing tool, which allows the user to draw traces that connect one pin to another based on the airwires. The trace widths were determined by the current expected to be going through each connection. While routing, it's important to make turns with 45-degree angles instead

of 90-degree ones, since sharp corners can disrupt current flow and introduce problems with signal integrity or even overheating in higher current situations.

Once routing is complete, a design check is performed to catch any issues which can be done in the errors tab. In the TEXRAY design, several errors popped up right away. Many of these were related to incomplete or missing connections, even though everything looked visually fine. By clicking through each error, the affected areas were highlighted on the board. It turned out that in some cases, the traces were very slightly off from the pins, meaning they weren't actually connected even though they appeared to be. These were corrected by zooming in and snapping the traces directly to the pin pads to ensure a solid connection. Another issue involved a footprint compatibility problem with one of the transistors. The original footprint was either incorrect or incompatible with Fusion's rules, so to resolve this, a different but functionally similar transistor was selected with a footprint that worked better with the software while being able to satisfy the requirements.

After making these fixes and confirming that no more errors were present, the board was now fully routed, with all components properly placed and connected. The design was then ready to continue the fabrication phase, approaching where the final files would be exported and sent out for manufacturing. By taking the time to carefully go through each step, from schematic to layout to error correction, a functional and manufacturable PCB would ideally be created, ready for testing in the actual system.

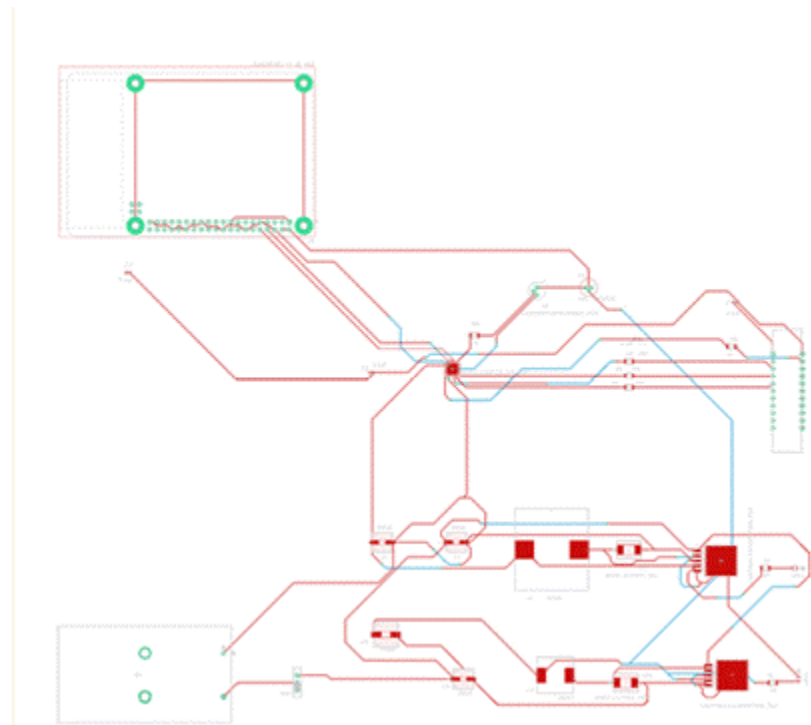


Figure 8.1.1 PCB Routing

After completing the routing process for the TEXRAY PCB, the layout of the components and traces began to take shape, as shown in the image above. Looking closely at the major components, it can be seen that the placement was done with both functionality and space

optimization in mind. One of the key placements is the TCD1304DG CCD sensor, which is located along the edge of the PCB. This is intentional, as it needs to be positioned where it can directly receive the spectral light that enters the spectrometer. Since it plays a central role in detecting the optical signal and converting it to an analog output, its placement along the boundary ensures that no other components obstruct the light path.

The battery, being a relatively large and bulky component, is placed at the bottom left corner of the board. This helps balance the overall weight distribution and keeps it away from more sensitive circuitry to reduce potential interference. By giving it its own space, it's easier to route power lines and provide safe mechanical clearance, especially important when dealing with heat or vibration. On the opposite side of the board, the Raspberry Pi is positioned at the top left, making it easily accessible and providing straightforward integration with an LCD. This setup allows for clean GPIO alignment, especially since the LCD connects directly to the Pi via DSI connection. There's also a conscious effort to leave the top right portion of the PCB relatively open, reserving that space in case a housing or enclosure for the LCD is needed in the future.

For routing the signal and power lines, a two-layer PCB structure was used, with the top layer shown in red and the bottom layer in blue. This dual-layer approach makes it significantly easier to manage trace congestion and avoid wire crossovers, which is especially important in a compact design with a lot of interconnections. When a trace on the top layer encounters another trace and can't be routed around it, a via is used to drop that connection to the bottom layer, effectively allowing it to pass underneath. Once it clears the obstruction, another via brings the trace back to the top layer so it can complete its connection to the appropriate pin. This method of jumping between layers helps keep the design neat and electrically reliable while reducing the risk of short circuits or signal integrity issues.

Once all the connections are in place and verified to be error-free through the errors tab, the next important step is setting up the ground plane. The ground plane acts as a solid reference voltage for all components and essentially covers all space of the PCB that isn't a component or a wire that isn't already set to ground. To create it, the polygon tool in Fusion is used to outline the entire perimeter of the board. After closing the outline, the polygon pour tool is used to fill the defined area with copper, which will automatically connect to all nets assigned to ground. A 20 mil isolation is specified to keep the copper pour safely distanced from any traces or pads that are not connected to ground, preventing unintentional shorts. This results in a well-distributed ground plane that helps stabilize the system.

Finally, one last step remains before the board is ready for fabrication — organizing the component labels and values. Each component comes with a reference label (like R1, C2, etc.) and sometimes a value (like 10k Ω or 100nF). These labels are critical for assembly and troubleshooting, especially during soldering. To ensure they're visible on the final board, these designators must be placed on the top silkscreen layer. If they're left on another layer or obscured by a component or trace, they won't be printed on the PCB during

manufacturing. This can cause confusion during assembly, especially when placing components by hand or working from a visual guide.

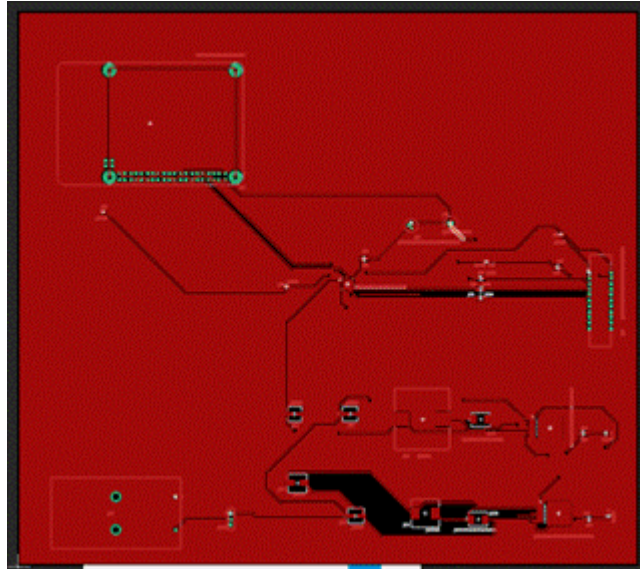


Figure 8.1.2 PCB with Ground Plane

The final design, with all connections completed, the ground plane filled, and the labels properly moved to the silkscreen layer, is shown above. It represents a fully-prepared PCB layout, optimized for both performance and ease of assembly, and ready for the next phase of manufacturing.

At this point, once all the routing, ground planes, and silkscreen adjustments have been completed, the final step before fabrication is to open the manufacturing preview window. This gives a digital representation of what the physical PCB will look like once it's produced. In this view, it's possible to closely inspect every detail of the board which includes trace routing, via placement, component alignment, silkscreen labels, and the copper pour areas. Seeing the board laid out this way is helpful to ensure that everything looks correct and matches the intended design. It acts as a final checkpoint before committing to manufacturing. If something appears off, whether it's a misplaced label, incorrect trace width, or a missing via, any last-minute corrections or improvements can be done right before generating the Gerber files.

8.1.1 Main Board layout

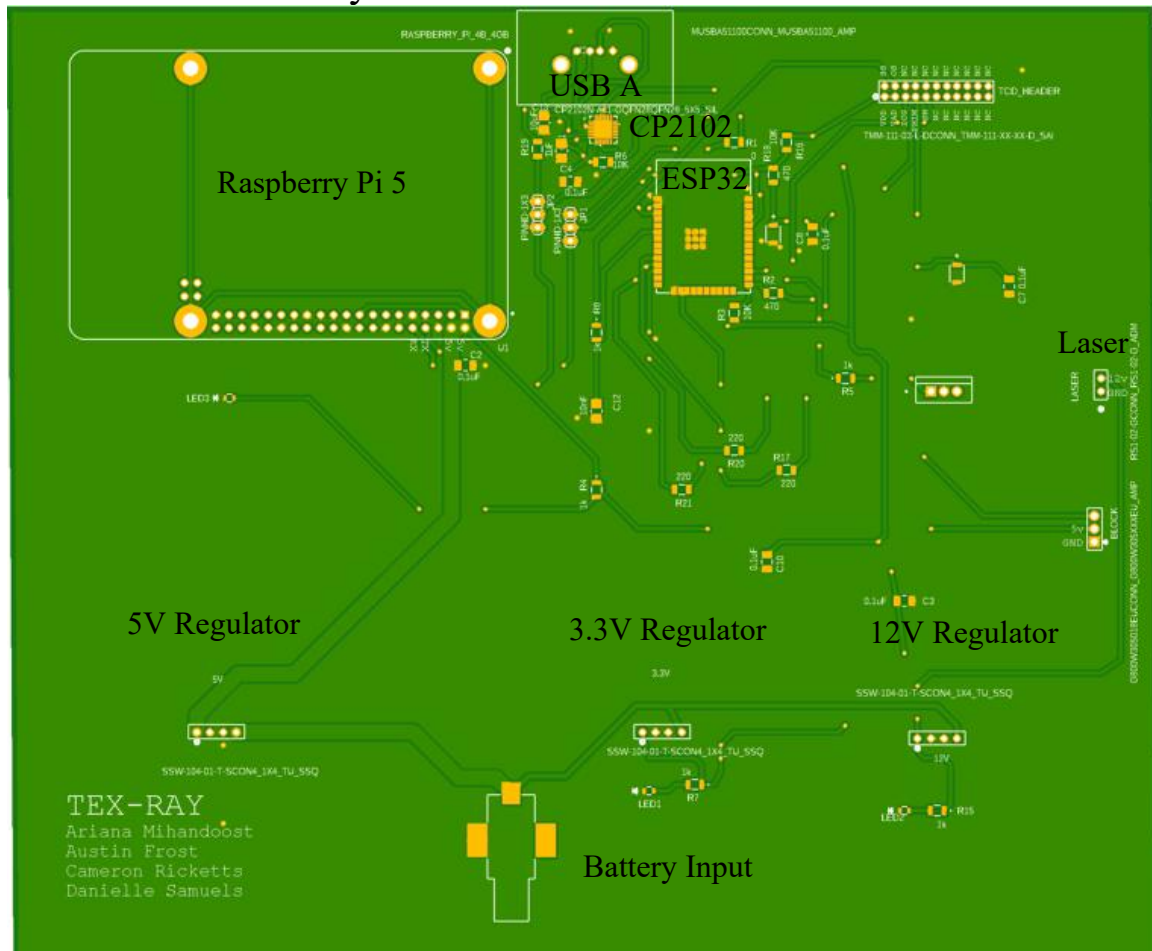


Figure 8.1.3 Final PCB Preview

The PCB layout displayed in the preview represents the finalized design for the TEXRAY spectrometer system, showing how the various components are positioned and interconnected for proper system operation. At the center of the board is the ESP32 microcontroller, which serves as a primary controller for the laser. Traces extend from the ESP32 to multiple peripherals, including connections to the MOSFET transistor. The gate of the transistor is connected through a resistor limiting the current, and the drain-source path interfaces with the laser circuit, enabling switching operation. The ESP32 is also routed to the Raspberry Pi, receiving the input signals via the RX and TX pins to turn off the laser or turn it on. The CP2102 is placed slightly above the ESP32 and connected to its RX and TX pins to receive data for programing. Being that the RX and TX is routed to both the CP2102 and the Raspberry Pi 5, jumpers are put in place to switch between the connections.

On the bottom of the board is the battery input, where power is supplied to the system. This power flows into the 3 voltage regulators slightly above, all of which ensure low-noise, regulated power for the ESP32, Pi, laser, and supporting circuitry.

8.1.2 Voltage Regulator Layouts

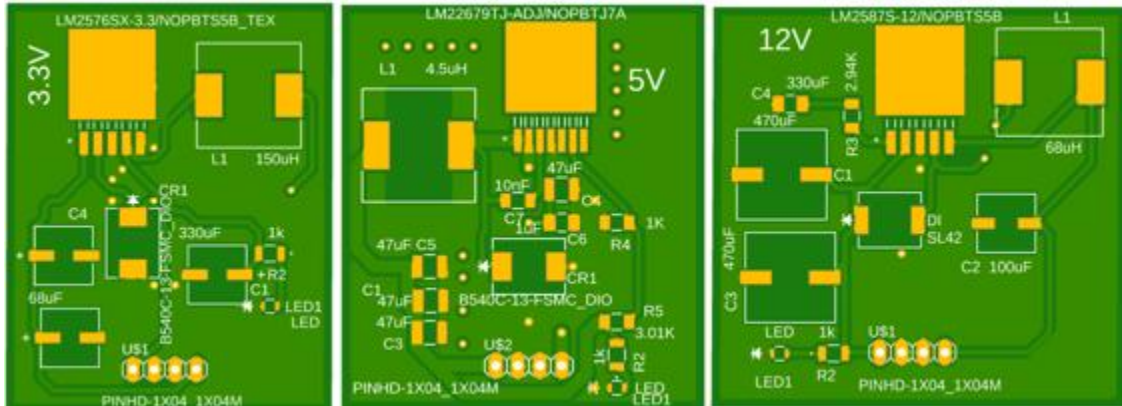


Figure 8.1.4 Voltage Regulator Layouts

Above are the layouts for the voltage regulators. When designing these layouts, sizing was a key factor in aiming to make them compact to be able to be placed onto the main board with ease. For stability, it was essential to have the inductors as close to the regulator chips as possible as well as having the capacitors not far off, due to the small sizing of the boards in general this was easily achieved. With exception of the 5V regulator, the current being drawn from these regulators are relatively low so the traces were made with a 20 mil trace width which is more than sufficient for the max 500mA current draw expected. As for the 5V regulator, due to it supplying the Raspberry Pi, it is expected to need to supply up to 5A. Therefore the trace widths on the 5V regulator's input and output rails were increased to 55mil traces with the boards thickness being set to 2oz.

8.1.3 STM32 Board Layout

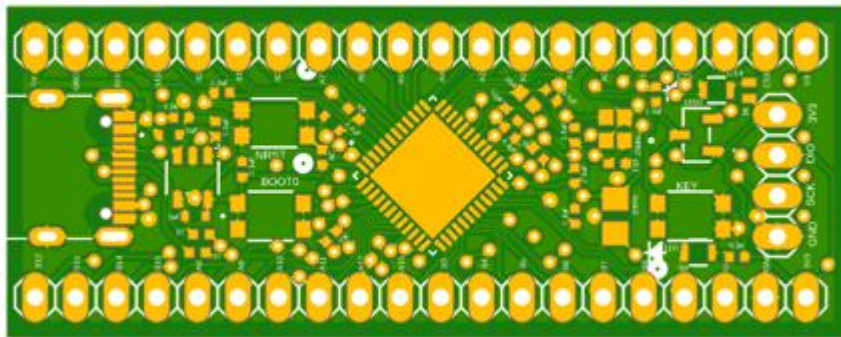


Figure 8.1.5 STM32 Board layout

Above is the STM32 board layout. This board was designed with the goal of replicating the STM32 Black Pill development as precise as possible. The main factors in doing so are the boards dimensions and the spacing for the pin header connections. Once that was complete the components had to be placed accordingly with the black pill board as reference.

8.1.4 Signal Amplification Board Layout

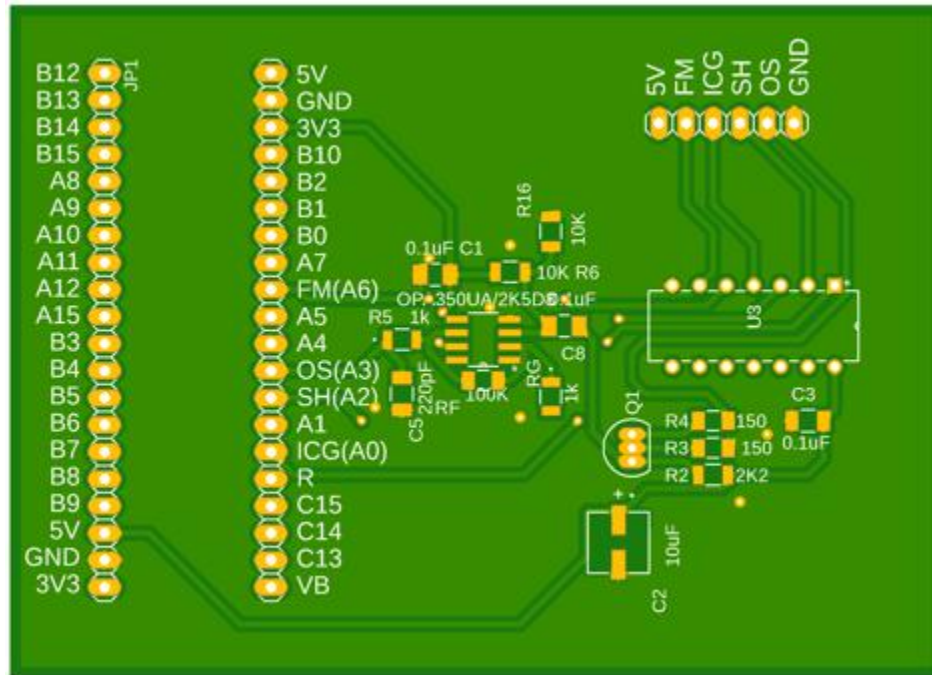


Figure 8.1.6 Signal Amplification Board Layout

This board is the layout of the signal amplification board. The pin headers on the top right connect to the TCD1304DG via female to female wires, allowing for non-restrictive repositioning with testing. The hex inverter is directly below it connected to the the CCD's timing signal pins which are provided by the STM32. The output signal flows through the transistor connection to the coupling capacitor to remove the offset. The signal feeds through the OPA350 in the middle and the lowpass filter then is connected to the corresponding pins where the STM32 will be placed. The spacing of the female headers were made precisely to match with the STM32 Black Pill development board, as well as the STM32 Board created, allowing for them to be easily placed and removed.

9 System Testing and Evaluation

9.1.1 Dispersion Demo

The final demo for SD1 tested the fundamental nature of the spectrometer portion of TEXRAY. The components involved were a 633 nm HeNe laser, 520 nm green laser pointer, 25 μ slit, and a 1200 lines/mm holographic, reflective diffraction grating. The 520 nm and 633 nm wavelengths were meant to simulate the range of wavelengths observed after being diffracted by the grating. The general design displaying dispersion is a rudimentary one. Unlike the Czerny-Turner configuration, which uses a spherical mirror to collimate the beam onto the diffraction grating and another spherical mirror to focus the dispersed light onto the detector. The slit in the demonstration allows us to measure the power losses from the slit and grating. While although not comprehensive enough to

estimate the power that will ultimately incident upon the linear CCD detector, it does remain insightful for general concessions.

The configuration involved propagating a 633 nm HeNe laser and a 520 nm green laser pointer colinearly along the same linear axis. A beam splitter at the beginning of the optical axis combined the red and green beams. Alignment of the two beams was conducted with the two designated mirrors for each laser into the two pinholes on the optical axis. The alignment and collimation of the beams in this context is particularly important. Ensuring that the beams are collimated improves the spectral resolution and misalignments can leave a spectrometer vulnerable to signal losses. Especially related to the use of spherical mirrors in the final spectrometer design, misalignments can contribute to increased aberrations.

This system directed the colinear beams through a vertically oriented 25 micron slit. The slit will diverge our light horizontally and improve the spectral resolution of the dispersed light from the grating by also spatially filtering our beam. This horizontally diverged beam is then incident upon a 1200 lines/mm holographic diffraction grating. This follows the same grating density we plan on implementing into our system, the specifications of which have been detailed in chapter 6. The 1200 lines/mm groove density allows for greater spectral dispersion, making the subtle wavelengths changes more discernable.

We continued to qualitatively demonstrate that the distance from the diffraction grating to the image plane is related to the amount of dispersion. These expressions have been defined in Chapter 6. The farther away the image plane the greater the dispersion. The opposite holds as well, where the closer the image plane to the grating, the closer the first order mode is to the central mode. The TCD1304DG linear array CCD has an active area of 29.1 mm. When the image plane is ~19 mm away the diffracted image of the red and green slit is ~29 mm separated from each other.

Overall, we demonstrated the importance of an aligned optical system, wavelength dispersion off of a reflective grating, and the effect of dispersion under changed positional circumstances.

9.2 Laser Diode Quality Testing

The excitation laser largely dictates the quality and intensity of our received Raman spectrum. This demand prompted extensive considerations in deciding on the most beneficial laser for Raman spectroscopy to discern textile types, outlined in Section 3.4. It is therefore important to conduct quality assurance testing on the lasers to ensure a properly performing device. Laser diodes are inherently sensitive to changes in temperature and input current [147]. Decreases in temperature and current can result in a peak wavelength that shifts towards shorter wavelengths, where increases in temperature and current can shift the peak towards longer wavelengths. Further, increasing the input current can lead to broadening of the Full Width at Half Maximum (FWHM). Confirming that the center wavelength of our laser diode matches the desired specification of 520 nm is important for cooperation with the rest of the chosen Raman illumination optics. It is further relevant to confirm that the laser diode produces a narrow FWHM, which contributes to a more

resolvable Raman spectrum. Therefore, we assessed the spectral characteristics of three laser diodes with a specified center wavelength at 520 nm. We further tested one Diode-Pumped Solid-State (DPSS) laser with a specified center wavelength at 532 nm, to compare diode versus solid-state laser quality.

Our previously chosen laser diode, the ams-OSRAM PL 520B, before switching to the Q-Baihe module, professed an outpower power level of 100mW, a typical central wavelength of 520 nm, and a spectral linewidth of 1 nm. The data sheet further specifies a varying peak wavelength range from 515 nm to 520 nm. The laser diode was purchased assembled with the driver component and collimating lens. We attached the anode and cathode to the input and ground of a power supply respectively. The operational voltage is 3V to 6V, and the diode calls for a greater than or equal to 1 mA of current. Varying the input voltage and current resulted in 80mW and 100mW power readings, as expected. Using the StellarNet BLUE-Wave miniature spectrometer, we characterized the spectral qualities of the diode. Specifically, the peak wavelength and FWHM. We placed a Neutral Density filter (Thorlabs NE40A) in front of the laser diode as to not oversaturate the spectrometer. Figure 9.2.1 (a) shows the measured center wavelength at of the LD at 526.84 nm, we further noted the FWHM measured at 5 nm. This completely contradicts what the supplier specified and potentially changes the design of our illumination optics.

With the realization of the discrepancy from the ams-OSRAM PL 520B specification versus operation, we continued to test other laser diodes to develop a sense of their reliability. We conducted tests on two identical laser diodes, the ams-OSRAM PLT5 518FB P. The two laser diodes were originally purchased with the intent of integrating one of them into TEXRAY in its earlier stages of development; these laser diodes were abandoned simply due to its low, 30 mW, power for our desired use. The specified typical operating wavelength is 520 nm and the FWHM is at 1 nm. The data sheet further specified a varying wavelength range from 510 nm to 530 nm. The laser was connected to the temperature-controlled laser diode mount for 5.6 mm diameter laser diodes (Thorlabs TCLDM9) and the benchtop LD/ TEC controller (Thorlabs ITC4005). The specified threshold current stood at 35 mA and the operating current stood from 80 mA to 100 mA. From the first laser diode, an 80 mA input current paired with a 10°C operating temperature provided a peak wavelength of 522.28 nm and a FWHM of 3.04 nm. Upon increasing the temperature to 43°C, the peak wavelength slightly shifted to 522.66 nm, increasing the input current to 90 mA had no effect on the spectral characteristics of the diode. No changes in the FWHM were noted with the changes. The second laser diode showed somewhat comparable results. An input current at 80 mA and temperature control at 25°C resulted in a peak wavelength of 523 nm and a FWHM reading of 3.04 nm. Decreasing the input current to 50 mA, while maintaining the same temperature lowered our peak wavelength to 521 nm and the FWHM maintained itself at 3.04 nm. Decreasing the current to -10°C didn't change the nature of our diode.

We continued to test the DPSS at 532 nm. A stable center wavelength and narrow FWHM is characteristic of a solid-state laser [147], [148]. The resulting spectral reading is shown in Figure 9.2.1(b). This test served as reassurance for this notion. The infrared pump (not pictured in the figure) does reveal itself in the spectral response at ~800 nm.

Implementation of a the DPSS would require an additional laser line filter to eliminate the IR pump extinction, as to not overcome our Raman signal. While some spectral drifting may occur by virtue of a degrading system, DPSS lasers are considered robust and reliable.

The testing of the various lasers has been important in ensuring a reliable operation of our Raman spectrometer. Our originally chosen laser diode, the ams-OSRAM PL 520B, proved itself unusable with the current illumination optics setup. The tests from the two previously considered laser diodes showed similar performance, and their spectral characteristics changed in accordance with theoretical expectations. However, when implementing our excitation source, we must remain mindful of the subtle disparities from the specifications of the lasers versus the operation. With laser diodes, a shifted center wavelength may not be compatible with our illumination optics and a larger FWHM may degrade our spectral resolution. Even if the ideal laser diode is found, it important to consider whether it would maintain its spectral characteristics under the same operating conditions, or if drifting would occur. We were previously more concerned with a center wavelength being less than or equal to 520 nm and as small of a FWHM as possible. While the inconsistencies in the operation of laser diodes versus its specifications can be a major inconvenience, its tuneability could be advantageous in some contexts. This testing prompted considerations towards pivoting to a DPSS 532 nm laser, which would overhaul our previous illumination optics selections, but offered a more reliable operation. Ultimately, we did end up switching to a 532 nm source.

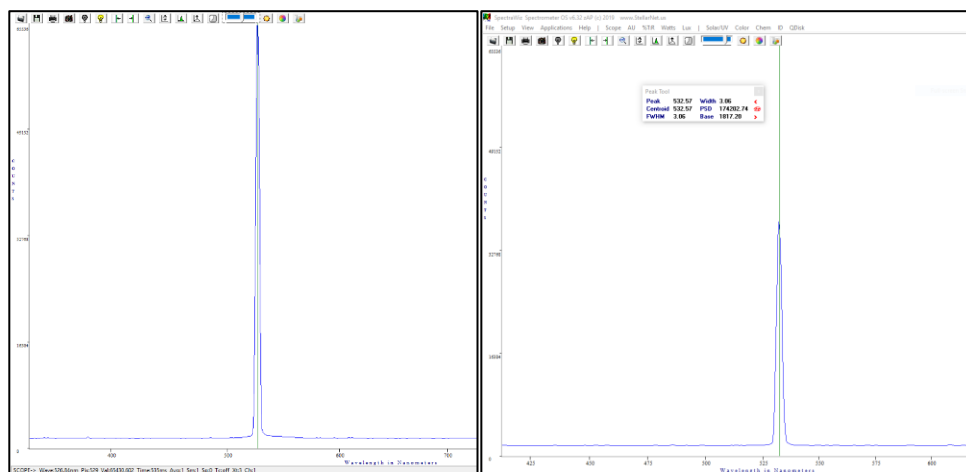


Figure 9.2.1 (a) Spectral Response of ams-OSRAM PL 520B Laser diode (b) Spectral Response of DPSS laser

9.3 Optoelectronics Feasibility

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 involved 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 advanced this testing by connecting our illumination optics with the StellarNet spectrometer in Raman mode. This helped 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 involved 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.

9.3.1 Early Collection Optics Mockup

As a preliminary attempt to generate a Raman signal and assess the efficiency of our system, we attempted to recreate our signal collection optics setup using only materials available to us in the CREOL undergrad lab, aside from a laser source and a 550 nm cut-on longpass filter loaned to us temporarily. We tested two laser sources, a laser diode module at 520 nm, 80 mW and a 532 nm, 100 mW DPSS laser pointer. A picture of our rough setup is shown in figure 9.2.1. Due to lack of materials and wanting to minimize power loss as much as possible for such a crude setup, we opted to test a transmissive Raman signal generation layout rather than the reflective setup we plan to use in our final

design. This enables us to avoid using a beamsplitter and eliminates complexity so that we may just have a simple test of our ability to generate Raman signal.

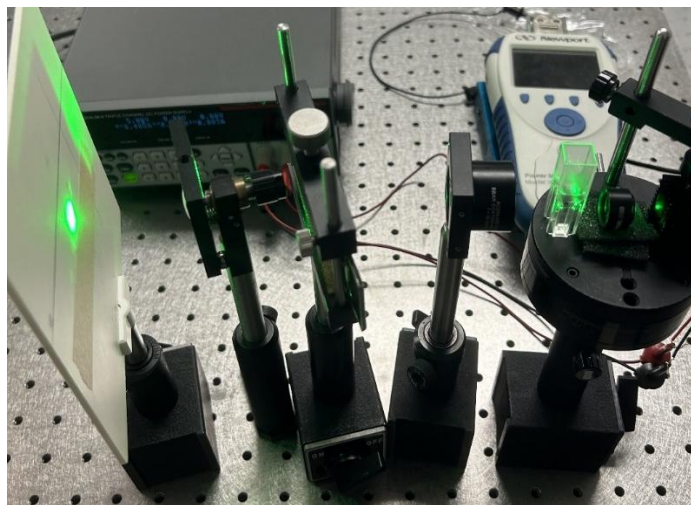


Figure 9.3.1 Preliminary collection optics test

Our laser source was focused into a 50 mm lens to create a high-intensity spot onto the cuvette filled with an ethanol sample. As we have discussed previously, a higher intensity spot directed onto the sample should increase Raman signal generation. The 550 nm cut-on longpass filter we had borrowed for this test limited the lower spectral range of our attainable Raman peaks to 840 cm^{-1} , but because ethanol has distinct Raman peaks at around 2900 cm^{-1} , we should still have been able to observe some Raman shift occurring. The light that passed through the cuvette was then collimated by a subsequent lens and passed through a 600 grooves per mm grating, which was used to separate the Rayleigh wavelength from the potential Raman shifted wavelengths. Not shown in the above picture, the long-pass filter was placed after the grating prior to another focusing lens meant to focus the Raman signal to a point. Also not shown in the above figure, a single-photon camera was placed at the focused point to attempt to detect any differences in signal generated when the sample was present vs. when the sample was absent.

Though we were able to distinguish some clear difference between the signal detected with the sample was present vs. when the sample was removed, we were unable to determine with 100% certainty that this difference was due to the Raman signal and not due to some scattered light or reflections near the detector. As a result, this test was inconclusive with regards to our ability to detect Raman shift. There were many improvements that could have been made to this test had we the proper opto-mechanical components. For example, the 50 mm focusing lens directly in front of the diode was not able to be properly mounted at the time, leading to it wobbling and shifting around. Factors like this could have significantly contributed to difficulty gathering a discernable signal.

9.3.2 Raman Signal Acquisition

Following our early collection optics mockup, many additional tests were conducted to analyze and address potential missteps in our approach to generating and collecting our

Raman Signal. We rebuilt our initial mockup multiple times with slight variations in configuration to locate problem areas in our testing. It is important to once again note that at this point in the testing we did not have our ideal components and needed to work with the equipment available to us in the CREOL undergrad lab and components that had been temporarily lent to us. After multiple attempts, our most recent testing configuration conclusively produced and detected an identifiable Raman shift.

Again, we conducted our testing using a sample of 70% Ethyl Alcohol, which has a notable Raman peak that occurs approximately between 2900 cm^{-1} to 2980 cm^{-1} [149]. Demonstrated in Fig. 9.2.2, we set up a 532 nm 100 mW DPSS laser with an 800 nm pump along our optical path. This laser was directed into a bandpass filter centered near 532 nm which was meant to block the 800 nm pump and enable only the 532 nm laser line to pass through. This laser line was then passed through a 50 mm focal length focusing lens which increased the intensity of the light incident on the sample. The Raman signals excited by the sample, along with the laser line, was directed into a 50 mm focal length collimating lens which was then sent through a 550 nm cut-on longpass filter. This filter was used to block the laser line and enable only the Raman signal to continue in the system. The Raman signal was focused by a 50 mm focal length lens into a spectrometer fiber to display the spectral reading.



Figure 9.3.2 Successful Raman collection configuration

The spectrometer settings needed to be tuned to the ideal configuration for Raman signal acquisition before any shift could be observed. Trying to view the signal with the StellarNet BLUE-Wave miniature spectrometer default settings would not allow any signal to be

viewed. Notably, our setup for this test was not significantly different than that of prior tests which we had conducted and were ultimately unsuccessful. For this reason, we believe the adjustment of spectrometer settings was a key factor in finally being able to observe a definite Raman shift. The dark measurement of the spectrometer was first recorded in the software to reduce the overall noise of our acquired signal. Additionally, the acquisition time was adjusted to 10 seconds rather than the default setting of 1 second. Using these settings, the spectra was recorded with the a) sample being absent in the system and b) the sample being present in the optical path. These spectra were saved and uploaded to MATLAB for precise viewing, shown in Fig. 9.3.3.

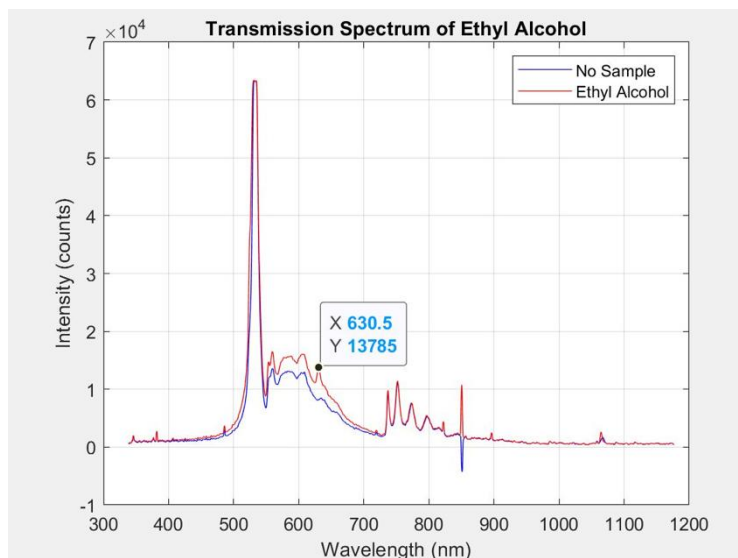


Figure 9.3.3 Received Raman signal with ethyl alcohol sample and no Raman signal without the sample

The spectra clearly demonstrate that when no ethyl sample is present in the system, there is no spectral peak occurring at 630.5 nm. However, when the sample is placed back into the system, a clear and noticeable peak is shown at 630.3 nm. The wavenumber equivalence of this value is 2936 cm^{-1} , which corresponds to the anticipated wavenumber characteristic of the Raman spectrum of ethyl alcohol. This result was consistent and reproducible, as we removed and placed the sample back multiple times to be completely certain that the signal was being accurately detected, and that it was not just coincidental.

The StellarNet spectrometer further reaffirmed our spectrometer design and detector decisions, as our implemented spectrometer portion is comparable. The StellarNet BLUE-Wave model has a 600 lines/mm groove density, from which we were able to discern the Raman spectrum of Ethyl. The 1200 lines/mm groove density that was chosen for our spectrometer will have higher resolving capabilities. Further, StellarNet has the Czerny-Turner configuration implemented into this model, which is the characteristic spectrometer configuration of most of their commercial spectrometers, and further contributed to a received Raman signal.

The optoelectronics feasibility of our system as it pertains to the detector's capacity to receive the Raman signal— which is expected to be on the order of picowatts— has been a contentious point in our project. Though the CCD used in the BLUE-Wave spectrometer

is not explicitly specified, the StellarNet Manual states, “The most common UV-Vis detector StellarNet uses is the SONY ILX CCD that has 2048 elements with $14\mu\text{m} \times 200\mu\text{m}$ tall pixels each with a $14\mu\text{m}$ pitch. These detectors are the best made for spectroscopy” [150]. Which further corroborates with the only mentioned specifications for the detector being, “2048-pixel CCD detector” with having a “ $14 \times 200 \mu\text{m}$ pixel size”. Our chosen CCD linear array detector, the Toshiba TCD1304DG, shows similar operational capabilities to the SONY ILX CCD. However, the offered 3648 pixels results in a larger detector width, and thus, a wider receivable spectral range. Referring to section 3.6.7 offers a more comprehensive comparison of the Toshiba TCD1304DG CCD against the SONY ILX511 CCD. Therefore, use of the Blue-Wave spectrometer has experimentally implied linear CCD arrays, like the one chosen for our system, have the necessary sensitivity to detect Raman signals.

As previously mentioned, the acquisition time for the received spectrum of ethyl alcohol stood at 10 seconds. One of the issues with the preliminary Raman tests we conducted was that our integration time was too low. An increased integration time of our system can compensate for low excitation powers and low sensitivity detectors to receive a discernable Raman signal. However, as TEXRAY is being developed as the equivalent to a consumer grade product, there are certain timely expectations we are expected to meet. The wait during the 10 second acquisition time offered an important perspective into the relevance of a desired low integration time specification.

Overall, though this test used a transmissive configuration rather than the reflective setup we implemented into our final design, and the sample is a liquid rather than textile, it proved to us that we could generate a discernible Raman signal using the materials available to us. After further optimizing our system and using higher quality components which we hand selected for our project, our signal readings should become even more clear and precise.

9.4 CCD Software Testing

Both the LCD module and CCD sensor were tested for the final three-minute demonstration video at the end of Senior Design 1. The LCD was attached to the Raspberry Pi using a display serial interface (DSI) connection, allowing for the display screen of the RPi to be viewed on the LCD. Files and command line terminals could be opened through the touchscreen ability of the display, and so the LCD was used to display a graphical user interface (GUI) through a pop-up window by running a Python file coded on the RPi. The GUI allowed the user to switch between a main screen and a “Hello World” message inside the window by pressing a touchscreen button at the bottom of the screen.

The CCD sensor was made to send a continuous stream of spectral data to an ESP32 development board using the Arduino IDE. The CCD was set up on a miniature breadboard with each communication pin connected to the ESP32 board. Male-to-female jumper wires were used to connect these pins and signal activation for the shift gate, master clock, integration clear gate, and output signal on the CCD through the Arduino code uploaded to the ESP32. The analog voltage signal output of the sensor was received and converted by

the embedded ADC in the development board. The resulting digital spectral data was displayed through the serial monitor in the IDE, writing each integer value to a serial data transmission line at a specified baud rate. It was during this testing that the ESP32's embedded analog-to-digital converter was found to be far slower than described on the microcontroller's datasheet. While the specifications of our system required a 500 kHz data rate between the CCD and the ESP32's ADC, the highest rate of transfer achieved through memory dump testing in Arduino was a little over 100 kHz, well below even the floor of the recommended operating range for the TCD1304 of 200 kHz. It was these results that ultimately led to the STM32F401CCU6 being chosen as the MCU to drive and handle the transmission of the TCD1304 data.

Once the STM32 was interfaced with the CCD, testing of input signal timing commenced, analyzing the analog voltage signal output of the TCD1304 using the oscilloscopes available in the engineering building's Senior Design laboratory. This process was lengthy due to the trial-and-error involved with learning the timing requirements of the TCD1304. The device is built intentionally to operate with high sensitivity to all voltages throughout its running process, this means that if the timing of the input signals is not aligned to the point of less than a microsecond, then the output signal will not be usable for optics systems such as ours. Operating ranges given in the TCD1304's datasheet provided a useful jumping-off point, as optimal frequencies for both the master clock signal and data transfer rate are provided. The datasheet also provided diagrams explaining the timing relationship between the shift and clear gate signals, detailing minimum delays between the rising and falling edges, given that the polarities of the two signals were opposing. The frequencies of the shift and clear gate were also set early on in testing, as once the most optimal master clock frequency was determined to be 2 MHz, at this clock rate, the readout time of the CCD was 3694 pixels multiplied by a period of 2 microseconds. From this, the clear gate was set at a frequency of 133.33 Hz to create a period of 7.5 milliseconds, and in early testing, the shift gate was set at the same frequency to ensure that the integration time produced a constant readout. Once the frequencies and duty cycles of both the CCD input signals and the embedded STM signal, used for ADC coordination, were determined, the output signal of the CCD could be verified at increasing integration times with a Python GUI showing the converted digital data sent from the STM32.

An issue presented itself in the CCD display described before, as even after the CCD was verified to be operating perfectly using the input signals determined in the previous set of tests, with these signals directed straight from the output pins of the STM32, there was an issue of frame corruption in the ADC output. Frames would be cut off midway through a readout, despite the oscilloscope presenting a perfect output signal at the CCD's end. After comparing this oscilloscope data with the input voltage from the STM supplying the CCD, it was found that there was a correlation between corrupted frames and voltage increases at the 5V pin on the STM32. Capacitors were placed between the STM32's supply voltage pin and the CCD to counteract this, but the issue remained present, though at less frequent intervals. The problem was finally resolved by increasing the size of the direct-memory-access buffer being used by the STM32. While the frame corruption issue was still seen in 7.4 kB buffers, at 14.5 kB, it was eliminated. At this point, the transmitted CCD data was usable for integration testing with the optics system.

Unfortunately, this is where the final complications of our system presented themselves. During testing of the fully integrated optics system, the noise generated from extreme integration times became apparent. These tests could only begin once all breadboarding present in earlier phases of the project was replaced with the finalized printed circuit boards so that the entire system could be fit within our enclosure. This replacement process only finished during the final phase of the summer semester, leaving little time to determine the best approach to counteract the problems present at the integration times necessary for Raman spectroscopy systems.

9.5 Diffraction Grating Efficiency

The efficiency of a diffraction grating describes the proportion of incident power diffracted into a specific order. Optimizing the diffraction efficiency for our low-light application is particularly important, and a higher diffraction efficiency ensures that as much of the input light is preserved through the dispersive process. This efficiency is dependent on both the angle of incidence and the wavelength of the light.

Section 3.6.4 outlines our diffraction grating selection. The selected grating has a blaze wavelength of 500 nm, which is the closest blaze wavelength to our region of interest available commercially. Therefore, to maximize efficiency, we must regard the incident angle of the grating. This typically involves placing the grating at the blaze angle this corresponds to the Littrow configuration, where the incident and diffracted angles are the same. However, this is difficult to achieve with our reflective setup as the diffracted beam reflected onto the incident beam path. Therefore, in the initial designs of the spectrometer simulated through Zemax, an incident angle of -10° was chosen, as this was the closest we could get to the blaze angle while allowing for comfortability in placing the focusing lens and the detector. A transmissive grating was briefly considered to circumvent this issue, but its specified general efficiency for our spectral range was too low.

To test the efficiency of grating at various incident angles—we proceeded with the configuration shown in Figure 9.5.1. We ensured a collimated green laser pointer was aligned along an optical axis, then placed the diffraction grating mounted on a rotation mount in the path. We proceeded to measure the power of the +1 and -1 orders given varying incident angles. The grating from Thorlabs designates an arrow which describes the more efficient order relative to the incident beam. For further reassurance, we tested the efficiency when flipping the arrow.

Table 9.5.1 denotes the various power measurements for a given incident angle and first-order mode direction. The upwards arrow designates a right pointing arrow when faced with the incident beam, and the downward arrow designates a left point arrow when facing the input beam.



Figure 9.5.1 Diffraction grating testing setup

Table 9.5.1 Power measurements based on incident angle and first-order mode direction

		10°		0°		-10°	
		Trial 1	Trial 2	Trial 1	Trial 2	Trial 1	Trial 2
↑	M ₊₁	0.493	0.497	0.595	0.598	0.629	0.627
	M ₋₁	0.185	0.185	0.110	0.111	0.74	0.79
↓	M ₊₁	0.63	0.89	0.89	0.107	0.185	0.180
	M ₋₁	0.513	0.628	0.488	0.595	0.500	0.499

Given the results from Table 9.5.1, we found that the more efficient left and right first-order beams at an incident angle of 10° and -10° was diffracted at 26.8 degrees. Our desired spectral range would be diffracted at 29.1° to 36.5°. A 29.1° diffraction angle would be placed too close to the optical axis to fit the 50 mm lens and detector with regards to the mounts. At a 0° angle of incidence, we see that the power is maintained between the efficiency from the 10° and -10° angles of incidence. For our spectral range, this angle of incidence would diffract 550 nm at 41.3° and 640 nm at 50.2°, leaving enough space to fit our focusing lens and detector. Therefore, a 0° incident angle was chosen which would balance efficiency and comfortability in configuring the spectrometer system.

9.6 Spectrometer Performance

To evaluate the spectrometer's performance, we will use a fluorescent light source to assess the receivable spectral range and the system's resolvability. Fluorescent light bulbs are ideal for calibration due to their strong mercury and phosphor emission bands in the visible wavelength range. Specifically, the emissions bands from approximately 542 nm to 631 nm closely aligns with the expected detectable range of our system. Notably, some peaks are spaced by about 3 nm. Therefore, we can further estimate the system's spectral resolution by its capacity to differentiate between these peaks.

The resultant images of the fluorescent spectrum shown in figure 9.6.1 were taken with a Thorlabs CMOS camera. The photo containing the emission bands along the CCD was to get a sense of the wavelength spread across the detector. As a disclaimer, the resolution and spectral range of a spectrometer system are heavily determined by detector used. While we do expect different results when our system is interfaced with the CCD, this testing offered a sanity check.

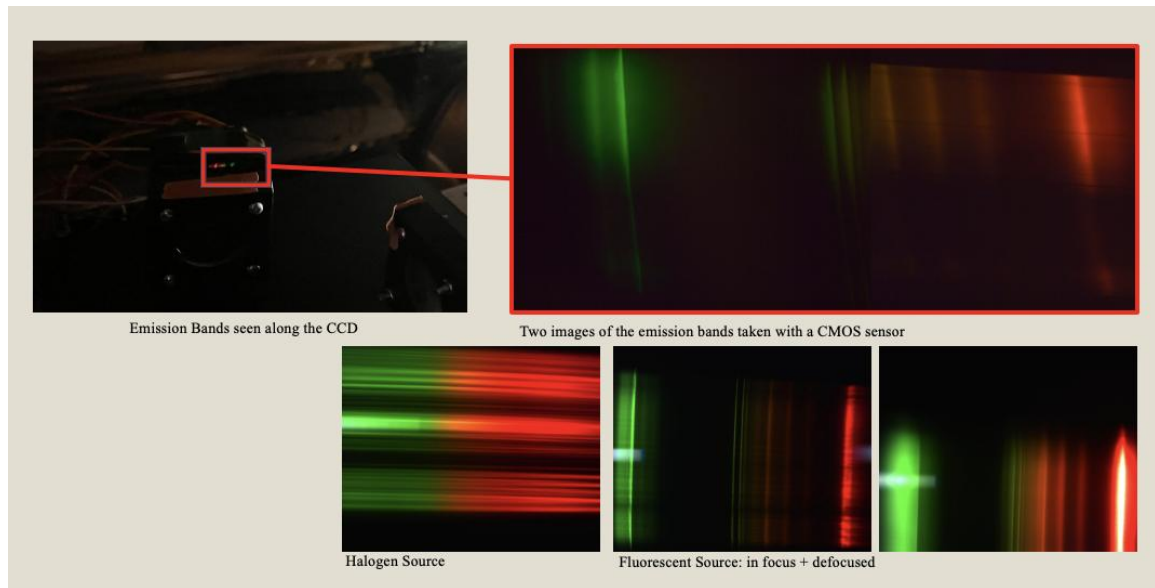


Figure 9.6.1 Spectrometer images

Using MATLAB, images from the Thorlabs camera were processed and calibrated by manually matching the most intense peaks from a fluorescent reference spectrum to the image, as seen in figures 9.6.2 and 9.6.3. A polynomial fit was used to convert pixel position to wavelength, followed by smoothing and normalization to produce clean, well-defined peaks. This experimental spectrum ultimately aligned with the reference spectral lines. To assess the resolution, we took the average full width at half maximum (FWHM) of the peaks across the two images, this resulted in an average 0.4579 nm FWHM. Which is within our spectrometer's resolution requirement. We know our spectral range requirement is met.

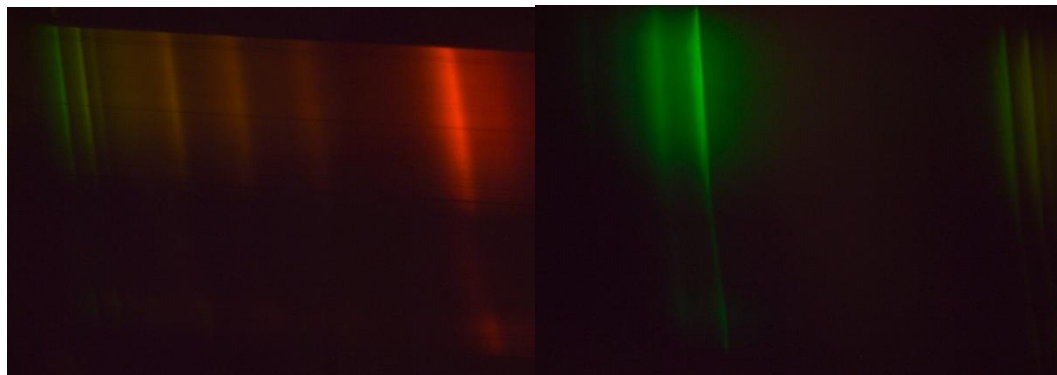


Figure 9.6.2 Spectral image of fluorescent bulb. Spectrum (a) left, spectrum (b) right.

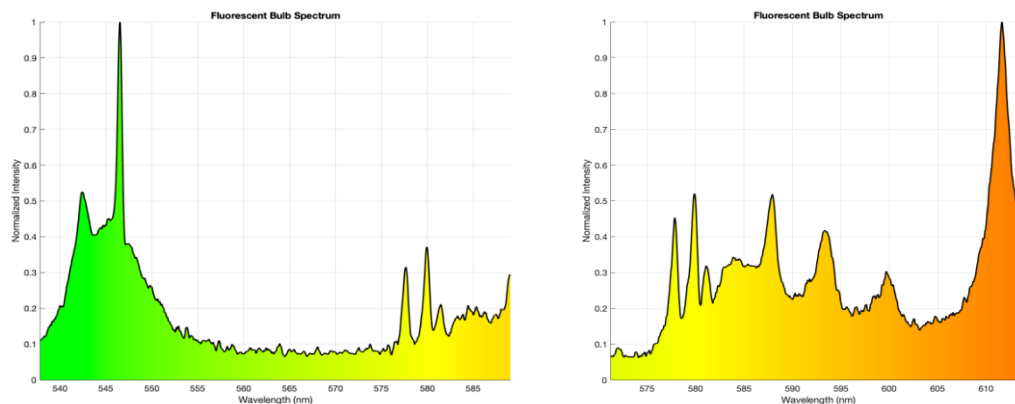


Figure 9.6.3 Corresponding spectral plot to spectrum (a) left, and spectrum (b) right.

Figure 9.6.4 shows a visual comparison of the same spectral portion of a fluorescent bulb from the Stellar Net commercial spectrometer and the spectrometer under TEX-RAY. One can see the peaks are more resolvable in our system.

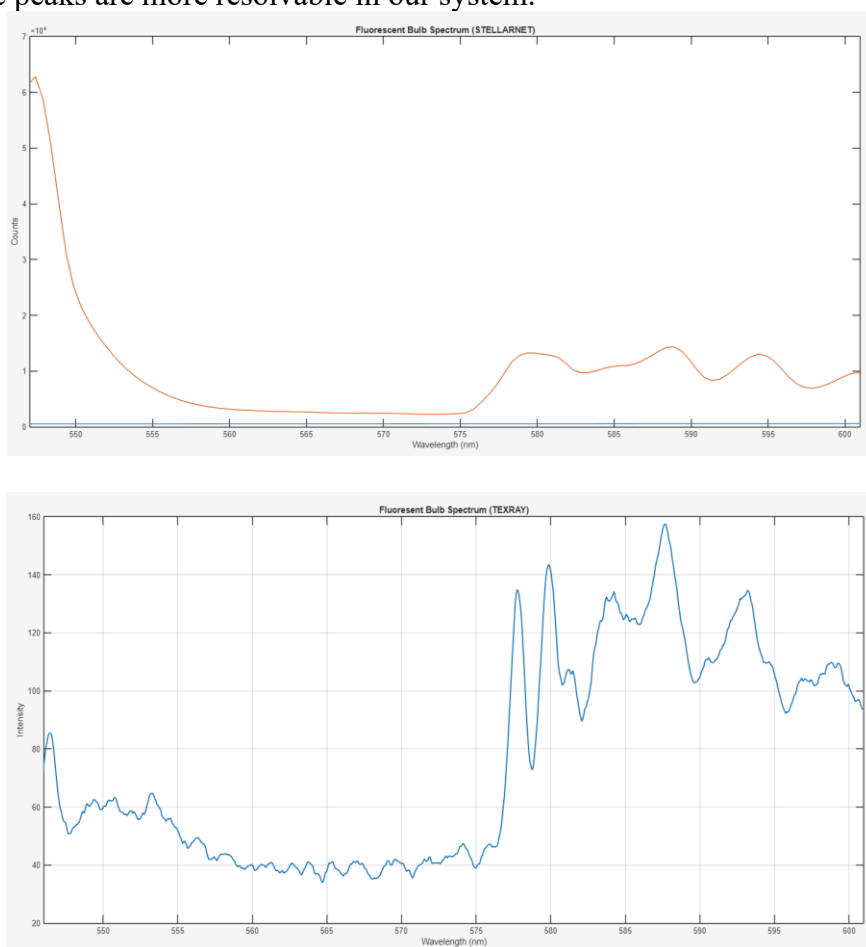


Figure 9.6.4 Fluorescent bulb spectrum from commercial spectrometer (top) and from TEX-RAY spectrometer (bottom).

We did ultimately get our CCD functional enough to detect the fluorescent bulb. The top of figure 9.6.5 shows the continuous frame input, while the bottom allows us to assess a single fluorescent bulb spectrum frame.

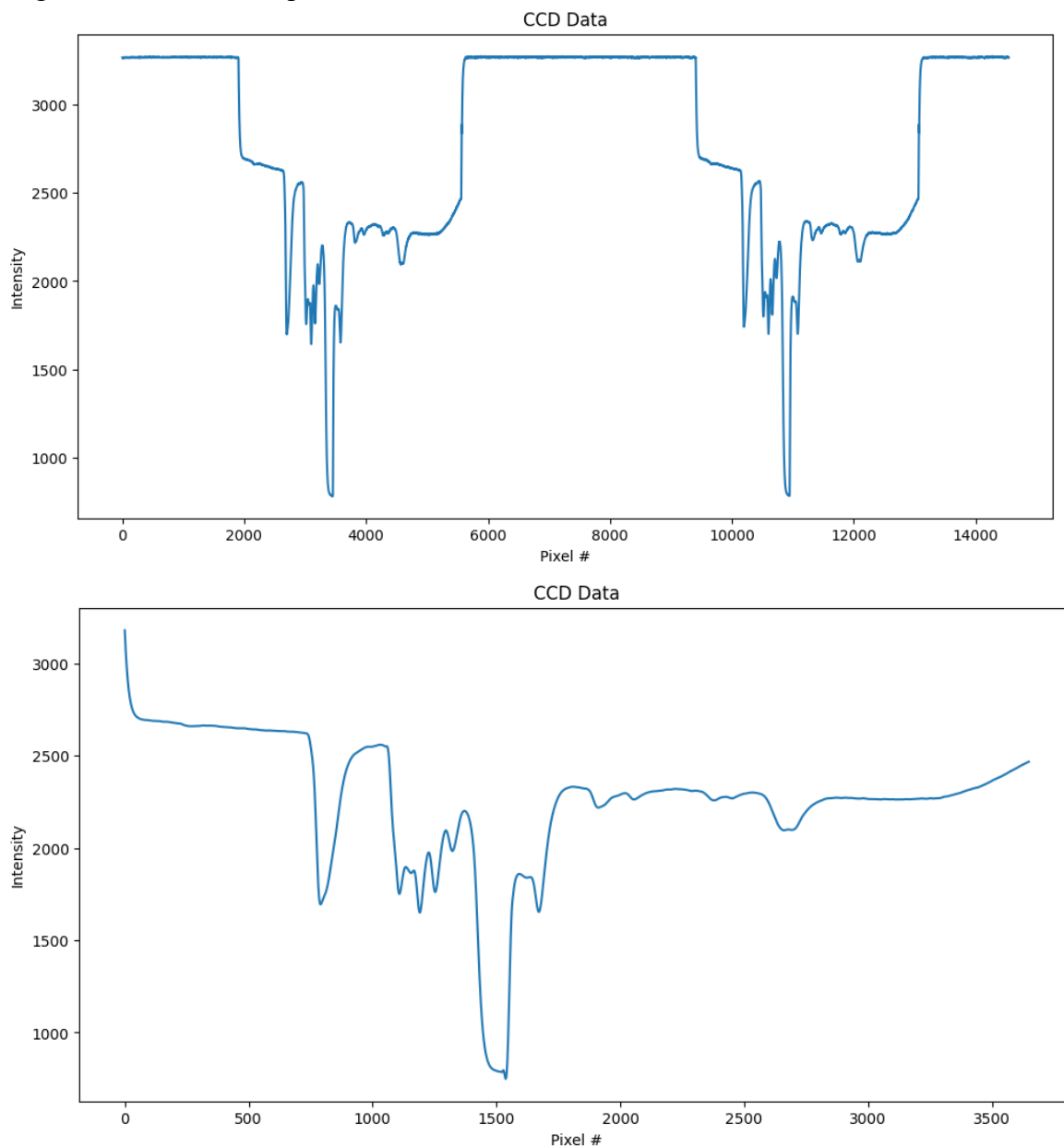


Figure 9.6.5 Continuous incoming signal from fluorescent bulb onto CCD (top) single frame freeze (bottom)

9.7 Aligning the Probe Optics with the Spectrometer

In the Raman spectrometer, the Chroma T550lpxr dichroic mirror paired with the Chroma ET542lp longpass filter were implemented to cutoff our excitation wavelength, 532.5 nm, to properly isolate the Raman shifted wavelengths. The filtering of our pump wavelength

paired with the low light nature of Raman scattered light does not allow one to discern light past the longpass filter, and consequently align the optical system past this point.

While the optomechanical design of the system with the use of rods and kinematic mounts on the mirrors help mitigate misalignments, visualizing the beam path past the filter is critical to maintain a properly aligned optical axis. To overcome this blind spot, we introduced light sources with a longer wavelength than 550 nm to align our system.

Rhodamine 6G is a fluorophore with an excitation wavelength at 532 nm and an emission wavelength between 550 nm to 580 nm, which can be detected past the 550 nm cut-on wavelength of the longpass filter. A solution of 1 μM of Rhodamine 6G and Methanol was prepared and placed at the sample location. With the 532-pump wavelength focused onto the solution, the dye fluoresced brightly, and the 580 nm wavelength emission was detectable throughout the system. We were then able to properly move the positions of the 75 mm achromatic focusing lens to ensure were properly coupling the light onto the spectrometer. Since the Rhodamine 6G 580 nm emission lies within the spectral range of the spectrometer, we were able to detect it onto the Thorlabs CMOS camera we were using in testing as seen in figure 9.7.1.

A HeNe can also be used along the sample pathway for alignment purposes as well. The HeNe's at our availability are pre-collimated, so to get the expected light activity throughout the system, it should be focused onto the 18 mm Edmund optics lens.

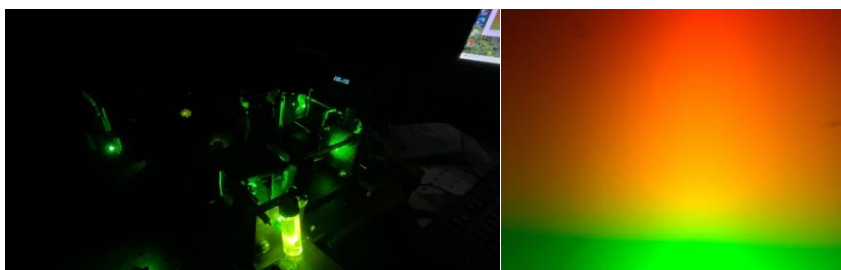


Figure 9.7.1 Rhodamine at sample input (left) Rhodamine spectrum (right).

9.8 Raman Signal Acquisition via CMOS

We tested the integrity of our Raman system using a Thorlabs CMOS detector since as discussed in Section 9.4, we could not get the CCD fully integrated into our system. After calibrating our system with a fluorescent bulb, we then took and processed an image of the Raman scattered light from acetone. The peak found at 552 nm shown in figure 9.8.1 aligns with references we've seen in literature regarding prominent acetone Raman peaks. Since the resultant images of the spectra were taken with a Thorlabs CMOS camera, and not our intended detector, this only gives an approximate sense of the performance of the system. However, this verifies our systems ability to produce, collect, and identify a Raman signal.

We were further able to produce an image of a Raman signal from cotton and polyester. Figure 9.8.2 and 9.8.3 explore the images and spectrum of the Raman signals from cotton and polyester at various input laser power levels. At lower power levels, the peaks are more

defined for both cotton and polyester. At higher power levels, we can see the broadening of the peaks which correspond to higher rates of fluorescence. Overall, both signals are saturated with fluorescence, these results are similarly seen as we couple the commercial spectrometer to the probe optics.

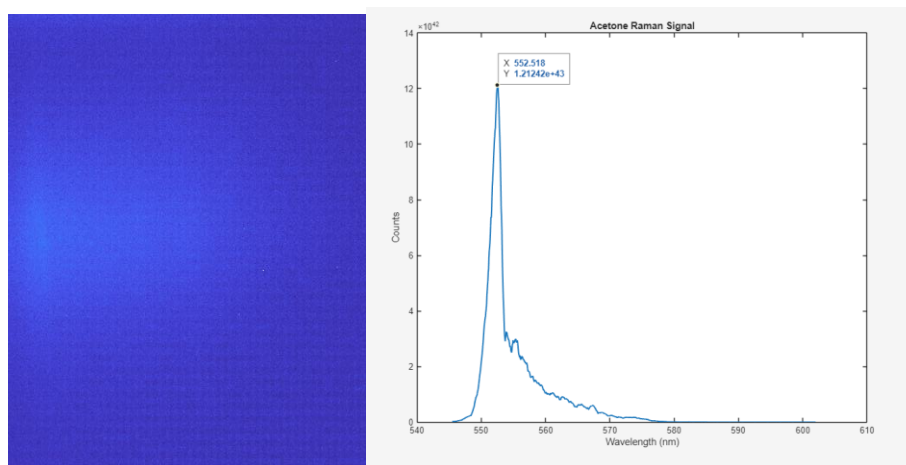


Figure 9.8.1 Raman spectrum of acetone acquired via CMOS.

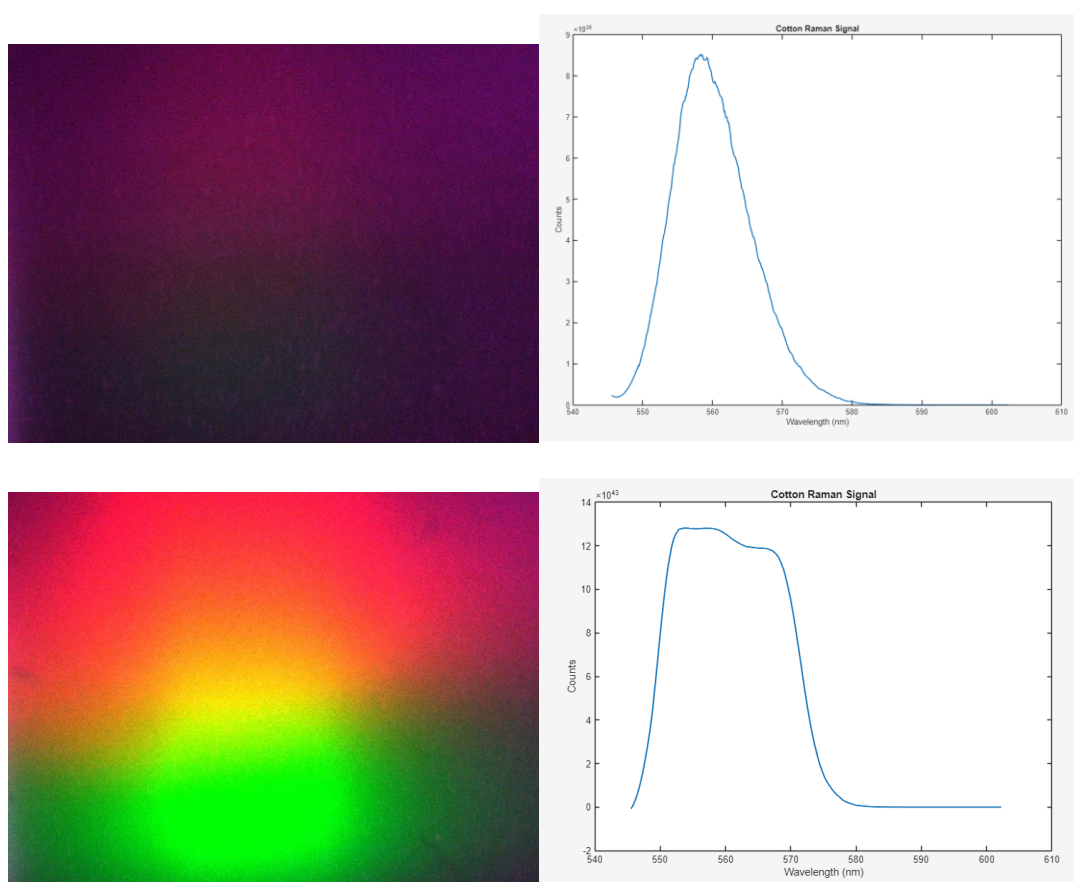


Figure 9.8.2 Image and corresponding spectrum plot of cotton with a lower power (top) and with a higher power (bottom)

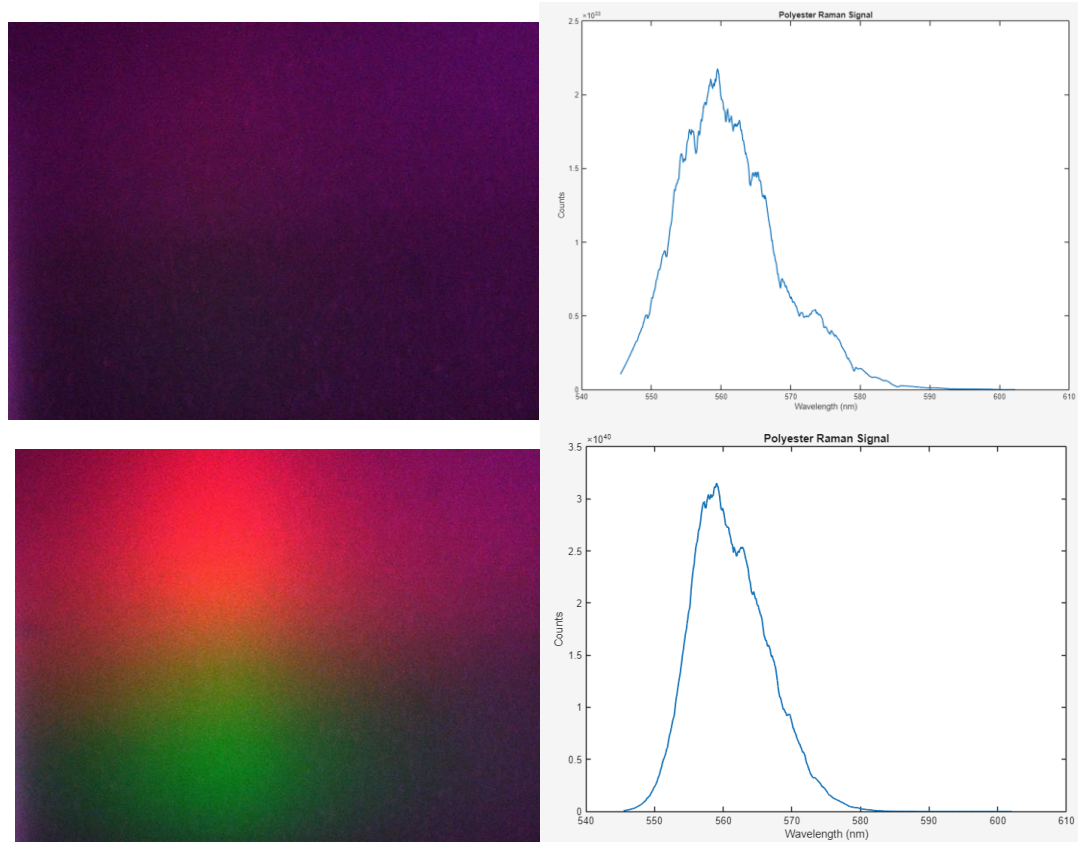


Figure 9.8.3 Image and corresponding spectrum plot of polyester with a lower power (top) and with a higher power (bottom)

10 Administrative Content

This section will give a detailed outline of the financial planning and budgeting that was implemented into the design process for our project, as well as the time management strategies used to keep project delivery on track for the course deadlines. Such strategies involved setting project milestones and dictating work distributions.

10.1 Budget and Financing

This Senior Design project did have two loaned optics courtesy of Chroma, and a few fabric samples courtesy of Test Fabrics Inc., but did not otherwise have an external sponsor, and was funded entirely by the 4 members of the team. We actively searched for a sponsor throughout the documentation and production of our system so as to improve system performance and implement higher quality components. The budget breakdown table lays out our initial estimates of the total project cost and the portion of our overall budget allocated to each individual component at the beginning of the research period.

Table 10.1.1 Budget Breakdown

Item	Cost per unit	Quantity	Total Cost
Laser diode	\$250	1	\$250
Laser diode driver	\$40	1	\$40
Dichroic mirror (Beamsplitter)	\$100	1	\$100
Long Pass Filter	\$50	1	\$50
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	\$67
Raspberry Pi	\$35	1	\$35
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			\$1,256.70

Our initial estimates for the overall cost of the fabric identification system were just over \$1200, which is less than half the price of the cheapest commercial fabric identification device. Every penny cheaper that we could make the project would be beneficial, as it would be further justification for our pursuit of this Senior Design project. Of course, while conducting research and actually choosing our workable components, performance had to

be equally balanced with the budget so as to make a genuinely competitive product compared to those currently on the market.

10.2 Bill of Materials

The Bill of Materials details the actual costs of all individually purchased components and reflects a more accurate total cost of our overall system, enabling a better comparison of our final product to commercial competitors.

Table 10.2.1 Bill of Materials

Item	Part number	Cost per unit	Quantity	Total Cost
Laser diode module	Q-BAIHE 532 nm laser module	\$43.98	1	\$43.98
Dichroic mirror (Beamsplitter)	Chroma T550lpxr	\$250	1	\$250
Long Pass Filter	Chroma ET542lp	\$365	1	\$365
Plano-convex Focusing Lens	Edmund Optics #48-423	\$31	1	\$31
VIS 0° Coated Achromatic Lens	Edmund Optics #47-639	\$120.84	1	\$120.84
Bandpass filter	Edmund Optics #26-981	\$74.20	1	\$74.20
Plano-concave lens	Thorlabs LC2969	\$30.74	1	\$30.74
Plano-convex lens	Thorlabs LA1509	\$25.04	1	\$25.04
Mirror	Edmund Optics #36-043	\$35.51	2	\$71.02
Slit	Thorlabs S50K	\$119.13	1	\$119.13
VIS 0° Coated Achromatic Lens	Edmund Optics #47-637	\$120.84	2	\$241.68
Diffraction grating	Thorlabs	\$128	1	\$128

	GR25-1205 Grating			
CCD	Toshiba TCD1304DG	\$34	1	\$34
PCBs		\$25.46	1	\$25.46
LCD	B0CXTFN8K9	\$32.99	1	\$32.99
Raspberry Pi	B0CK3L9WD3	\$69.49	1	\$69.49
ESP32 Development Board	B0718T232Z	\$9.99	1	\$9.99
3.3 Volt Regulator	LM2576SX- 3.3/NOPB	\$3.72	1	\$3.72
5 Volt Regulator	LM22679TJ- ADJ/NOPB	\$6.10	1	\$6.10
12 Volt Regulator	LM22679TJ- 5.0/NOPB	\$13.10	1	\$13.10
Battery power supply	PS12-BK60- LF60NA	\$53.47	1	\$53.47
CP2102	CP2102N-A02- GQFN28	\$4.32	1	\$4.32
STM32 Chip	STM32F401CCU6	\$5.20	1	\$5.20
ESP32 Chip	ESP-WROOM-32D	\$5.20	1	\$5.20
IC Components (Resistors, Capacitors, Inductors, LEDs, etc.)		\$56.14	NA	\$56.14
Fabric Samples		\$0	1	\$0
Total Cost				\$1819.81

The actual total cost of our project ended up being closer to \$1800, which is quite a bit more than we anticipated in our original budget. However, this price point is still significantly cheaper than the commercial products for fabric identification currently on

the market, which start at a base price of \$2500. This means that even though we went over budget, we were still able to achieve our goal of building a fabric identification system at a more competitive price point than the current market, without sacrificing quality and functionality.

10.3 Purchasing Status Summary

In order to help the team keep track of what components had been purchased and received, and what components still need to be purchased going into Senior Design II, this table was made and will be continuously updated.

Table 10.3.1 Part Purchasing Status

Part Name	Status
ams-Osram PL 520B Laser Diode	Received
Lazeerer Nanodrive V6 buck/boost driver	Received
Raspberry Pi 5	Received
Liquid Crystal Display	Received
Chroma T525lpxr Dichroic Mirror	Received
Chroma ET525lp Longpass Filter	Received
DTR-G-2 Collimating Lens	Received
MKS Newport KPX382-C Lens	Received
Edmund Optics #48-423	Received
MKS Newport F-MCC-T	Received
DIY- Optics Slit	Received
Edmund Optics #43-471	Received
Thorlabs GR25-1204 Grating	Received
Toshiba TCD1304DG	Received

10.4 Project Milestones

This section lays out important project deadlines that the group needed to adhere to for Senior Design I and II, as well as personal deadlines set amongst the group for the purpose of keeping the design process on track.

Table 10.4.1 Senior Design I Project Documentation Milestones

Task	Time Period	Start Date	End Date	Responsibility
Brainstorming	1 week	1/11	1/17	All
Finalize Project Idea	1 week	1/17	1/24	All

Divide and Conquer Document	1 week	1/17	1/24	All
Divide and Conquer Revision	1 week	1/24	1/31	All
30-Page Milestone	~1 month	1/31	2/24	All
80-Page Milestone	~1 month	2/24	3/23	All
80-Page Milestone Revision	10 days	3/23	4/4	All
110-Page Milestone	1 week	4/4	4/11	All
120-Page Milestone	1 week	4/11	4/18	All
Finalize and Submit Paper	4 days	4/18	4/22	All

While the above table set deadlines for progression in the 120-page report, the following tables allocated tasks to team members starting in Senior Design I and following into Senior Design II, based on major and respective responsibilities. This helped the team move along smoothly while focusing on separate overarching tasks concurrently.

Table 10.4.2 Senior Design I Project Design Milestones

Task	Time Period	Due 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 10.4.3 Senior Design II Project Design Milestones

Task	Time Period	Dates	Responsibility
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All Components Purchased	~2 weeks	5/31	All
PCB Testing	~1 month	6/9	Austin & Cameron
Data processing testing	~1 month	6/9	Austin
Illumination Path Alignment	~1 month	6/9	Ariana
Spectrometer alignment	~1 month	6/9	Danielle
Optical Systems Integration	~1 month	6/15	Ariana & Danielle
Total Systems Integration	~1.5 months	7/10	All
Short-form Report	~2 weeks	7/7	All
Peer Report	1 day	7/29	All
Practice Final Presentation	~2 weeks	7/24	All
Final Presentation	1 day	7/24	All

11 Conclusion

With TEXRAY, our Senior Design team set out to create an attainable at-home method of fabric authentication that rivals current market competitors in price and functionality. The average modern consumer is growing increasingly conscientious about the quality and ethics of the goods they purchase and the power of their dollar. In today's economy, people wish to invest their money into goods that they know will last and that they can feel good about buying. However, though buyers' attitudes towards shopping are changing, this change isn't always necessarily reflected in the attitudes of manufacturers and suppliers. Especially in the textile and clothing industry, it is not uncommon to find retailers who claim to be selling high-quality goods when, in fact, they are simply peddling knock-offs. For a consumer who is searching for a 100% cotton t-shirt, whether for environmental, aesthetic, comfort, or quality reasons, there is a significant chance that any listings that seem to meet this requirement are misleading or outright lying. Outside of attempting to vet retailers prior to purchasing from them as best as you possibly can, there are few means for the average consumer to be certain that the clothing they receive is truly as advertised.

There are existing products on the market available for consumers to purchase that are able to discern textile type and would enable at-home fabric authentication. However, the floor price for such products is still quite expensive and unreasonable for the average household, with the cheapest option still being about \$2500. This is because most of these authentication devices rely on NIR spectroscopy, which requires the use of very expensive InGaAs detectors, inflating their overall costs. Motivated by these issues, our group set out to design a textile identification device that can address consumer needs while reducing the price point as much as possible. To achieve these goals, we needed to identify an alternative to NIR spectroscopy that would still enable high-quality, accurate readings of spectra and would yield identifying characteristics distinct to each fabric type. In researching possible alternatives, we eventually found and settled on utilizing the concept of Raman shift and Raman spectroscopy in designing our system.

Raman spectroscopy in particular is a spectroscopy method that has a lot of potential for DIY and at-home system fabrication. In our research, we even came across systems that used broken CD's as a replacement for a diffraction grating and were still able to generate highly accurate Raman signals. There are countless scholarly and hobbyist examples of budget Raman spectroscopy systems, which was one of the primary motivating factors for our team landing on this specific technology, though we aimed to strike a balance between budget and system design quality. More importantly, however, Raman spectroscopy is particularly applicable to fabric identification, as the unique vibrational and rotational modes within the molecules of the fabric enables each textile type to have a characteristic "fingerprint" Raman shift, enabling highly accurate material identification.

Throughout the semester, our Senior Design team worked hard towards understanding the considerations that need to be made to create a functioning Raman spectroscopy system, and invested significant time into selecting what we believe to be the best components suited to accomplishing our goals. By dividing our system into sections and assigning these sections to our members individually based on major, we fostered the expertise necessary for each sub-system of our project to be designed with great attention to detail. The Raman signal collection optics were carefully chosen to ensure compatibility with our center wavelength while maximizing the spectral range of our system as much as possible, keeping budget in mind. Along these lines, lens diameters and focal lengths had to be carefully chosen such that Raman signal acquisition could be maximized. Given the low-power nature of Raman signals, and especially considering the absorptivity of textiles compared to, for example, liquid samples, every effort had to be made to maintain as much of our signal as possible as it propagates through the system before reaching the CCD detector. These same considerations were applied to all of the spectrometer optics, such as the collimating mirrors. The diffraction grating was selected such that the optical resolution of our system was as high as possible while maintaining the spectral range necessary to identify the key characteristic peaks of our fabrics of interest. One of the most integral components in our design was the CCD, as it had to be delicately chosen so as to ensure that it has the capabilities to detect very low power signals, likely in the picowatt range. Without a highly sensitive linear CCD array, we would not be able to detect any Raman signal or identify any fabrics. This component also contributed to dictating the spectral range we would be able to observe of our chosen fabrics' Raman signals. Additionally, the

proper electronics needed to be implemented into the system to be able to support these integral optical components. The PCB was designed with supporting these optical components in mind, powering our laser source as well as the CCD and enabling components like the Raspberry Pi to conduct signal analysis and display our acquired signal.

With so many factors to consider in mind, we conducted much testing throughout the semester to aid in understanding and achieving our goals. Most notably, we designed a rudimentary optics collection setup using mostly components available to us in the CREOL undergrad lab and demonstrated that we were, in fact, able to detect an accurate Raman signal from a liquid sample. This preliminary test gave us the confirmation we needed to prove that our system was feasible and could reasonably be accomplished within the Senior Design curriculum. It also gave us very useful insight into the spectrometer settings and configurations that we would need to implement into our handmade spectrometer to maximize Raman signal quality. Additionally, because CCD datasheets are known to be notoriously confusing, we set up preliminary wiring of our selected CCD to test its operation and responsivity, generating useful insights into what integration of the CCD into our full system will look like.

In Senior Design II, our team focused on integrating the components together into a fully assembled and operational Raman spectrometer for the purposes of textile identification and product authentication. This entailed fine-tuning our optical setup for maximizing alignment and signal acquisition, testing electrical wiring and PCB functionality, integrating signal analysis software, and finalizing the user interface to emphasize ease of use and simplicity. While we faced a series of problem regarding the full integration of our system, Chapter 9 details some of the major testing that demonstrates the extent of the functionality of TEX-RAY. Since the conception of the project, we knew that compensating for the low signal nature of the Raman signal would be difficult. With more time for testing and troubleshooting, we may have ultimately received a Raman signal from our integrated system alone. Nonetheless, the efforts put towards this project were not in vain. We were ultimately able to generate, collect, and differentiate Raman signals. We implemented a fully 3D-printed housing, developed a probe optic and spectrometer system, drove our system with custom electronics, and got the CCD functional for higher power signals after extensive troubleshooting.

Having committed a significant amount of time towards laying a solid foundation of knowledge and testing into our system, we believe that TEX-RAY represents a promising material authenticator prototype that is attuned to the needs of the modern consumer.

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14 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 WavelengthOptical 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.

$$v_0 = \frac{10^7}{\text{Excitation Wavelength (nm)}}$$

$$v_0 = \frac{10^7}{520 \text{ nm}} = 19230.77 \text{ cm}^{-1}$$

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

$$v_{\text{scattered}} = v_0 - \text{Raman Shift}$$

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

Step 3: Convert the scattered wavenumber to wavelength using:

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

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

✅ **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, $dv/dl \text{ (cm}^{-1}/\text{ mm)} = (d \cos(\theta)(v_0 - v_j)^2) / (mF)$. Where d is the spacing between grooves, $\cos(\theta) = 1$. v_0 is the absolute wavenumber of the laser, v_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

```

Prompt 5:

What are the most lightweight or fastest methods of implementing dynamic time warping?

Output 5:

The fastest and most lightweight implementations of dynamic time warping (DTW) focus on reducing computational complexity while maintaining accuracy. Below are the key approaches and algorithms:

Constraint-Based Methods

These methods limit the search space in the cost matrix:

- **Sakoe-Chuba Bands** and **Itakura Parallelogram**: Restrict the warping path to a fixed-width window around the diagonal, reducing the number of evaluated cells [1][2][6].
- **Implementation**: Adjust the window width parameter K to balance speed and accuracy (e.g., $K=10$ in FastDDTW) [4].

Multilevel Approximation (FastDTW)

FastDTW is a leading linear-time approximation:

1. **Coarsening**: Downsample time series to lower resolutions.
 2. **Projection**: Compute a low-resolution warp path and refine it iteratively at higher resolutions.
 3. **Refinement**: Apply constrained DTW within a small window around the projected path [2][6].
- **Complexity**: $O(N)O(N)O(N)$ time and space, vs. $O(N^2)O(N^2)O(N^2)$ for standard DTW <https://cs.fit.edu/~pkc/papers/tdm04.pdf> [2].

Specialized Variants

- **PrunedDTW**: Prunes unpromising paths early using heuristics [1][6].
- **SparseDTW**: Exploits sparsity in the cost matrix for efficiency [6].
- **MultiscaleDTW**: Combines multiple resolutions for faster computation [1][6].

Lower Bounding Techniques

Accelerate similarity search by filtering out non-promising candidates:

- **LB_Keogh**: Computes a lower bound using envelope constraints [1].
- **LB_Improved** and **LB_Enhanced**: Tighter bounds with similar computational efficiency [1].

Code Example (FastDTW)

python

```
from fastdtw import fastdtw
distance, path = fastdtw(series1, series2, radius=5)
```

This uses a constrained search window (radius) to approximate DTW [2][4].

Comparative Trade-offs

Method	Speed	Accuracy	Use Case
FastDTW	High	Moderate	General
Sakoe-Chuba	Medium	High	Constrained alignment
LB_Keogh	Highest	Low	Pre-filtering

For lightweight applications, **FastDTW** or constrained DTW with small window sizes are typically optimal [2][4][6].

Thread Link:

(<https://www.perplexity.ai/search/what-is-the-most-lightweight-o-J7hGxYBhRAykyIRpNzNP1g?0=d>)