Raman Analyzer for Illicit Drugs

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ABSTRACT — THIS PROJECT AIMS TO INNOVATE DRINK SAFETY IN BAR SETTINGS DEVELOPING THE RAMAN ANALYZER FOR ILLICIT **DRUGS** (RAID), RAMAN **SPONTANEOUS UTILIZING SPECTROMETER** RAMAN SPECTROSCOPY. RAID OFFERS AN ACCESSIBLE AND USER-FRIENDLY SOLUTION FOR DETECTING SPIKED DRINKS, COMBINING ADVANCED SPECTROSCOPY WITH INTUITIVE INTERFACES. BY**USER** INTEGRATING **PRECISION OPTICAL COMPONENTS** ADVANCED **SIGNAL** PROCESSING. RAID RELIABLE **ENSURES** ACCURATE AND ILLICIT OF SUBSTANCES IN DETECTION BEVERAGES. THE **SYSTEM EMPLOYS ANALYSIS REAL-TIME** AND FEEDBACK, ALLOWING CONSUMERS TO EFFORTLESSLY VERIFY DRINK SAFETY. OUR DESIGN INCLUDES A ROBUST, PORTABLE HOUSING SUITABLE FOR BAR ENVIRONMENTS AND AN INTERACTIVE DISPLAY THAT CLEARLY INDICATES THE CONTAMINANTS. **PRESENCE** OF RAID'S INNOVATIVE APPROACH PROVIDES A VITAL **FOR ENHANCING SAFETY** CONFIDENCE IN SOCIAL DRINKING SETTINGS. **SOPHISTICATED SPECTROSCOPY** MAKING ACCESSIBLE TO THE AVERAGE CONSUMER.

INDEX TERMS — AC-DC CONVERTER, RAMAN SPECTROSCOPY, GABA, STEPPER MOTOR, AVALANCHE PHOTODIODE.

I. INTRODUCTION

With the goal of improving drink safety and accessibility in social contexts, this project intends to create the Raman Analyzer for Illicit Drugs (RAID), a portable Raman spectrometer designed to detect spiked drinks in bars and other comparable settings.

The RAID system uses spontaneous Raman spectroscopy and a simple interface to allow regular consumers to easily test their drinks for illegal drugs. RAID, which combines scientific spectroscopy with easy design, promises to improve public safety and customer confidence in social drinking environments. The primary goals of this project encompass several key aspects.

First, RAID aims to develop a system capable of presence detecting the accurately Gamma-Aminobutyric Acid (GABA) in liquid samples at and above a predefined experimental threshold, serving as proxy a Gamma-Hydroxybutyrate (GHB) [1]. Achieving a spectral resolution of approximately 1nm or better is crucial for finer analysis of molecular structures and Efficient data compositions. acquisition methodologies will be established, involving the development of algorithms for rapid and reliable Raman spectra acquisition, and optimizing exposure times and signal-to-noise ratios. To ensure ease of use, a user-friendly touchscreen interface will be created, enabling researchers and consumers of varying expertise levels to operate the spectrometer effortlessly. Cost optimization is another critical goal, focusing on delivering high performance at an affordable price, thereby maximizing accessibility. Additionally, incorporating a motorized rotation stage will enable precise measurements and automated homing after spectrum acquisition.

To attain these fundamental goals, numerous objectives have been established. The threshold for GABA detection will be determined by calibrating the Raman spectrometer with known concentrations and comparing the results to a baseline spectrum. To achieve the desired spectral resolution, several optical setups will be tested, together with narrow-band advanced dispersive filters elements. Implementing real-time spectral processing software. which includes background subtraction and baseline correction, will make spectra acquisition more efficient. The user interface will be designed to include straightforward controls, real-time feedback, and configurable liquid identification options. Cost-effective optical components will be analyzed to compromise between performance, dependability, and cost. The motorized rotation stage will be programmed for precise movement and auto-homing, improving measurement precision.

Beyond basic goals, advanced objectives include improving laser power to improve signal-to-noise ratios and sensitivity, broadening the wavelength spectrum for more comprehensive material research, and creating a sophisticated sample handling system. This includes fine-tuning laser parameters like strength and duration, incorporating new or modified laser sources, and creating automated sample positioning and manipulation systems. Stretch goals for the RAID project include achieving a compact and portable design to improve accessibility and field-based analysis, enabling multi-substance detection and discrimination, and focusing on advanced spectral resolution enhancement techniques. This would entail investigating as Fourier-transform Raman approaches such spectroscopy and incorporating modern data processing and machine learning techniques to automate workflows, enhance detection accuracy, and enable real-time decision-making.

Overall, the RAID project is an integrated approach to developing Raman spectroscopy for drink safety applications. By addressing these specific goals and objectives, RAID strives to provide a reliable, easily accessible, and effective device that improves public safety while making specialized spectroscopy available to the average bar owner/customer. This concept has the potential to transform how drink safety is managed in social settings, giving people a reliable way to protect themselves against the dangers of spiked beverages.

II. SYSTEM DESIGN

The Raman Analyzer for Illicit Drugs (RAID) required careful component selection and integration to obtain a high-performance Raman spectroscopy system. Our system is built around a 532 nm, 500 mW laser that is designed to optimize Raman while scattering efficiency avoiding fluorescence. This wavelength is ideal for getting clear and distinct Raman spectra from a wide range materials, including the detection Gamma-Aminobutyric Acid (GABA), which is a surrogate for Gamma-Hydroxybutyrate. The laser's intensity is accurately regulated by a function generator, which controls the power output, pulse duration, and repetition rate. This modulation is crucial for increasing the Raman signal and limiting thermal damage to sensitive samples, resulting in reliable and accurate detection.

Many optical components are used to precisely regulate the spatial properties of the laser beam. A

4.0 OD Neutral Density (ND) filter initially reduces laser intensity, followed by perfect focusing with a 38 mm focal length lens. This lens focuses the laser on the sample site, increasing power density and spatial resolution, both of which are necessary for successful Raman signal production. Additionally, the lens collimates the dispersed light from the sample, increasing the system's optical efficiency. A dichroic mirror is used to focus the modulated laser light on the sample while allowing longer wavelength Raman-scattered light to pass through. This gap is necessary for effectively isolating the excitation light from the Raman signal. Following interaction with the material, the scattered light is further filtered by a long-pass filter, which eliminates any leftover excitation light, guaranteeing that only Raman-scattered light enters the spectrometer.

The spectrometer, which includes a diffraction grating and a photodiode detector, disperses incoming Raman-scattered light over a wide range of wavelengths. This technique captures extensive spectral information, allowing for exact identification of molecular vibrations and insights into the sample's chemical characteristics. The spectral data is then processed with powerful signal processing methods to improve the signal-to-noise ratio, resulting in high-resolution and accurate spectroscopy. The RAID system features an easy touchscreen interface to allow for real-time analysis and user involvement. This interface enables users to simply control the spectrometer, view statistics, and receive fast feedback on the presence of illicit chemicals in their beverages. The system is housed in a durable and portable shell that can resist the rigors of bar environments while protecting the sensitive optical components [2].

Overall, the RAID system's design incorporates a high-performance 532 nm laser, precise optical components, and advanced signal processing techniques to provide a dependable and user-friendly tool for identifying illegal chemicals in beverages. This unique solution improves drink safety in social settings by making sophisticated Raman spectroscopy available to the common consumer.

III. SYSTEM COMPONENTS

There were various components meticulously chosen and integrated to develop the RAID system. The following section will detail each of these components incorporated into the final build and provide a concise overview of each selected part.

i. 532nm Laser

The choice of a 532 nm laser for our Raman spectroscopy system is critical because of its high Raman scattering efficiency, low fluorescence interference, and compatibility with conventional optical components. This wavelength amplifies the Raman signal due to the $\lambda^{-}(-4)$ dependency, considerably increasing scattering efficiency. Furthermore, the 532 nm laser effectively reduces fluorescence from organic and biological samples, resulting in cleaner spectrum data. Its interoperability with widely available optical filters, mirrors, and lenses simplifies and optimizes our system, resulting excellent sensitivity and an increased signal-to-noise ratio for precise molecular analysis.

ii. Longpass Filter

In the development and optimization of Raman spectrometers, the selection of suitable longpass filters is crucial for enhancing instrument performance and measurement accuracy. Longpass filters play a pivotal role in blocking undesired Rayleigh scattered light while transmitting the Raman scattered signal, which is essential for capturing high-quality spectral data. This comparison table presents a concise overview of three popular longpass filters from renowned manufacturers: MKS Newport (20CGA-550), Thorlabs (FELH0550), and Edmund Optics (#47-505). Each filter is evaluated based on critical parameters such as size, cut-on wavelength, transmission wavelength range, thickness, and clear aperture. Such a comparative analysis is invaluable for researchers and engineers in selecting the most appropriate longpass filter for their specific Raman configurations, spectrometer taking consideration the specific requirements of their applications.

iii. Rotating stage

In our Raman spectrometer, the grating lens needs to be rotated to properly disperse the different wavelengths of scattered light and direct them to the photodiode. This rotation allows for selecting specific wavelengths or scanning a range of them for analysis. The results of our make/buy analysis confirmed that external procurement of a prefabricated motorized rotating stage was too cost prohibitive. Given that information, we decided to source the necessary raw materials and self-manufacture the rotating stage. So, our budget remained within the allowable range, and portability and accessibility of the testing aligned with our publicly stated goals, one being cost-effective.

iv. Power supply

The laser we chose for our project came with its own built-in power supply. For the rest of the project, we decided to use an ALITOVE DC 12V 5A Power Supply Adapter Converter Transformer AC 100-240V input. This 12V power supply built-in features, automatic overload cut-off, over Voltage cut-off, automatic thermal cut-off, and short circuit protection, made it a well-suited candidate to power the Raspberry Pi 3 B+, the motorized rotating stage, and the 7-inch LCD for the touchscreen application. This ALITOVE offers no voltage fluctuations at power on, during transmit, receive, or at power off. Ideal to protect our electronic components.

IV. SOFTWARE DESIGN

The software design of the Raman Analyzer for Illicit Drugs system is critical for achieving accurate detection and user-friendly operation. The software design of the Raman Analyzer for Illicit Drugs system, developed in Python, is vital for ensuring accurate detection and a user-friendly interface. This allows for integrating data acquisition, processing, and user interface management to provide a seamless experience for detecting gamma-Aminobutyric acid (GABA) concentrations in beverages using Raman spectroscopy. An outline of the software architecture detailing the functions and their responsibilities within the RAID system is described below.

i. Software Architecture

From a software standpoint the RAID system is designed to handle specific tasks independently. The four main categories of the software design are as follows:

- 1. **Initialization**: Setting up hardware interfaces and loading necessary data.
- 2. **Data Acquisition**: Reading data from the photodiode.
- Data Processing & Analysis: Analyzing the collected data to extract the Raman spectrum and determine GABA presence and concentration level.
- User Interface Management: Providing a user-friendly interface for displaying detection results.

ii. Initialization

Initialization of the software involves setting up the SPI interface for the MCP3008 ADC and configuring the ADC channel for the photodiode. Loading of the pre-recorded GABA spectra for analysis comparison is included in this as well. Our preloaded GABA spectrum data as well as a normalized water spectrum file is imported via the 'import_data' function responsible for importing data from the Excel files to a NumPy array

iii. Data Acquisition

The 'run_analysis' function initiates data acquisition once the begin button is clicked by running the motor, reading the spectrum data samples from the photodiode, processing this information, and estimating final GABA concentration. The Raman spectroscopy signal is read through the photodiode and translated to a digital signal by an ADC converter using the 'read_spectrum_from_mcp3008' function ensuring the analog data can be processed, digitized, and analyzed in both an effective and precise manner.

iv. Data Processing & Analysis

The data processing and analysis side of the program can be broken down into several steps:

- 1. Crop the signal: The 'read_spectrum_from_mcp3008' function reads and captures a specific number of samples from the photodiode cropping the signal to read a certain amount of the sample.
- **2. Normalize the data:** The 'safe_normalize' function is responsible for normalizing all data to prevent errors

- **3. Divide out water signal:** The 'divide_out_water_signal' function divides sample data by the water data to remove the water signal
- **4. Smooth the data:** The Savitzky-Golay filter is applied to reduce noise via the 'smooth data' function.
- 5. Calculate peak differences: Peaks in both the sample and reference data of 500mg, 750mg, and 1000mg are identified in order to aid in detecting characteristic peaks commonly found in GABA.
- 6. Compare peak differences: The function 'estimated_gaba_concentration' compares the processed sample data with the previously loaded reference data to estimate the amount of GABA present in the sample if any at all.

Together these functions work to intake, process, and analyze Raman spectroscopy data in order to detect and estimate GABA concentrations within beverages.

v. User Interface Management

The Tkinter GUI setup handles user interactions, displaying the Raman spectrum, GABA concentration levels, and GABA detection status. Buttons for both starting and stopping analysis are provided as well.



Fig. 1. RAID GUI results displayed to the user. Image provided by the RAID project team.

The RAID system's software is carefully created to work in sync with the hardware components, to ensure we can accurately and efficiently detect GABA levels using Raman spectroscopy. Its simple design, clear organization, and user-friendly interface make it easy to use, maintain, and improve in the future. With the use of Python and Tkinter, the RAID

system offers a powerful and user-friendly solution for detecting illicit substances.

V. HARDWARE DESIGN

i. Optical System

Introducing the optical system for the RAID project, our focus centers on the meticulous design and integration of both the Raman illumination system and spectrometer. These critical components are engineered to optimize signal generation and detection, ensuring robust performance in diverse environmental conditions.

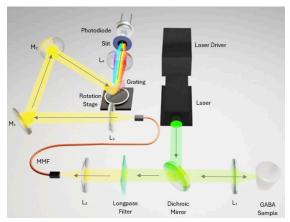


Fig. 2. Composite optical system overview showing the combination of the Raman illumination system with the spectrometer. Image provided by the RAID project team.

The system utilizes a 532 nm laser, chosen for its cost-effectiveness and high supply due to its extensive application in various fields. This laser wavelength also aligns closely with the expected shift Raman of our target molecule, gamma-aminobutyric acid (GABA), centered around 580 nm. To ensure optimal delivery of the laser beam onto the sample, we employ a dichroic mirror with a cut-on wavelength of 552 nm. This assists us in blocking out the excitation wavelength of our pump. The beam reflects off the dichroic mirror positioned at 45 degrees through a collimating lens with a focal length of 38.1mm, ensuring a parallel beam that minimizes divergence. This collimated beam is then directed through a focusing lens, which converges the light onto the sample, maximizing the intensity at the focal point. This design is crucial for enhancing the Raman scattering signal, which is inherently weak compared to the excitation light.

We also incorporate a beam expander in the optical path to adjust the beam diameter, ensuring it matches the acceptance aperture of the focusing lens (25.4mm). This step is essential to achieve a tight focus and maximize the Raman scattering efficiency. Moreover, we couple the light reflected off the sample into a multimode fiber which connects the Raman illumination system to the spectrometer. The entire illumination system is enclosed in a compact, rugged housing to protect the optical components and ensure alignment stability in the dynamic environments where the device will be deployed.

The spectrometer's optical design is tailored to capture and analyze the Raman-scattered light with high precision and sensitivity. At the heart of the spectrometer is a Czerny-Turner configuration, chosen for its excellent optical performance and versatility in dispersing light into its constituent wavelengths.

The Raman-scattered light from the sample is first collected and collimated by a lens positioned at the entrance (fiber end) of the spectrometer. We then take this collimated light and reflect it off 2 mirrors in order to ensure the light approaches at the Littrow angle of the grating, where diffraction is most optimized.

The guided light then encounters a diffraction grating, which disperses it into its spectral components. We opted for a ruled diffraction grating with 1200 lines per millimeter, as this specification provides an optimal balance between spectral resolution and light throughput for our target wavelength range. The grating is mounted on a precise rotational stage, allowing for fine adjustments to align the diffraction angle with the detector's position.

To maximize the light entering the spectrometer and enhance the signal-to-noise ratio, we utilize a lens to focus the dispersed light onto the detector. This lens is chosen for its high numerical aperture and minimal aberrations, ensuring that the light is sharply focused, and the spectral lines are well-resolved. The use of a lens over a fiber optic coupling was a deliberate choice to maintain spatial coherence and reduce modal dispersion, which could degrade the spectral resolution.

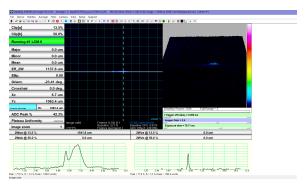


Fig. 3. This image shows that we were able to acquire a Raman signal for GABA. Image provided by the RAID project team.

The dispersed light is finally detected by an avalanche photodiode (APD), selected for its high sensitivity and rapid response time. The APD can detect weak Raman signals with high precision, making it ideal for our application. The slit is carefully placed in front of the APD and chosen to optimize the trade-off between spectral resolution and signal intensity. A narrower slit improves resolution but reduces the amount of light entering the system, while a wider slit increases light throughput at the cost of resolution. It also served to assist us in selecting which wavelengths we desire to measure. The detector is aligned to a stepper motor, which controls the movement of the diffraction grating, allowing for dynamic adjustments during spectral acquisition.

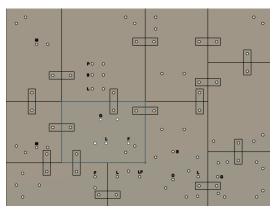


Fig. 4. This figure highlights our homemade breadboard the RAID project will be using for the combined system. Image provided by the RAID project team.

This comprehensive optical design ensures that the RAID Raman spectrometer can efficiently capture and analyze Raman signals with high accuracy and sensitivity, providing reliable results in challenging environments. By carefully selecting and integrating each optical component, we achieve a robust and efficient system while maintaining suitability for use in environments like bars and clubs.

ii. Microcontroller

The microcontroller, specifically the Raspberry Pi 3 Model B+, plays a central role in the operating system of the Raman Analyzer for Illicit Drugs by overseeing the entire detection process. It interfaces with various hardware components, including the Thorlabs DET 210/M photodiode and the MCP3008 analog to digital converter, to collect and digitize analog signals generated by the photodiode when it detects light. The Raspberry Pi model was selected based on its processing power, memory, and connectivity options with its useful features of a 1.4 GHz 64-bit quad core ARM Cortex-A53 processor and 1 GB of RAM which are beneficial for data-intensive analysis like Raman spectroscopy. The Thonny Python IDE with a preinstalled version of Python 3 was used for the development and debugging process. The microcontroller runs the script, which processes these signals to extract the Raman spectrum of the sample. It then compares the processed data against a pre-recorded GABA spectrum to determine the concentration of GABA in the sample. Additionally, the microcontroller manages the user interface through a touchscreen display, allowing users to initiate the analysis, view results, and interact with the system. By integrating signal acquisition, data processing, and user interaction, the Raspberry Pi ensures that the RAID system operates seamlessly and efficiently.

iii. Analog to Digital Converter

An analog-to-digital converter (ADC), specifically the MCP3008 in the RAID system, is an essential piece of our project and a widely used integrated circuit that converts analog signals into digital data, playing a crucial role in bridging the gap between the analog signals from sensors, such as the photodiode (Thorlabs DET 210/M) in Raman spectroscopy, and the digital processing capabilities of the Raspberry Pi microcontroller. This data represents the intensity of Raman-scattered light at different wavelengths, allowing for the analysis of molecular vibrations and structures. Our selection of the Brigold MCP3008 Analog to Digital Converter provided us with a 10-bit

analog-to-digital converter (ADC), 8 input channels for reading up to 8 analog sources/sensors at once, as Peripheral as Serial Interface communication for efficient data transmission to the microcontroller. Additionally, the MCP3008's ease of integration and low power consumption make it an efficient choice for portable and embedded systems like the RAID system. By converting the analog signals into digital data, the ADC facilitates accurate spectral analysis and real-time monitoring of current, which are essential for detecting GABA concentration and ensuring the operational integrity of the system. By interfacing the MCP3008 ADC with the Raspberry Pi 3 Model B+ microcontroller, we have built a cost-effective Raman spectroscopy system capable of collecting and analyzing spectral data with high resolution and accuracy.

iv. Motorized rotating stage

For our senior design project, we designed our own motorized rotating stage for the Raman spectrometer. The core of this design was the NEMA 14 stepper motor, chosen for its compact size and sufficient torque. To drive this motor, a TMC2209 stepper motor driver was used, which is known for its ability to handle micro-stepping, thus allowing for finer control and reduced vibrations.

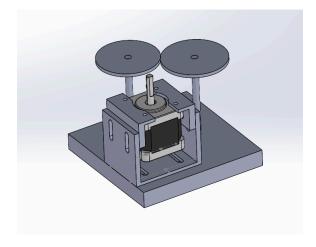


Fig. 5. Computer-aided design of stepper motor used in the Raman spectrometer. Image provided by the RAID project team.

The precision required for the rotating stage was quite high. We needed a step size of 0.005 degrees with a tolerance of ± 0.001 degrees. To achieve this, we configured the TMC2209 driver for 1/64 microsteps by setting the MS1 pin to LOW and the MS2 pin to HIGH. This

configuration increased the resolution of the motor's steps, making each step smaller and more precise.

In addition to the microstepping, we implemented a gear reduction mechanism to further enhance the precision. A 48-pitch 20-tooth gear pinion was paired with a 48-pitch 90-tooth gear. This setup created a gear ratio of 4.5:1, which in turn reduced the NEMA 14 motor's movement by a factor of 4.5.

To achieve our desired configuration, a series of calculations were performed. The basic step angle of the NEMA 14 stepper motor is 1.8 degrees per full step. With the 1/64 microstepping, this step angle is divided into 64 parts, resulting in a microstep angle of approximately 0.028125 degrees. Although quite small, this step did not meet our needs. Introducing our 4.5 gear ratio system helped us achieve our spec, the effective step angle becomes about 0.006 degrees per microstep. Although this is slightly larger than the target of 0.005 degrees, it still falls within the acceptable tolerance range of ± 0.001 degrees.

The mechanical design of the rotating stage was also critical to its performance. We designed a custom 3D-printed fixture to elevate the motor and gear assembly. This fixture played a crucial role in minimizing vibrations, which is essential for maintaining precision. Additionally, I used a flange ball bearing to secure the gear, providing smooth rotational movement and minimizing any wobble. Nylon washers were added on both sides of the gear to reduce friction and further stabilize the assembly.

Overall, the combination of precise micro stepping, effective gear reduction, and thoughtful mechanical design resulted in a highly functional and precise rotating stage. The final setup achieved a step size of approximately 0.006 degrees, which was sufficient for the needs of the Raman spectrometer.

v. Design of the PCB for the Motorized Rotating Stage and Peripheral Components

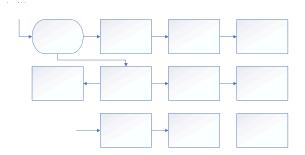


Fig. 6. PCB wiring diagram used to power the entire project. Image provided by the RAID project team.

We designed a custom PCB to manage and distribute power efficiently to all the components involved in the motorized rotating stage and the associated peripherals of the Raman Spectrometer. The entire setup is powered by a DC 12V 5A Power Supply Adapter Converter Transformer (AC 100-240V), providing a total of 60W of power. This power supply drives the TMC2209 stepper motor driver, which in turn powers the NEMA 14 stepper motor. Typically, a NEMA 14 stepper motor consumes around 1A at 12V under full load, translating to about 12W of power.

The 12V power supply also feeds into an LM2596S Adjustable DC-DC Buck Converter, stepping down the voltage to 5V to power the Raspberry Pi 3 B+. The LM2596S is highly efficient, with efficiency typically around 90%. Given that the Raspberry Pi 3 B+ typically consumes around 2.5W to 4W depending on the load and peripherals connected, the power drawn from the 12V supply through the LM2596S would be approximately 3W to 4.5W. accounting for efficiency losses. The Raspberry Pi 3 B+ also powers a 7-inch LCD touchscreen, which typically consumes around 5W, sourced directly from the 5V output of the LM2596S and managed by the Raspberry Pi's GPIO pins. Additionally, the Raspberry Pi powers the MCP3008 (Analog-to-Digital Converter). The MCP3008 ADC, used for various sensor readings, consumes minimal power, typically around 0.45mW in active mode at 5V.

To ensure the main power supply could adequately power all the components, we performed a series of calculations. The TMC2209 and NEMA 14 motor consume approximately 12W, the LM2596S buck converter output to the Raspberry Pi around 5W, the Raspberry Pi 3 B+ around 3W, the 7-inch LCD touchscreen around 5W, and the MCP3008 ADC 0.45mW. Summing these values gives a total power

consumption of approximately 25W, well within the 60W capacity of the 12V 5A power supply, leaving a comfortable margin for any additional minor components or unforeseen power spikes.

The LM2596S buck converter is close to the power input to minimize voltage drop and ensure a stable 5V output. The placement of the Raspberry Pi, stepper motor driver, and sensors minimizes interference and ensures clean signal paths, with a continuous ground plane reducing noise and providing a stable reference for all components. Overall, the PCB design ensured efficient power distribution and reliable operation of all components, creating a robust and reliable power management system for the motorized rotating stage and the Raman spectrometer's peripherals. This meticulous approach to power management was essential for the successful operation of the entire system.

In addition to the components integrated into the PCB, the system includes a laser and a laser driver, each with its dedicated power supply. The laser and its driver require a stable 120V power source, separate from the PCB, to ensure consistent performance and prevent interference with other components. This isolated power setup is crucial because the laser provides the excitation light necessary for the Raman scattering process. The laser was donated to us and already included its 120V wall adapter.

Lastly, the system uses a photodiode powered by a separate 12V battery, independent of the PCB. The photodiode, which detects scattered light, requires a stable power source free from electrical noise and interference.

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