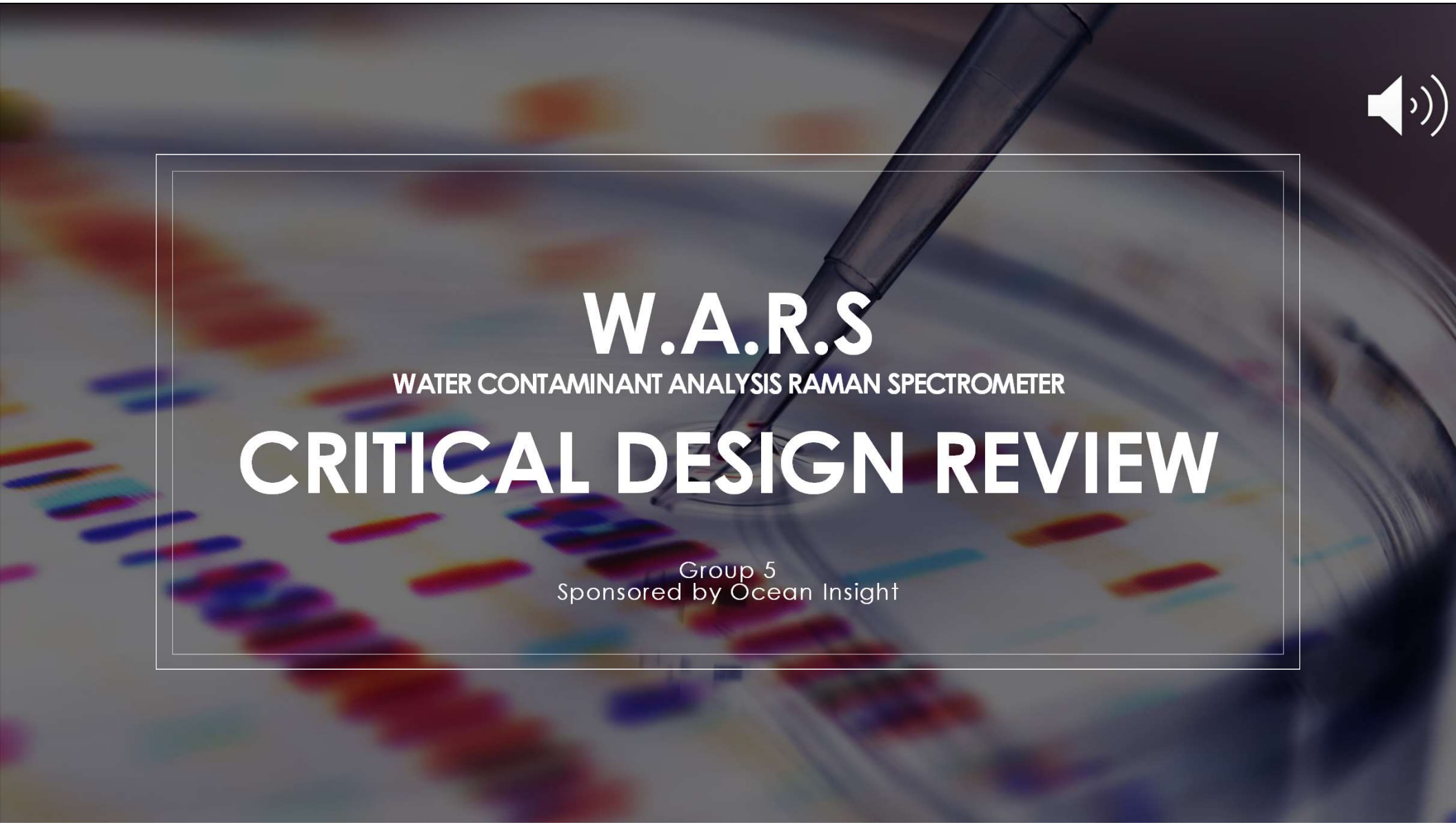


W.A.R.S

WATER CONTAMINANT ANALYSIS RAMAN SPECTROMETER

CRITICAL DESIGN REVIEW

Group 5
Sponsored by Ocean Insight

Our Team

George McDonald

Photonic Science & Engineering

Julia Augustin-Smith

Photonic Science & Engineering

Sebastien Jouhaud

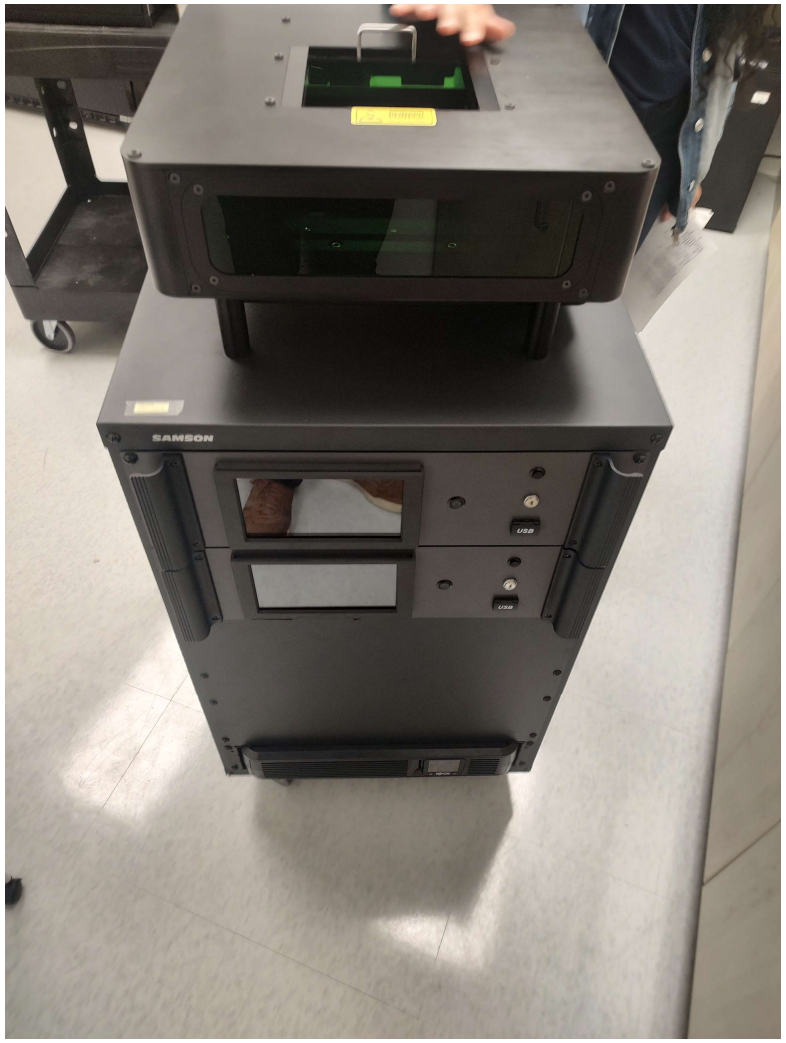
Computer Engineering

Gibran Khalil

Electrical Engineering

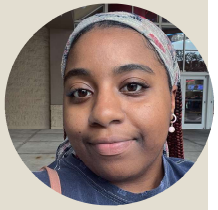
Juan Restrepo Diaz

Electrical Engineering



Water Analysis Spectrometer

- Owned by our sponsor Ocean Insight
- A spectrometer and its illumination system are important tools to help give knowledge that could not be acquired either way. It is a method of understanding molecules and how they interact with light. By analyzing the amount of light absorbed or emitted through a sample we can determine the characteristics of the sample.



Julia - CREOL

OceanOptics

Sponsor Benefits

Project Motivations

The overall quality of our drinking water is vital to the health and well-being of all living species on planet Earth, including humans.

Due to all the different sources of water, knowing which ones are safe to drink is essential to avoiding any kind of infections from water contaminants.

The goal behind our project is to create a water quality analyzer using Raman spectroscopy.

Julia - CREOL

Project Goals

The goal of this project is to build a portable, cost-effective Raman spectrometer that focuses on mainly measuring the contaminants in different water samples. The main goals of this project is the cost, size and ease of use.

- Cost
- Size
- Ease of Use

Julia - CREOL

Project Objectives

The **core objectives** of this project are to develop a compact spectrometer that contains simple mounted optics.

The **advanced objectives** use a combination of a well-plate reader and a detachable spectrometer to achieve a modular set-up. We will be using a 785 nm wavelength Raman laser and reduce fluoresce from signal.

Engineering Specifications

Requirement #	Requirement Specification
1.0	The system will have the ability to analyze 3 different contaminants that is in water.
2.0	Spectral range should be up to 885nm.
3.0	The system's processing time will be < 5 minutes.
4.0	Laser should be 785 nm
5.0	Sample size must not exceed 40 mL to fit in the reservoir of the reader.
6.0	Laser should not exceed 50 mW.
7.0	Spectrometer dimensions around 3.5" x 2.5" x 1.2"
8.0	Resolution of system no more than 20 cm^{-1}.
10.0	System will begin operating 1 second after safety interlocks are engaged.

Project Features

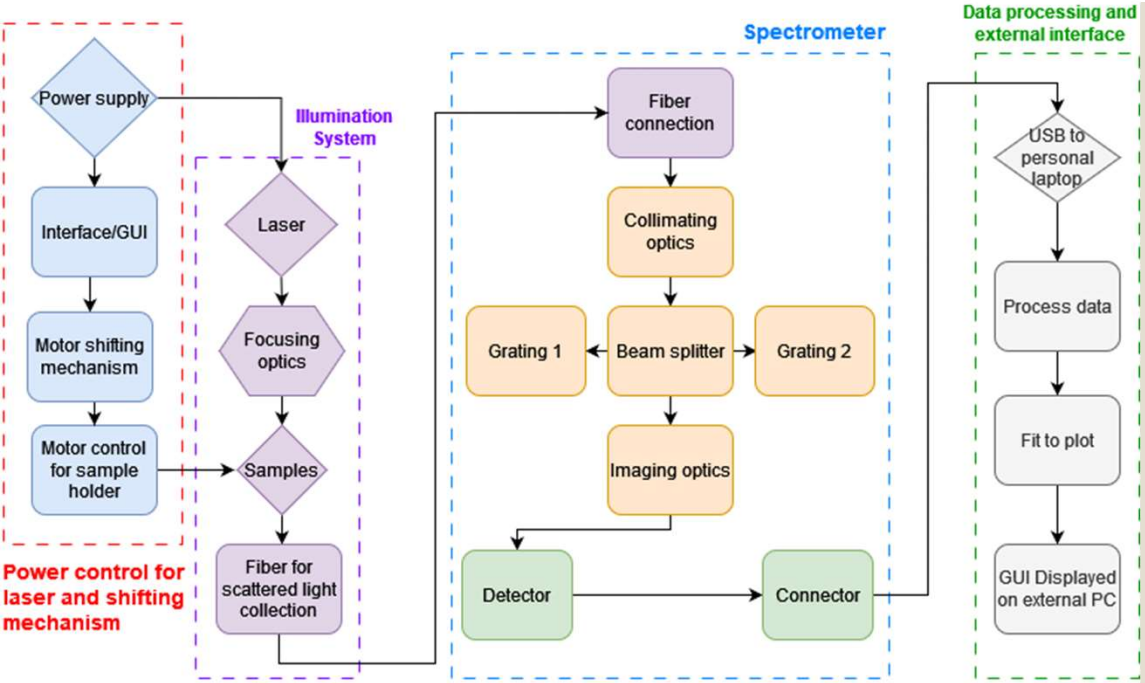
COMPUTER APPLICATION

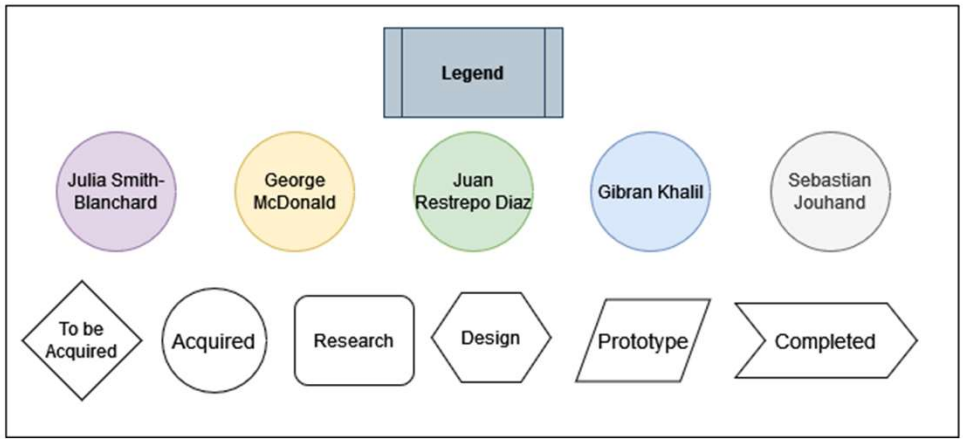
CONTAMINATION DETECTION

MODERATE SPEED

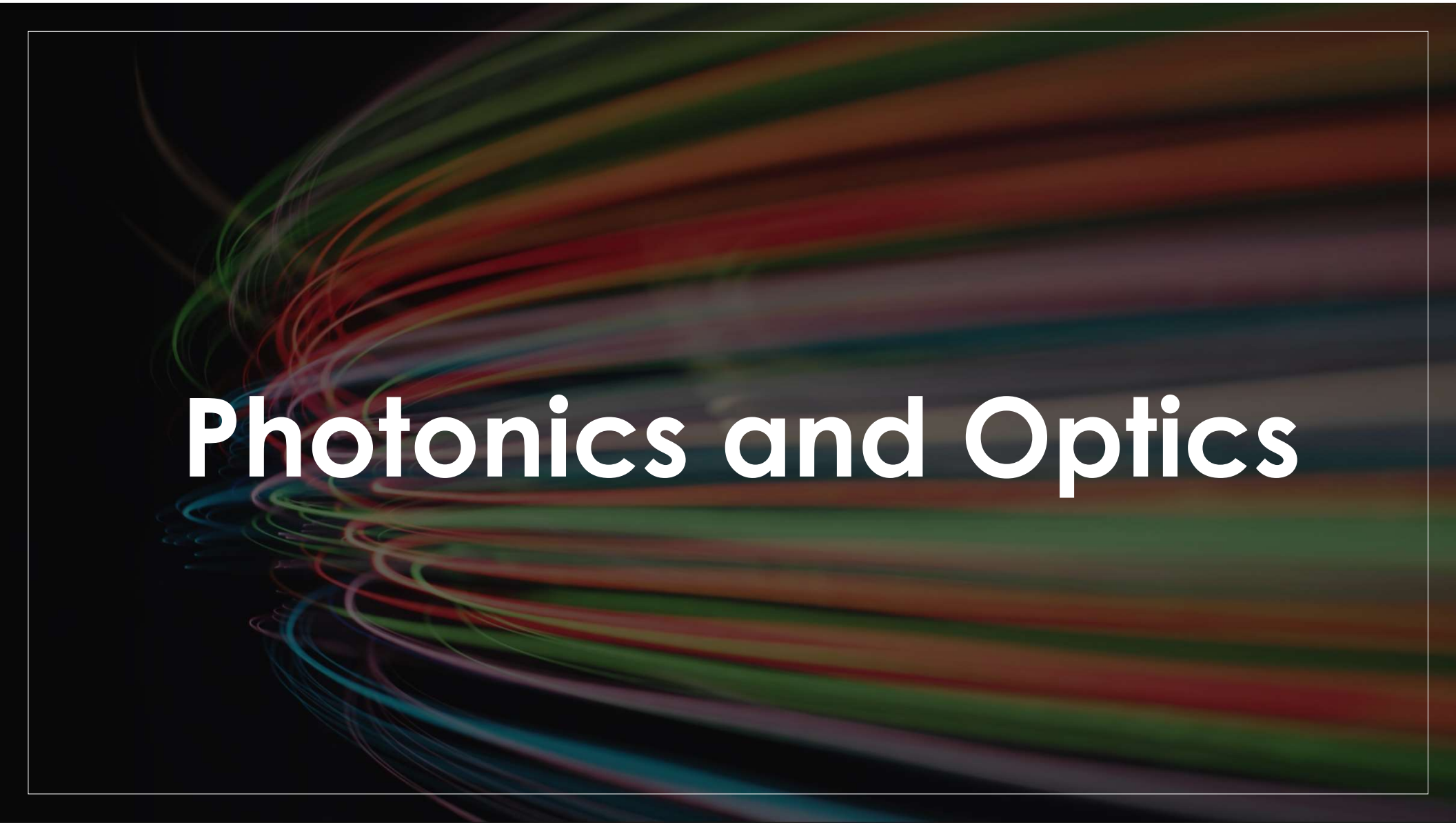
X AND Y TABLE

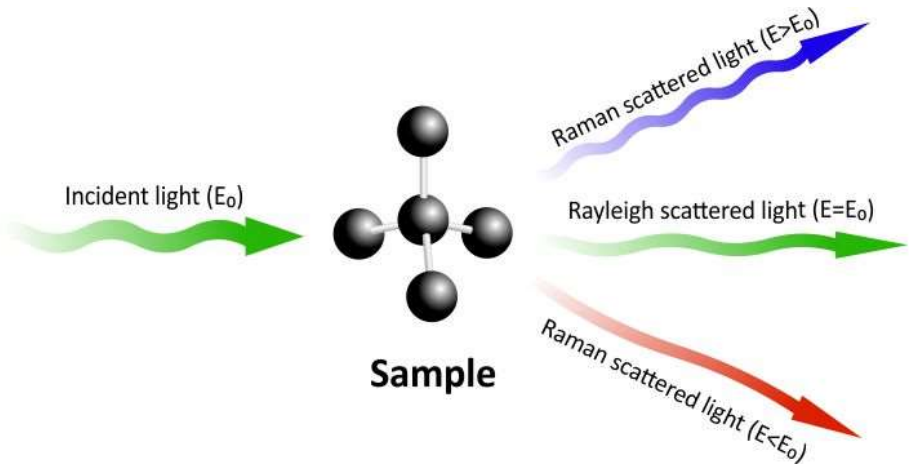
INSTANTLY MEASURE OVER 5 SAMPLES

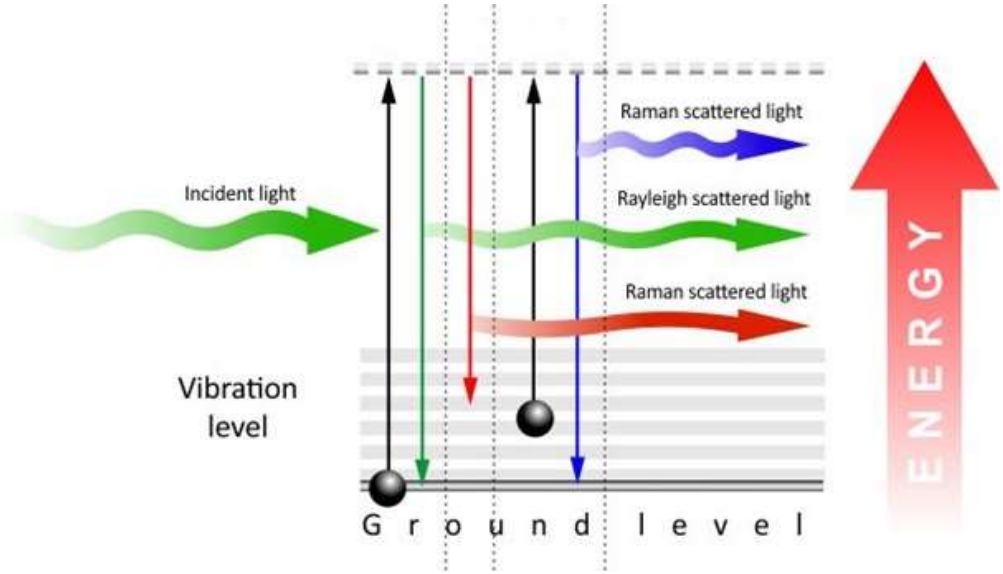




Block Diagram – Overall System


Photonics and Optics





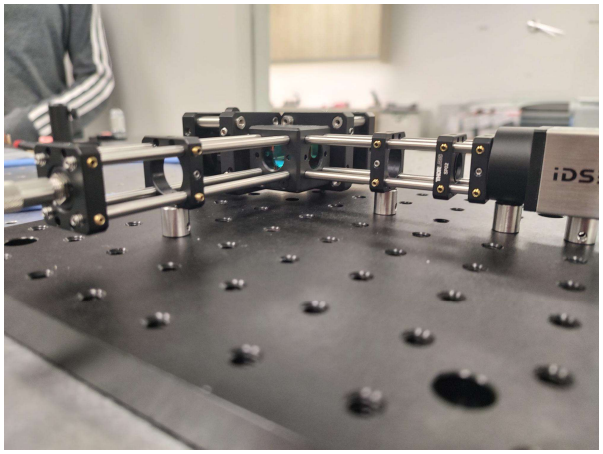
Brief Explanation of Raman Spectroscopy

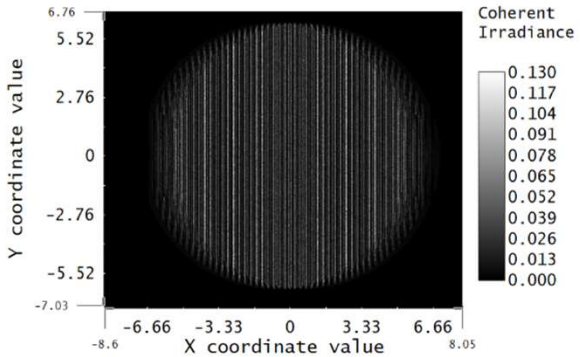
Light Interaction

- Laser light interacts with sample
- Laser light causes molecules to vibrate in *unique* ways.
- Small fraction of light is Raman scattered.

Sample Identification

- Scattered light contains information about molecular vibrations.
- For some scattered light, there is a wavelength shift.
- Analyze intensity and wavelength to identify the material.





Spatial Heterodyne Spectrometer (SHS) - 1

1) Light collection & processing

SHS collects and processes scattered light.

Light is split 50/50 and diffracts off two gratings.

Gratings must be of equal distance to beam splitter.

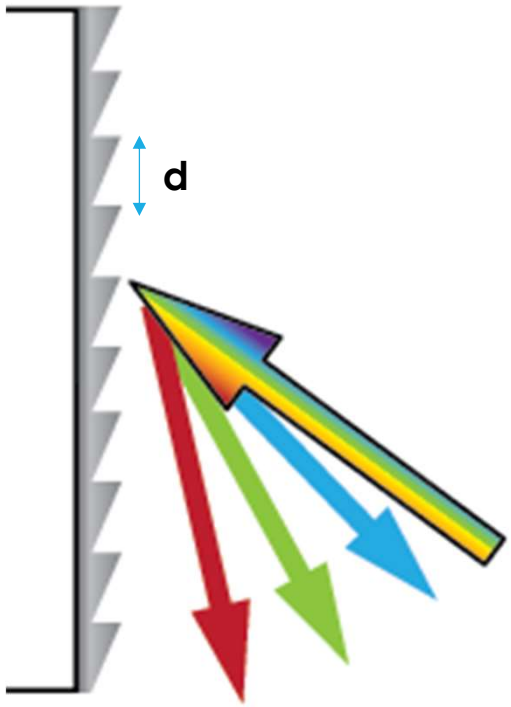
2) Image

Forms at detector.

Fizeau fringes form due to interference.

Image processing reveals different frequencies/wavelengths.

Julia - CREOL



SHS Design Equations

Grating Equation: $k[\sin(\theta_L) + \sin(\theta_L - \gamma)] = \frac{m}{d}$

Littrow Angle: $\theta_L = \sin^{-1}\left(\frac{n\lambda}{2d}\right)$

Fringe Equation: $v_F = 4(k - k_L)\tan(\theta_L)$

Resolving Power: $R = (2)(groove\ density)(grating\ width)$

Spectral Range: $SR = \frac{(number\ of\ pixels\ along\ detector)(\lambda)}{2R}$

Resolution (nm): $FWHM = \Delta\lambda = \frac{\lambda}{R}$

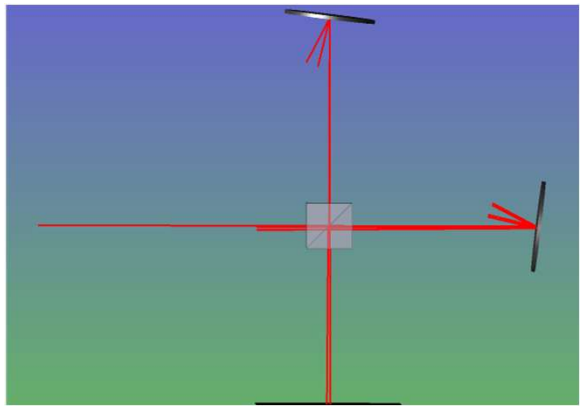
Resolution (cm^{-1}): $\Delta\omega = (10^7)\frac{\Delta\lambda}{(\lambda_{exc})(\lambda)}$

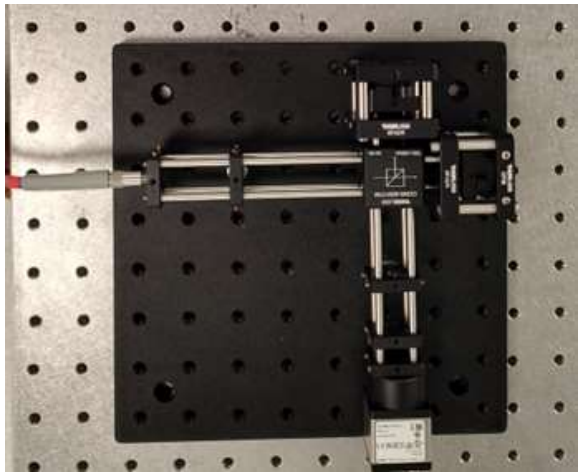
Raman Shift (nm) = $\lambda = \left(\frac{1}{\lambda_{exc}[nm]} - \frac{1}{\frac{Raman\ shift\ [cm^{-1}]}{10^7}}\right)^{-1}$

Design Parameter	Unit	Value
Laser Excitation Wavelength	[nm]	785
Number of pixels (N)	[#]	1936 (horizontal)
Groove Density	[Lines/mm]	300
Optics Width	[mm]	12.7
Calculation Result	**Unit**	**Value**
Littrow Angle	[°]	6.7623
Resolving Power	[Lines/mm][mm]	7620
Spectral Range	[nm]	99.7218
Resolution (FWHM)	[nm]	0.1030
Resolution (k)	$[cm^{-1}]$	1.6718
Band	[nm]	~885

Spatial Heterodyne Spectrometer - 2

- **Design Challenge:**
  - SHS compactness.
  - Resolving power and spectral range tradeoff.
  - Appreciate high resolution, increase spectral range to analyze a variety of contaminants.
- **Proposed Solution**
  - Using longer laser wavelength.
  - Balance grating size and groove density.
- Selected grating, detector, and laser determines a variety of factors.





Spatial Heterodyne Spectrometer - 3

- **SHS Prototype Key Specifications:**
  - ½ optics mounted on 16mm cage system.
  - Grating Angle – 6.7623°
  - Resolution – 0.1030nm
  - Spectral Range – Up to 885nm

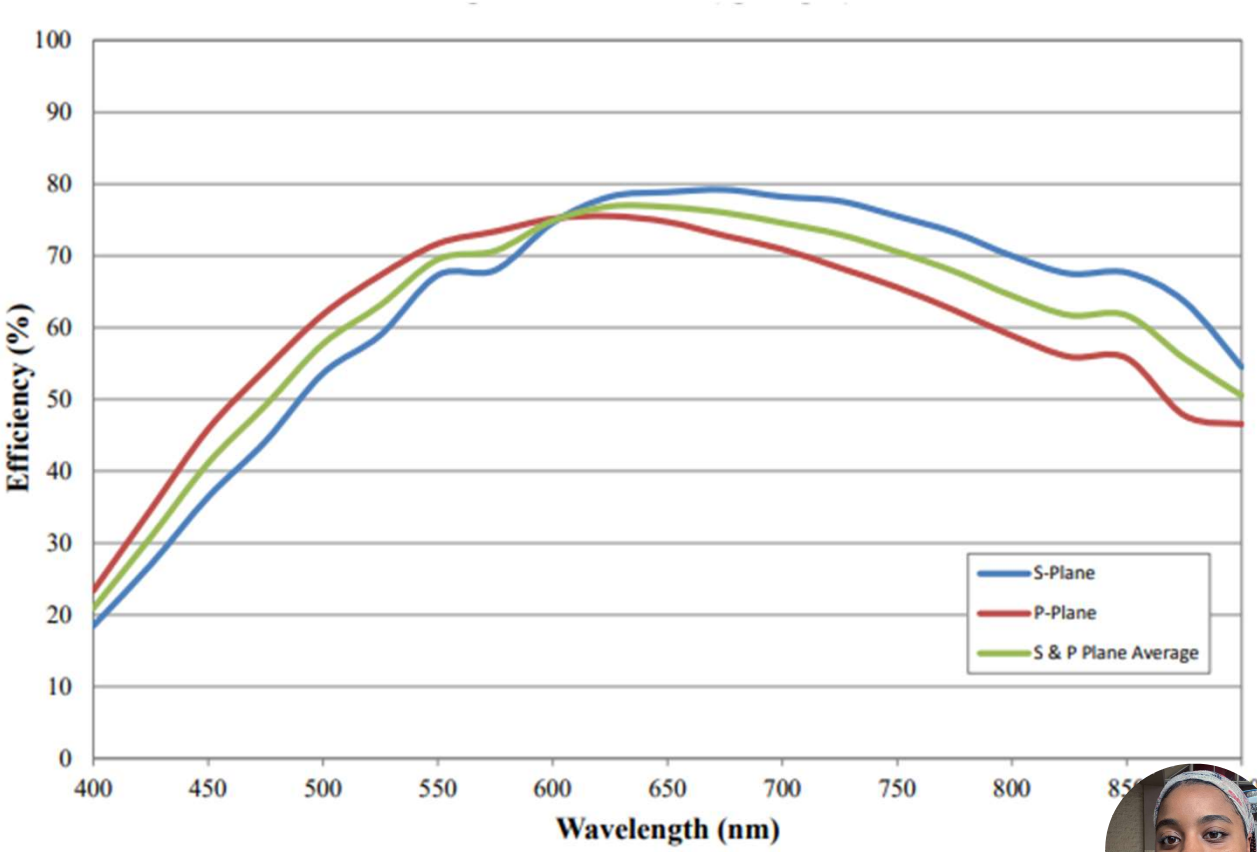
- Image above is a 3D model developed in ZEMAX.
- Image below is an image of the SHS prototype.

Optical Components - 1 Diffraction Grating Selection

Diffraction Grating	Edmund Optics (Richardson Grating)	Edmund Optics (Richardson Grating)	Thorlabs (GTU13-03)
Groove Density (grooves/mm)	300	150	300
Blaze Wavelength (nm)	760	300	235
Length x Width (mm)	12.5 x 12.5	12.5 x 12.5	12.5 x 12.5
Peak Efficiency (%)	79	61	- 55

Julia - CREOL

Optical Components - 2 Diffraction Grating Selection



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Optical Components – 3 Beam Splitter Selection

Diffraction Grating	CCM5-BS017 (non-polarizing)	CCM5-PBS202 (polarizing)
Wavelength Range [nm]	700 → 1100	620 → 1100
AR Coating	$R_{avg} < 0.5\% \; at \; 0° \; AOI$	$R_{avg} < 0.5\% \; at \; 0° \; AOI$
Material	N-BK7 1.5111 @ 785nm	N-SF1 1.7174 @ 785nm
Max Transmitted Beam Deviation	< 5 arcmin	< 5 arcmin
Reflected Beam Deviation	90±arcmin	90±arcmin

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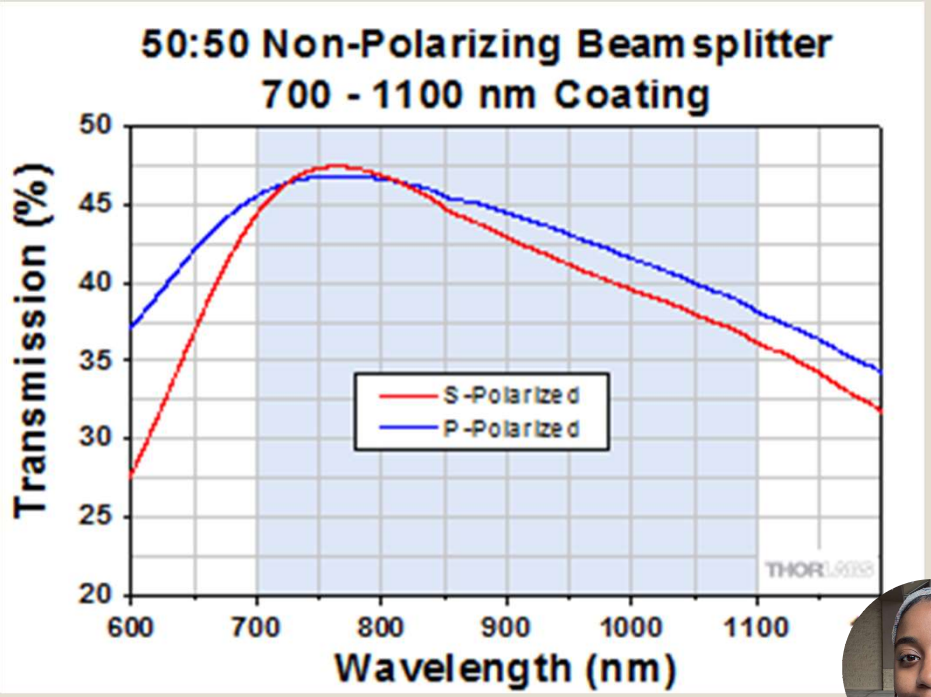
Optical Components - 4 Beam Splitter Selection



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Optical Components - 5 Laser Selection

- L1C-785 Oxxius laser communicates with PC through serial commands.
- Toggle emission, shutter, and intensity remotely.
- User may control laser through GUI.

IR Laser	L1C-785 Oxxius	Cobolt 08-NLD	Ondax LM-Series
Emission Wavelength [nm]	785 ± 10	784.8 ± 0.5	785 ± 0.5
Linewidth [nm]	≤ 1.2	≤ 0.07	≤ 0.0001
Fiber coupled output power [mW]	≤ 100	≤ 500	≤ 175
Beam Size (mm)	0.7 @ 100 mW (circularity ≥ 90%)	1.4 x 1.7 @ 500 mW	0.8 x 0.4 @ 175mW
Module Dimension (mm)	100 x 40 x 40	142 X 40 x 43	100 x 40 x 42.5

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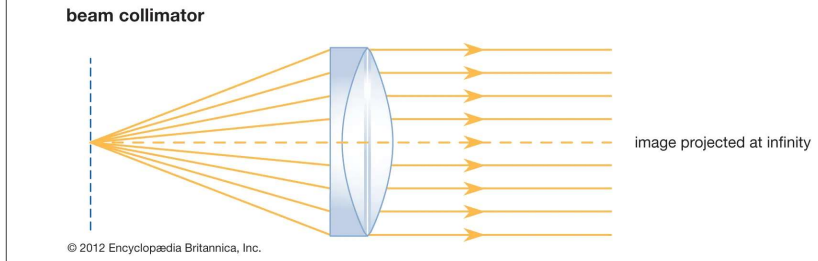
Optical Components - 6 Collimator Design



C20SMA-B - Achromatic Fiber Collimator, f = 20 mm, 650 - 1050 nm

- A collimator lens is important design of the spectrometer because it changes the diverging point source to a parallel beam.

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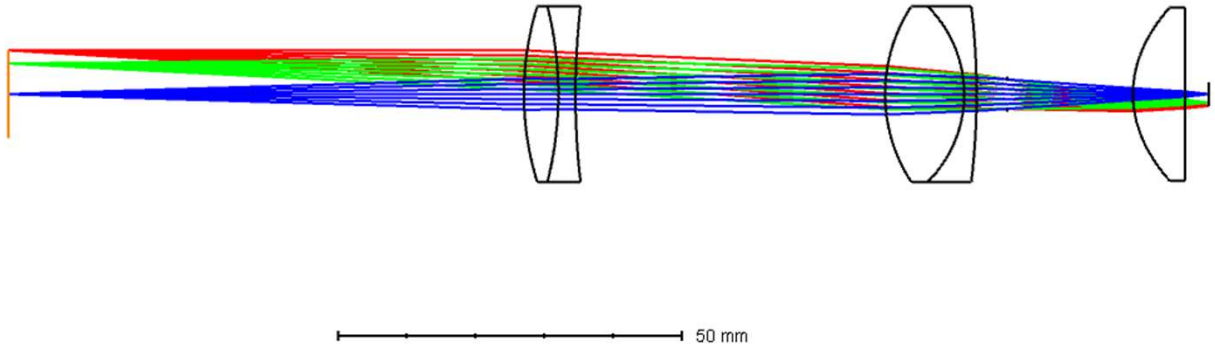
Optical Components - 7 Lens Design

Imaging Components	AC254-150-B	AC254-035-B	AL2520-B
Lens Type	Achromatic Doublet	Achromatic Doublet	Aspherical Singlet
Material/ Index @785nm	N-BAF10 / 1.6605 N-SF6HT / 1.7853	N-BAF10 / 1.6605 N-SF6HT / 1.7853	S-LAH64 / 1.7767
Thickness [mm]	Glass 1: 5 mm Glass 2: 2 mm	Glass 1: 11.5 Glass 2: 1.8	+7.6
Radii [mm]	Glass 1: 42.69 Glass 2: -52.00	Glass 1: 23.15 Glass 2: -17.87	+15.54
Diameter (mm)	25.4	25.4	25

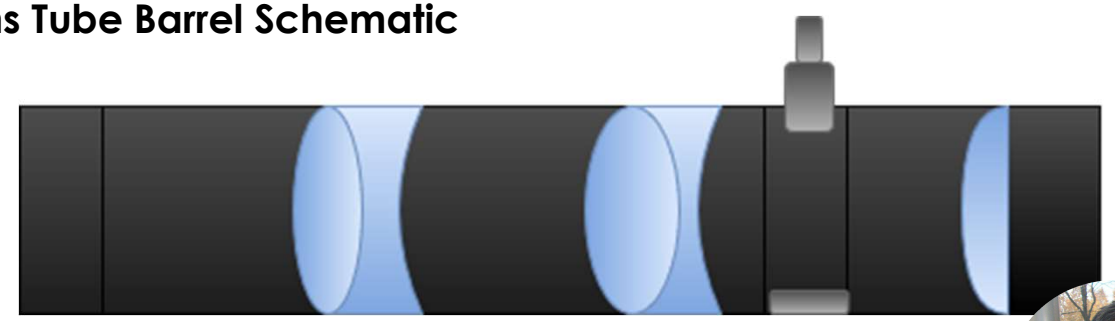
Optical Components - 8 Imaging Design

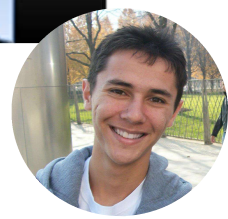
Zemax Design

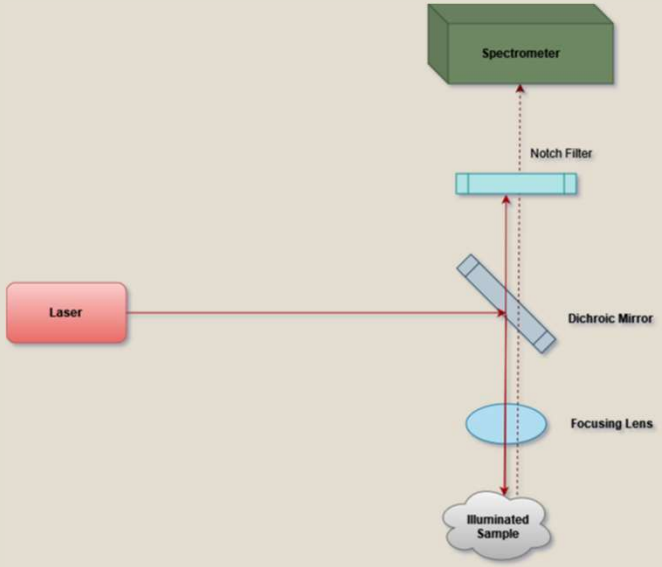
- Working Distance: ~75mm
- Image Distance: ~ 3.4mm from last surface
- Total optical track length: 99.6mm
- Effective Focal Length: 53.21mm

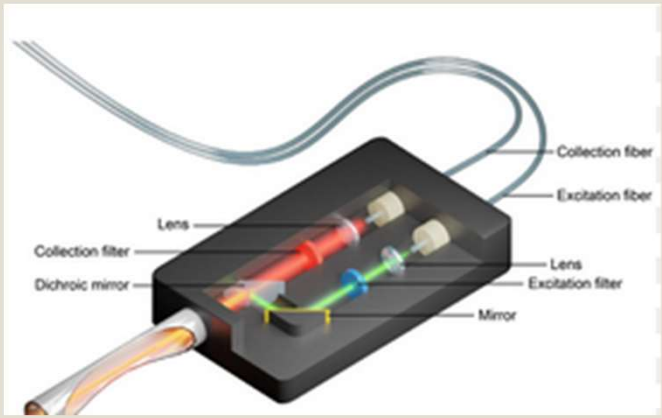


Lens Tube Barrel Schematic









Illumination System - 1

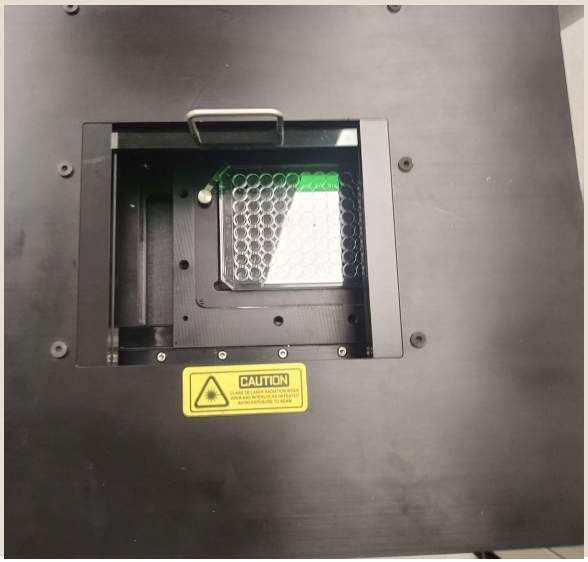
Laser is 785nm.

Dichroic mirror redirects laser beam to sample.

Scattered light passes through dichroic mirror.

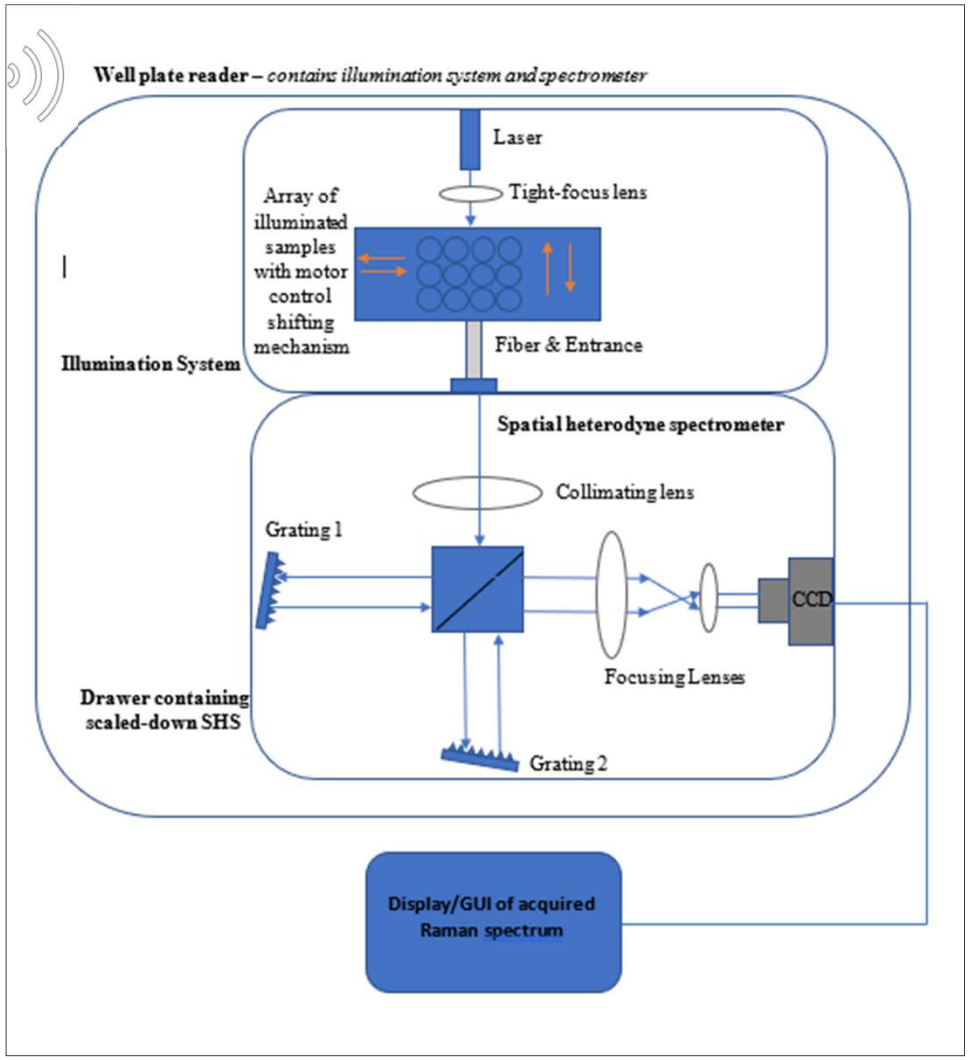
Directed through collection fiber.

Notch filter removes 785nm and preserves all other wavelengths passed to the SHS.



Illumination System - 2

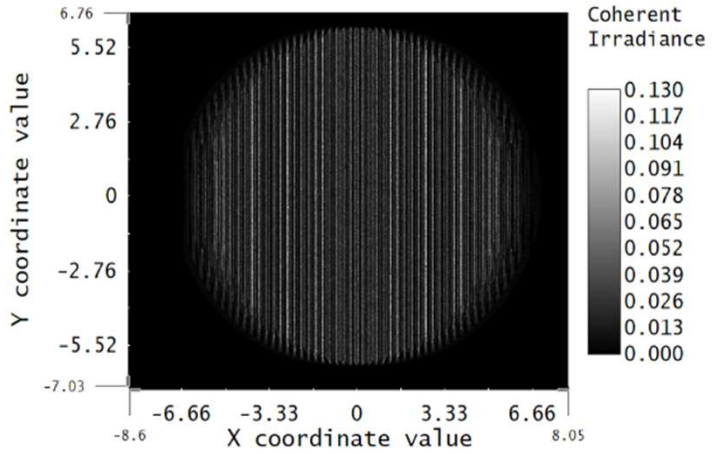
Component	Quantity	Important Characteristic
Notch Filter	1	Stops 785nm
IR Laser (Oxxius)	1	785nm
Shielded Fiber PM-780-HP	2	Wavelength Range: 780-1100nm
Emitting Fiber	1	Large Numerical Aperture
Achromatic Fiber Collimator	1	Focal length TBD
Well-plate	1	Round-cuvettes with flat strike surface



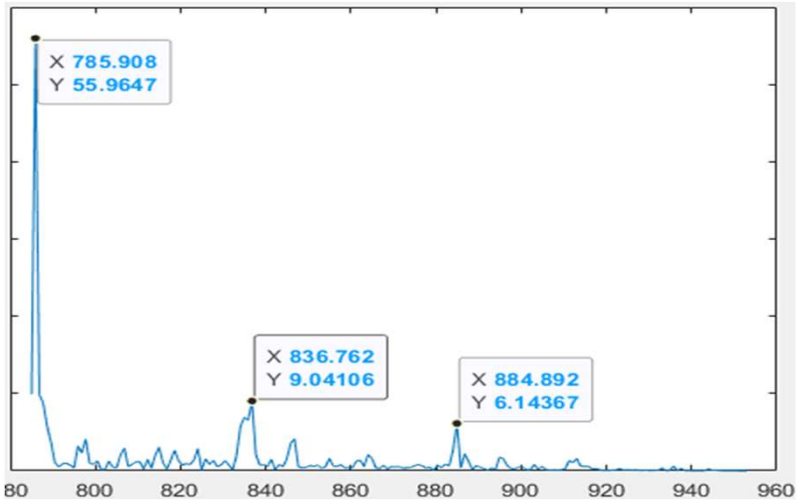
Layout of optical components

- **Illumination System**
  - Laser light guided to sample through emission fiber.
  - Sample is struck by laser light.
  - Collection fiber accepts scattered light.
- **SHS**
  - Accepts input light.
  - Composed of laser light, scattered light, Raman signal.
  - Scattered light splits, diffracts, and recombines.
  - Fringe image lands on detector to be processed.

Julia - CREOL



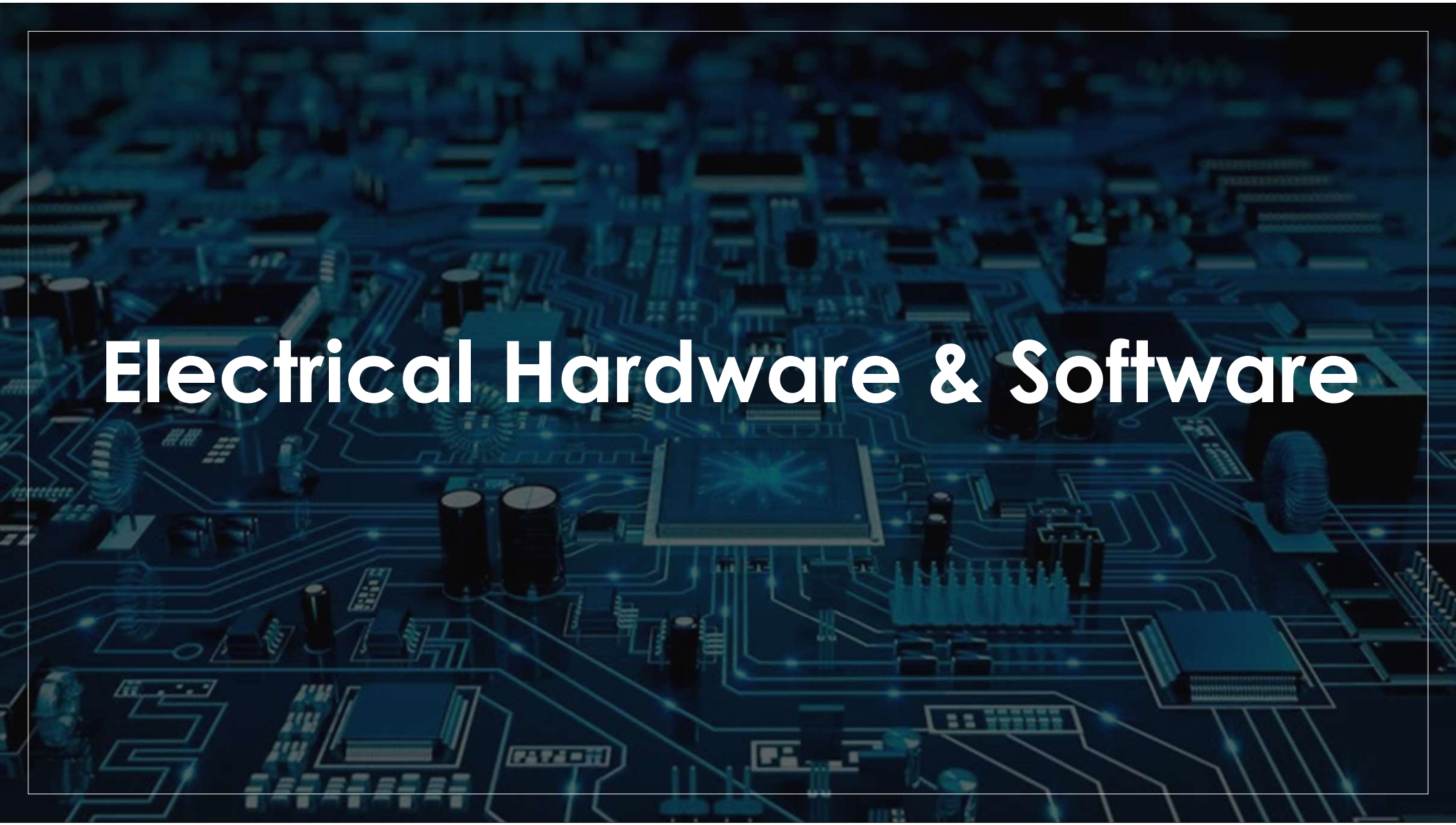
Inverse Fourier Transform



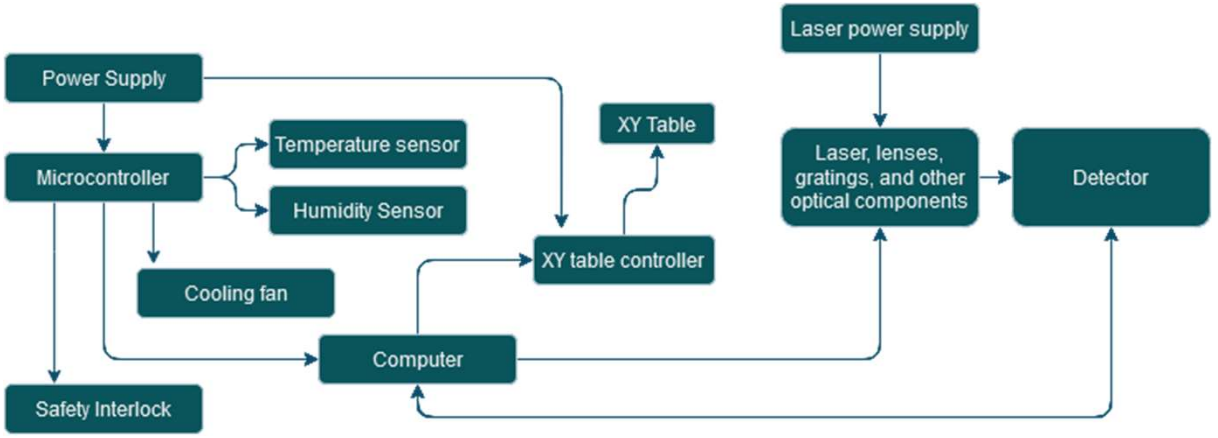
Optical Simulation and Inverse Fourier Transform Result

- **ZEMAX**
  - Input three wavelengths into non-sequential ray trace.
    - 785 nm, 830 nm, & 885 nm
- **MATLAB**
  - Image processing
  - *Note*: Wavelength axis (x-axis) is not configured to scale yet.

Julia - CREOL


Electrical Hardware & Software

Hardware Block Diagram

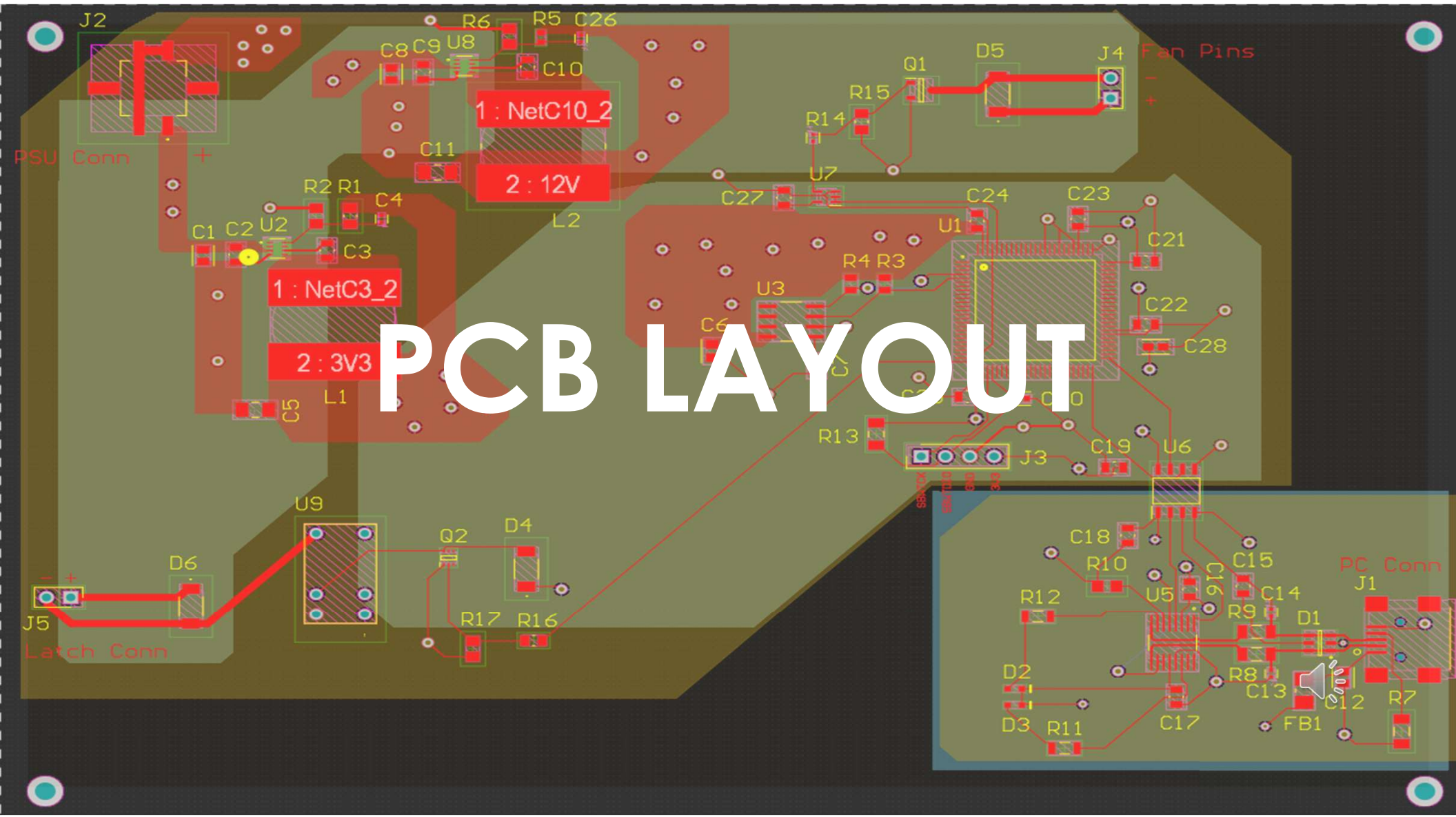


Humidity/Temperature Factors

- Performance and accuracy of spectrometer.
- Water sampling
- Overall system ventilation/moisture
- I2C
- Fan to draw <500mA

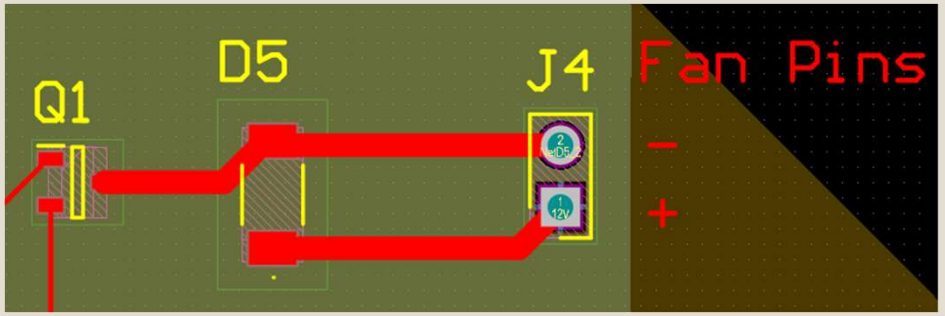
Feature	SHT33-DIS-B2.5kS	SHT40-AD1F-R2	HIH6030-021-001
Voltage Rating	2.15-5.5V	1.08-3.3V	2.3-5.5V
Current Drawn	6mA-15mA	3.2mA-5mA	6.5mA
Size	2.5mm x 2.5mm	1.5mm x 1.5mm	SOIC-8
Pins	8	4	8
Price	$9.60	$3.12	$12.5
Diff. Description	DFN Package	Small functionality	SOIC-8 Package

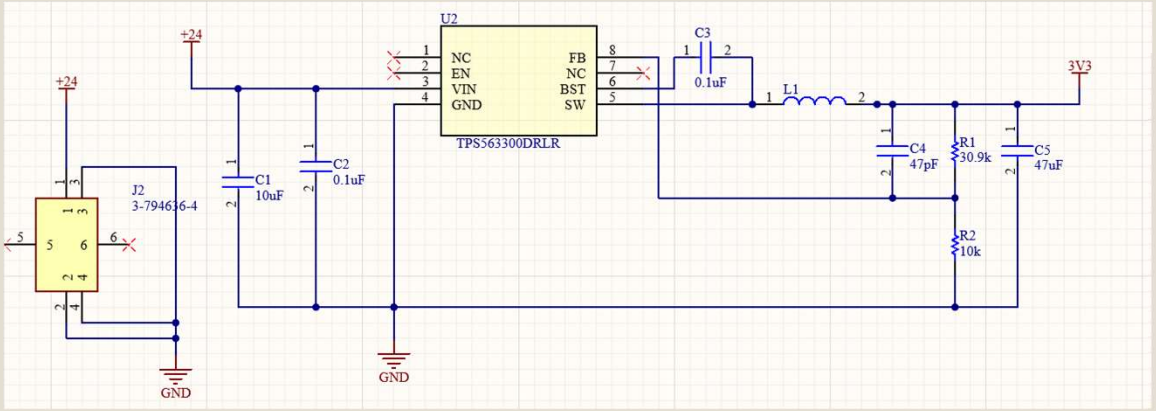
MODEL	input voltage rated (Vdc)	input voltage range (Vdc)	input current[1] max (A)	input power[1] max (W)	rated speed[1] typ (RPM±10%)	airflow[2] (CFM)	static pressure[3] (inch H_2O)	noise[4] typ (dBA)
CFM-8025BG-140-396	12	10.8~13.2	0.27	3.24	4,000	41.40	0.27	39.6
CFM-8025BG-150-444	12	10.8~13.2	0.35	4.20	5,000	51.74	0.43	44.5


PCB LAYOUT
J2
PSU Conn
R6
R5
C26
C8
C9
U8
C10
1 : NetC10_2
2 : 12V
L2
C11
R2
R1
C4
C1
C2
U2
C3
1 : NetC3_2
2 : 3V3
L1
C5
Q1
D5
J4
Fan Pins
R15
R14
U7
C27
C24
C23
U1
C21
R4
R3
U3
C22
C28
C6
C7
C20
R13
J3
C19
U6
U9
Q2
D4
D6
J5
Latch Conn
R17
R16
C18
R10
C15
PC Conn
J1
R12
U5
C16
C14
R9
D1
D2
R8
C13
C12
R7
D3
R11
C17
FB1

PCB Layout & Schematics

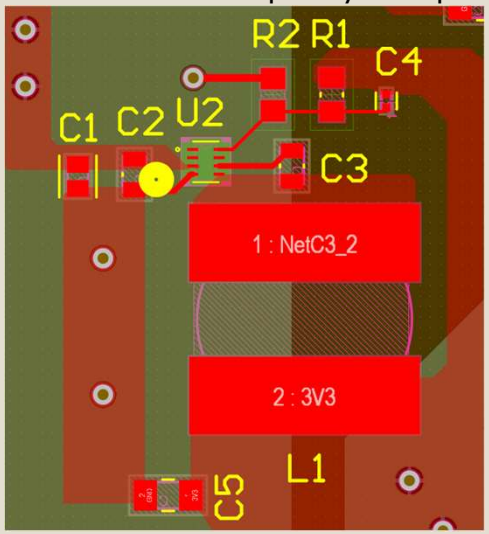
- Altium Designer
- Manufacturer Recommendations
- Challenge, Industry

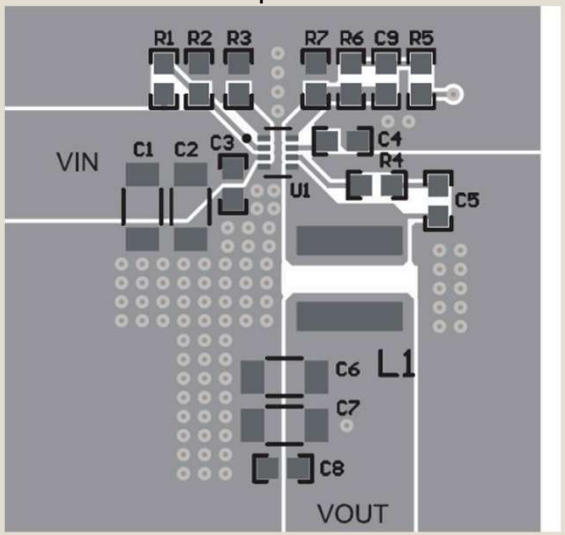




Power Distribution

- 24V Power Supply
- TI WEBench
- Buck Converters into 12V and 3V3 rails
- Current loop layout per manufacturer specifications



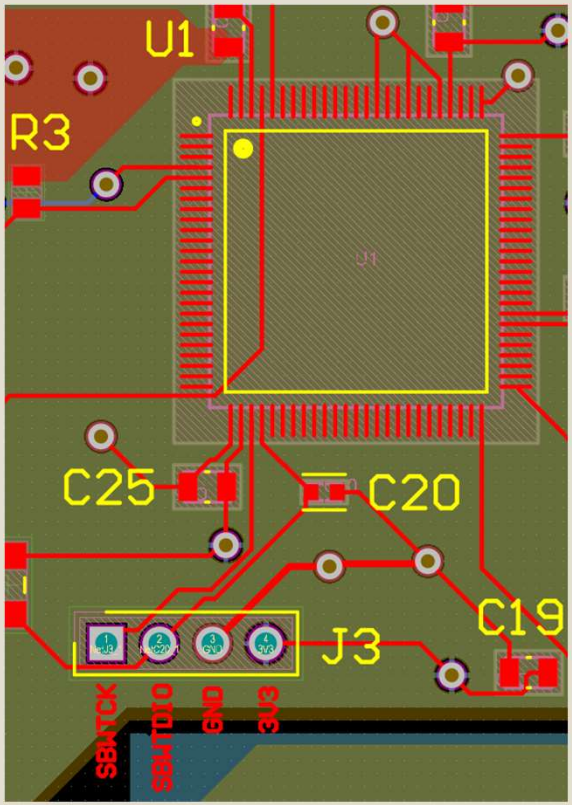


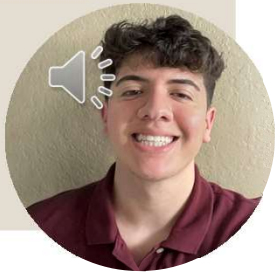
Feature	TPS563300DRLR	LM317MDT-TR	MAX25302BATD/V+
Voltage Rating	3.8V – 28V	4.2V – 40V	1.7V – 5.5V
Max Current Output	3A	1.5 A	2A
Voltage output	800 mV to 22 V	1.2 V to 37 V	600 mV to 5 V
Size	1.6-mm × 2.1-mm	2.4mm x 6mm	SOIC-8
Pins	8	4	14
Price	$1.70	$0.90	$1.94
Reasoning	Buck converter, TI webench simplicity	Outdated component	TDFN package, Does not meet new output requirements

MCU/ Programming

- Spy-by-Wire technology
- Logic gates for signal reinforcing
- MSP430EXP Development Board

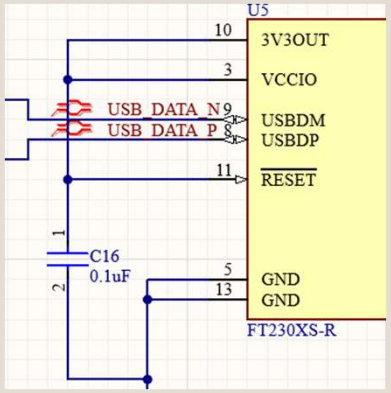
Feature	MSP430FR6989	STM32G431C6T6
Voltage Rating	1.8-3.6V	1.7-3.6V
GPIO Pins	74	38
Protocols supported	I2C, SPI, UART	I2C, SPI, UART, USART, USB
Pins	100	48
Price	$11.2	$7.1
Reasoning	CCS, familiar with programming. Spy-By-Wire programming through Dev board	STMCubeProg

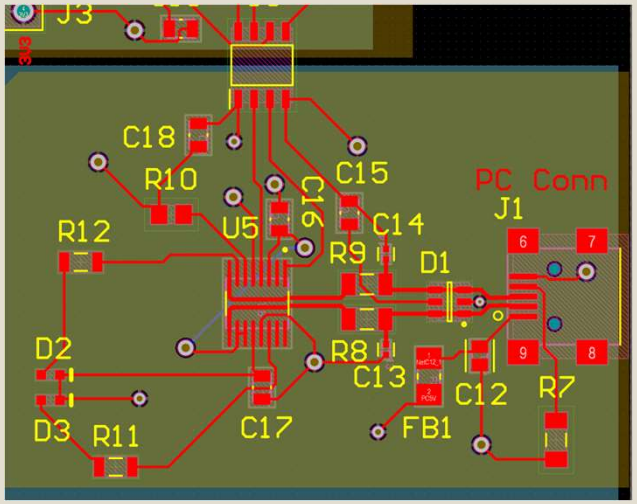




USB Layout

- Differential Pairs
- UART to USB connection with PC
- Isolation
- LEDs
- Trace specifications





Safety Interlocks

Safety interlock on laser.

Safety interlock on enclosure.

Layered safety system in case one of them fails.

Operation cannot be interrupted by user.

Safety lock specifications

	Banner Engineering SI-LS42DMMGF	IDEC HS1L	Omron Automation and Safety TL4019
Max Holding Force(Locked)	1500N	3000N	1200N
Operating Temperature Range	-20C to 70C	-20C to 55C	
Power Consumption	4.4W	4.8W	8W
Operating Voltage	110/230VAC or 24VAC/VDC	24VDC	24VAC/24VDC Or 110VAC
Switch Operations per hour.	600	900	
Maximum Actuator Speed	0.5m/s	1m/s	0.33m/s
Mechanical Life operations	1000000	1000000	1000000
Price	~426$	~200$	~552$

XY Table

Allows usage of well plate

Multiple samples allowed at once for mass data gathering

High resolution allows for accurate laser usage

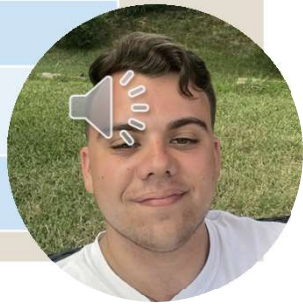
XY table specifications

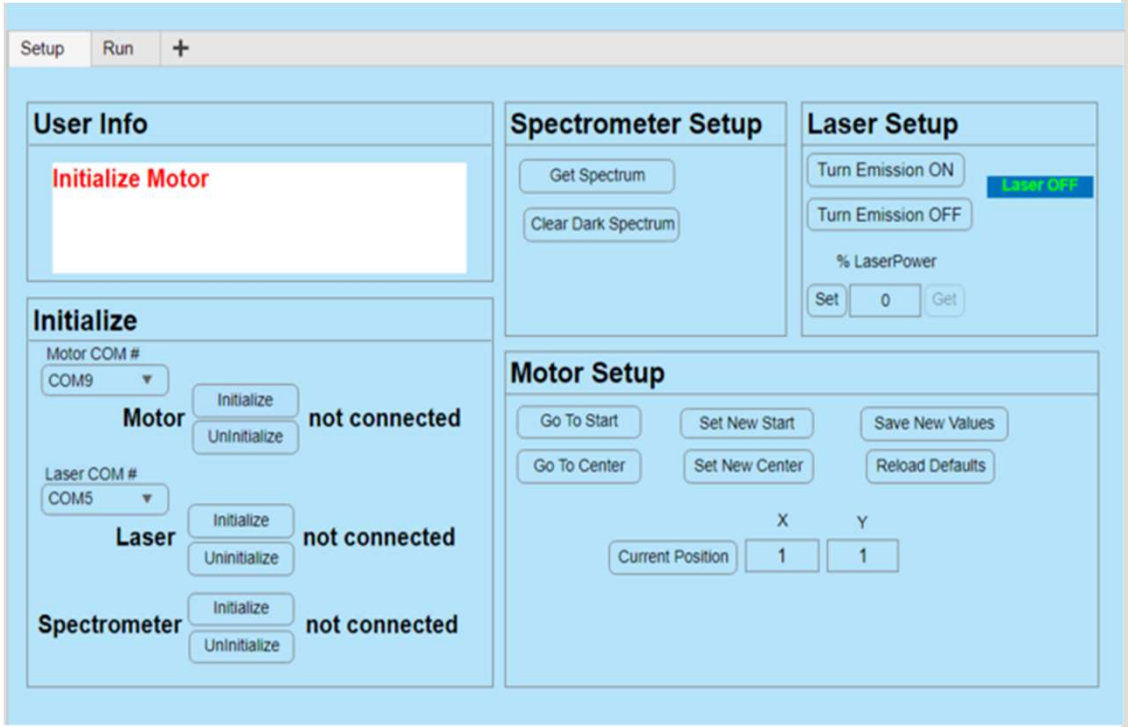
XY Table Model	ZABER ASR	PI L-731	MOXY-01-100-100
Controller compatibility.	XMCC With autodetect	None included manufacturer has recommended list	None included or sold by manufacturer
Travel Range	100x120	205x205	100x100
Resolution	0.15625um	1nm	1.25um
Motor type	Stepper (2 phase)	DC Motor	NEMA17 Stepper motor
Max Speed	85mm/s	50m/s-90mms	20mm/s
Price	Order Dependent	Order Dependent	2739$
Operating Temperature range	0C to 50C	5C to 40C	Unknown

Computer Specifications

- MATLAB and supporting libraries have specifications to be able to run
- Large storage is required to store all the data that will be used to perform calculations.
- RAM is an important aspect to be able to perform the calculations themselves.

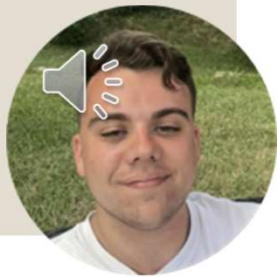
	Latte Panda	Dell XPS 13 9315	ASUS ZenBook Q526FA
Processor	Intel Atom x5-Z8350	Intel Core i5-1230U	Intel Core i7-8565U
Number of Cores	4	8	4
Storage Type	HDD	HDD	SSD-HDD Hybrid
Storage Capacity	64 GB	256 GB	1128 GB
RAM	4 GB	8 GB	16 GB
Operating System	Windows 10	Windows 11	Windows 11
System Type	64-bit	64-bit	64-bit



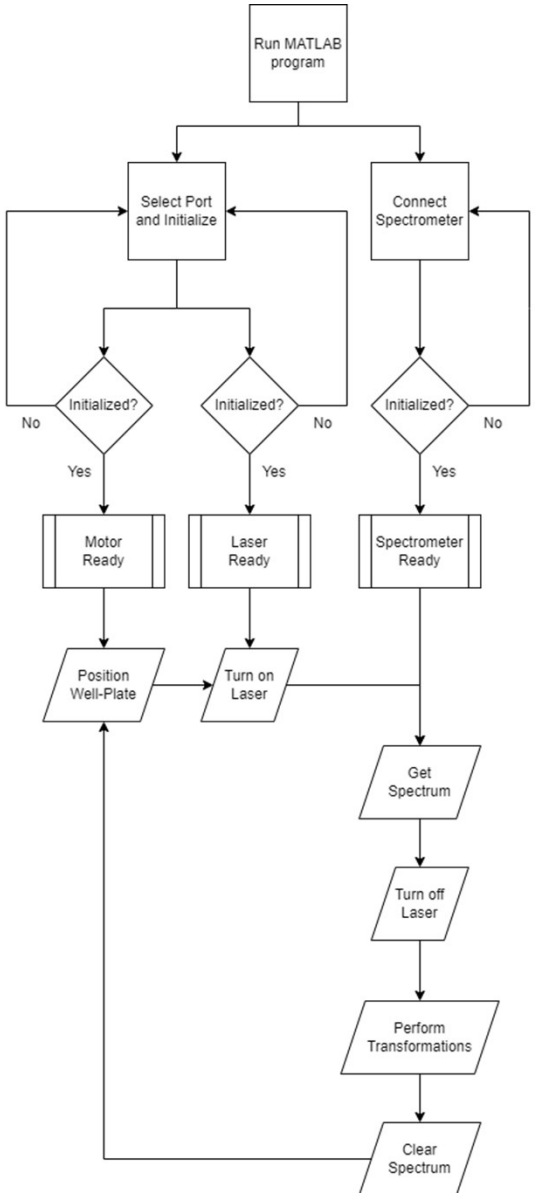


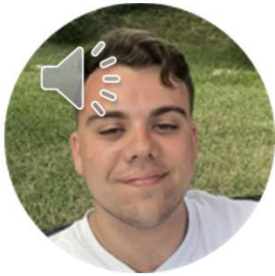
GUI

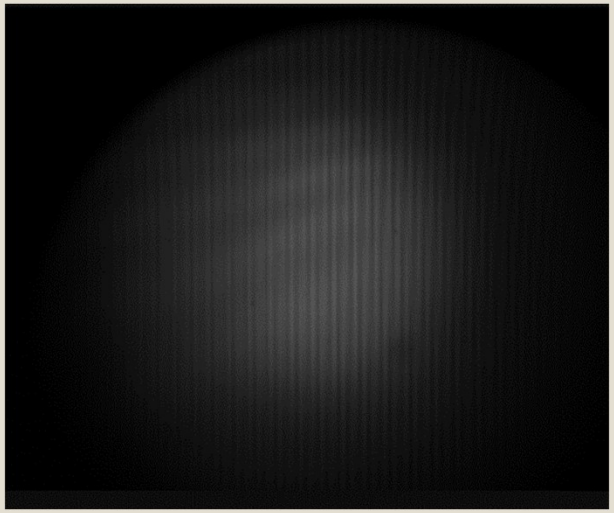
- The GUI is used to control the system as a whole and allows the user to make the adjustments available to them as they see fit.
- User input is required as the COM ports must be manually selected.
- Initialization of the various components is made through the GUI.
- Motor positioning and emission state is also controlled through the GUI.

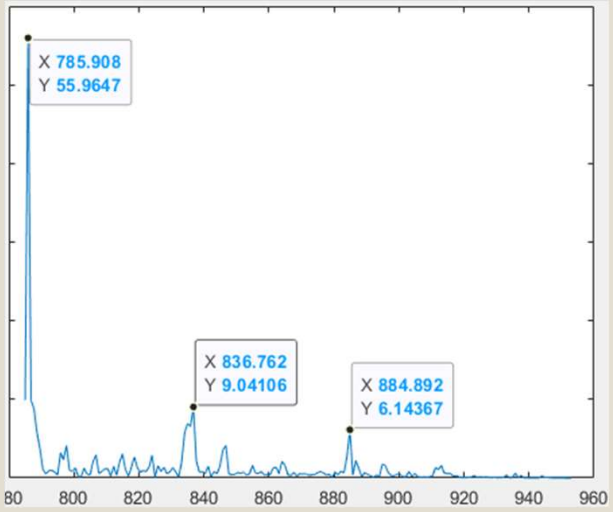


Software Block Diagram



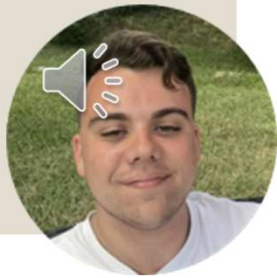






Fourier Transformation

- Camera takes multiple pictures of the fringes.
- The IDS Eye camera communicates with MATLAB in order to convert these images into mathematical matrices.
- A Fourier transform is then applied to the numerical matrix, and a graph is created.
- This graph has peaks at certain wavelengths that describe the chemical makeup of the sample.



Work Distribution

George

Julia

- Investigate imaging techniques **(Julia – P)**
- Lens design **(George – P)**
- Contaminant research and selection **(Julia – P)**
- Spectrometer assembly and design **(George – P)**
- SHS modeling and simulation **(Julia – P)**
- Search components **(George – P)**

Sebastien

- Spectral Analysis **(P)**
- Spectrometer Research **(P)**
- C++, MATLAB, Serial Commands **(P)**
- Software integration and communication with various devices **(P)**

Gibran

Juan

- PCB Design and Assembly **(Juan – P)**
- Power Supply Design **(Juan – P)**
- Research in humidity and thermal impact **(Juan – P)**
- System integration **(Gibran – P)**
- Precision motor design and selection **(Gibran – P)**
- Safety Design **(Gibran – P)**

Budget

ITEM	QUANTITY	PRICE ESTIMATE
Laser	1	Acquired
Gratings	2	~$160
Lens	3-4	~$260
CCD	1	$700
Motor translation stage	1	Acquired
Well plate reader with additional components	1	Acquired
Polarized beam splitter	1	$880
Power Source	1	$10
Custom PCB	1-2	$80
Custom Enclosure	1	TBD
Microcontroller	1	$15
Connectors	3	$10
Misc. Components	TBD	$30
TOTAL	N/A	~$2110

Work Progress

Laser is connected to computer and operating as needed

XY table is connected to the controller and the computer and is controlled by the computer as well.

Optical components are still being assembled and require installation before the spectroscopy can begin.

Thanks for listening!

Q&A?