The Development of a 3D-Printed Handheld Visible Spectrometer

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Abstract

This paper presents a design and implementation of a low-cost mini spectrometer that can be used for various applications in scientific research, education, and industry. The spectrometer was built using components already available in the lab and 3D printed housing and mounts, which reduced the cost significantly compared to commercially available spectrometers. The system is based on a flat diffraction grating and a CMOS sensor, and it covers the visible light spectrum from 460 to 620nm. The device is connected to a ThorLabs software for data analysis and visualization. The performance of the mini spectrometer was evaluated by measuring the spectra of different light sources and comparing them to the spectra obtained from literature. The results show that our mini spectrometer provides accurate and reliable spectral data with a resolution of approximately 2nm. The low-cost mini spectrometer presented in this paper can be a valuable tool for researchers, educators, and hobbyists who require spectral analysis but have limited budgets and/or space.

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1 Introduction

While sitting in an optics lecture in the autumn trimester of my final year, not long after I had chosen this project title as my final year physics project, the class was advised by Professor Dominic Zerulla to "Never build your own spectrometer, it is not worth the heartbreak". With this echoing in my mind, I decided then it was time to install an AutoCad programme and get to work. I now recommend to the reader: Never build your own spectrometer unless you have a lot of patience and an optics professor to prove wrong.

1.1 Goals/Aims of this Project.

The main goal of this project was to develop a 3D printed spectrometer which is handheld, low-cost and compact in nature. This was aimed to be achieved in conjunction with maintaining a high resolution and wide operational wavelength with the intent of being able to compete with other micro-spectrometers being offered on the market today.

I believe that this is an incredibly relevant project mainly since many micro-spectrometers available on the market today are extremely expensive. From my research on low-cost non-commercially built micro-spectrometers, many fall short of the mark due to their limited spectral resolutions. This limits the amount of information that can be derived from absorption and/or emission lines. My aim is to improve on this and maintain a 1-2nm spectral resolution all in a handheld portable device.

I also believe there is an important educational application of this project. The pedagogical benefit of teaching the principles of modern spectroscopy by utilizing a simple spectrometer setup can be majorly beneficial. Optical spectroscopy is an indispensable topic in scientific education for undergraduate physics students. Using this inexpensive setup, the quantum principles of light's interaction with matter can be explained by means of atom line emission and absorption in a classroom setting with minimal set up time. Being a final-year undergraduate experimental physics student, I believe that labs and practical experiments are just as important as the theory when it comes to fully understanding topics. Most experiments in the undergraduate physics course require highly expensive and complex instruments and equipment which highlights the importance of this low-cost project, which could be developed at home independently even, once again.

So, in this report I will introduce an optical setup that meets the criterion of high-resolution spectroscopy which remarkably remains around a factor of ten less expensive than other commercial spectrometers of similar specifications.

2 Spectroscopy

Our understanding of the universe comes from an expanded understanding of light as a wave across a much wider spectrum than what we can see. This in turn has led to a wave of modern technologies. Some aiming to utilize light's wave properties to transmit information, such as audio and visual communications. While others aim to measure spectral components of physical phenomena such as mass of particles, and the chemical make-up of matter both terrestrial and extra-terrestrial. [1]

Spectroscopy is a scientific measurement technique that investigates and quantifies the interaction of light with matter. These light-matter interactions at the molecular level, such as emission, absorption, fluorescence, and scattering, can be measured and analysed. These interactions are qualitatively and quantitatively analysed with light measuring instruments. The qualitative analysis is used to establish the identity of a sample while a quantitative analysis is performed to estimate the concentration of a substance. Every substance and element interact differently with light frequencies and the resulting patterns act like their own signatures or fingerprints making it possible to identify them. [1]

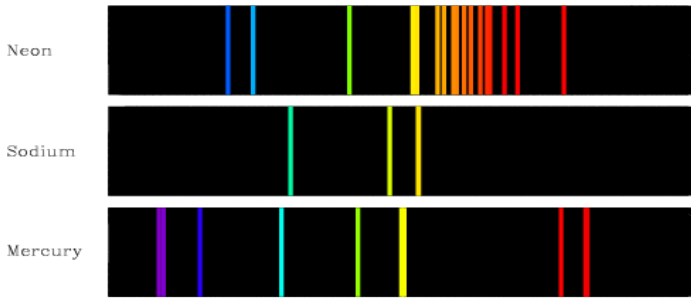


Fig 2.1: Emission Spectral Lines for Neon, Sodium and Mercury [2]

2.1 The Visible Light Spectrum

The reason that some things appear to be coloured at all to us is due to the fact that atoms and molecules absorb and emit different colours of light. So, a red shirt, for instance, appears red when sunlight shines on it because the shirt absorbs all the visible colours except the red light. Some of the red light passes through the shirt, and some is reflected from its surface. In this project, we are interested solely in the visible light spectrum.

The visible light spectrum is the segment of the electromagnetic spectrum that the human eye can view. This range of wavelengths, rather intuitively, is called visible light. Typically, the human eye can detect wavelengths from 380 to 700 nm. Cone-shaped cells in our eyes act as detectors tuned to the wavelengths in this narrow band of the spectrum. Other portions of the spectrum have wavelengths too large or too small and energetic for the biological limitations of our perception. [3] In this report, we will explore the spectral lines of Neon, Sodium and Mercury which fall inside the visible spectrum of light.

3 The Spectrometer

3.1 What is a Spectrometer?

The spectrometer is now a common scientific instrument used to determine characteristic information about a sample by analysing its interactions with light and its spectral components. They enable us to study light's wavelike properties to produce a spectrum and then measure the characteristics of the spectrum such as its wavelength, frequency and intensity. They can function over any range of the electromagnetic spectrum, but through their design and selection of appropriate optical components, as we will cover later, they typically operate in an application dependent region of the spectrum. [1]

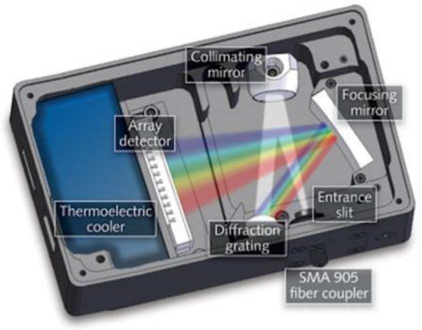


Fig 3.1: Typical Components of a Miniature Spectrometer [5]

3.2 How does a Spectrometer work?

So, what is a spectrometer and how does it work? The spectrometer as whole is a relatively simple device. The light from the sample first enters through the aptly named entrance slit and then is projected onto the collimating optic. The focal length of this optic is chosen so that it collimates the light emitted from the entrance slit and then directs the collimated beam of light onto the diffraction grating. After the light has been diffracted and separated into its chromatic components, the focusing or camera optic is used to focus the light dispersed from the grating onto the detector plane. In the case of a diffraction grating with given angular dispersion value, the focal length of the two mirrors/lenses can be designed to provide different linear dispersion values, which determines the spectral coverage for a given detector, resolution, and total length of the system. We will dive deeper into the workings of the spectrometer and its components later in this report.

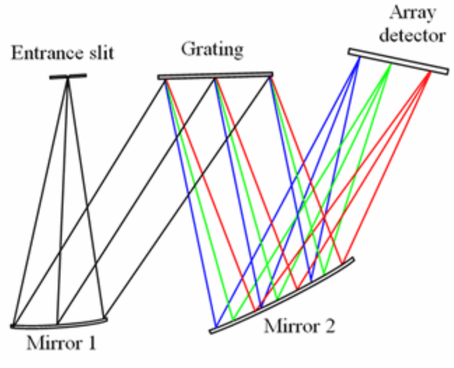


Fig 3.2: An Unfolded Czerny-Turner Spectrometer [1]

Perhaps the most common configuration for a spectrometer would be the Czerny-Turner configuration. A compact, flexible spectrograph design can be achieved by using the Czerny-Turner making it an ideal setup for what we are aiming to achieve in this report. However, there are many other variations in which spectrometers can be assembled.

3.3 Applications of the Spectrometer

Spectrometers have a whole host of applications both in research and industrial settings. They are often used as analytical tools in R&D and manufacturing laboratories as well as in the field. Some applications include but are not limited to; determining concentrations of an element in food and beverages, identifying contaminants, checking for counterfeit or illegal substances, analysing biological compounds, performing medical analysis, and identifying structural defects.

Spectrometers can come in all shapes and sizes and with different specifications. It is possible to develop a spectrometer system which implements your smartphone within its setup. [6] Miniature spectrometers are a desirable commodity as they can be easily inserted within an experimental setup without having to sacrifice much space. The miniaturization of spectrometers has been taken to the extremes. For example, there has been a 3D-printed miniature spectrometer developed that is so small that it can fit on the tip of an endoscope or on a miniature image sensor with a footprint of 100 x 100 microns. [7]

4 Key Components of a Spectrometer

As previously mentioned in Section 3.2, there were five main important components to consider when building our spectrometer. These were the entrance slit, the collimating and focusing optics, the diffraction grating and the detector. The choice of these components was then bounded by the initial constraints chosen such as resolution and wavelength range which is what makes constructing spectrometers so incredibly tedious. This is why it was so vital to have these ideal constraints and goals in mind when building our spectrometer, so it was then possible to choose the components carefully to achieve our goal.

4.1 The Entrance Slit

The slit is an opening that ultimately controls how much light enters the spectrometer. The width of the slit also controls the resolution. The narrower the slit is, the higher the resolution will become. However, narrower slits also decrease signal strength and throughput. These two factors are essential to balance when selecting a slit size. The angle of the light that enters the optical bench is also controlled by the slit.

Another function of the entrance slit is to define a clear-cut object for the spectrometer. One of the key factors that it impacts the throughput of the spectrograph is the height and width of this opening. The image width of the entrance slit is an important factor in finding the spectral resolution of the spectrometer when it is greater than the pixel width of the detector array. The image width of the entrance slit, W_i, can be estimated as: [8]

$$\mathrm{W}_i = (M^2 \times W_s^2 + W_0^2)^{\frac{1}{2}} \tag{1}$$

Where M is the magnification of the spectrometer that is set by the ratio of the focal length of the focusing optic to the collimating optic. W_o is the image broadening and W_s is the width of the entrance slit. The imaging broadening caused by the optical bench, W_o, is generally on the order of a few tens of µm for a Czerny-Turner configuration. [8]

Therefore, reducing the width of the entrance slit below this value will not significantly improve the resolution of the system. The pixel width of the detector sets another limit on spectral resolution, as we will explore later in this section. Reducing the image width below the size of the pixel width will not help increase the resolution of the spectrometer.

If the resolution requirement we set in the beginning is satisfied, the slit width should be as wide as possible to enhance the throughput and signal strength of the spectrograph.

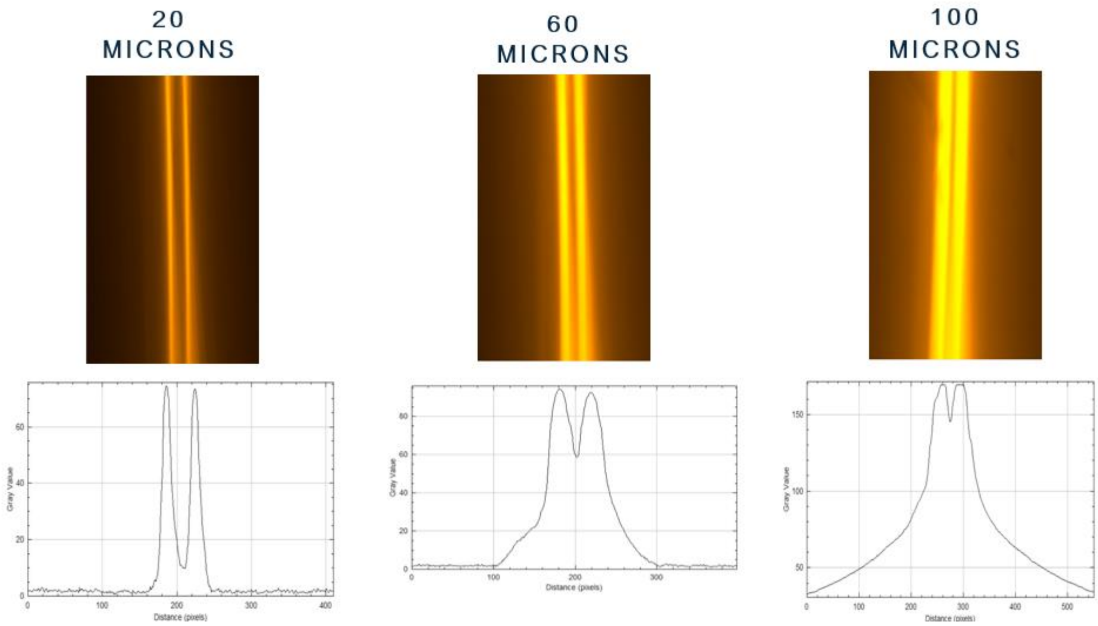


Fig.4.1: Images taken of the Sodium Doublet in the building stage of this project for different slit widths. The Sodium Doublet peaks are located at 589nm and 589.6nm respectively.

As can be seen from Fig.4.1, varying the slit width has a huge impact on the final image and profile plots taken of the spectral lines. As we see from the images, increasing the slit width has the effect of worsening the resolution and resolving power of our spectrometer. It also increases the irradiance of the image but in turn allows more background light to enter the spectrometer housing adding to the noise of the plots. It is clear to see that a large slit width would have a negative effect on our final build's resolving power which would hinder our ability to resolve peaks such as the sodium doublet shown above.

4.2 The Diffraction Grating

A diffraction grating is used to separate polychromatic light into its constituent wavelengths. In the spectrometers built during this project, diffraction gratings were used to separate the wavelengths of the collected light onto different pixels of the CMOS camera for detection. The grating of a spectrometer partially determines the wavelength range and the optical resolution that the spectrometer will achieve. Choosing the correct grating was a key factor in optimizing our spectrometer for the best spectral results. Different gratings would influence our optical resolution and our maximum efficiency for our specific wavelength range. The main factor considered when choosing our grating was the groove density.

4.2.1 Groove Density

A diffraction grating is essentially a surface spanning thousands of parallel grooves. It is because of these grooves, that a grating provides the ability to separate wavelengths based on the angle that they bounce from the grating, known as dispersion. Gratings can be reflective where the grooved surface is overcoated with a reflecting material such as aluminium [9], but they can also be transmissive allowing the light to pass through them and be diffracted. The amount of dispersion is determined by the number of grooves per mm ruled into the grating. This is commonly referred to as groove density, or groove frequency.

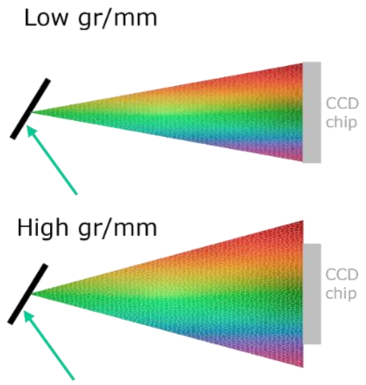


Fig.4.2: Dispersion of light by a low and high groove density grating. [10]

This groove density is the inverse of the groove spacing. From the groove spacing we can then obtain information about the diffracted orders and incident and diffracted angles using the basic grating equation:

$$m\lambda = d(\sin\alpha + \sin\beta) \tag{2}$$

where m is the diffraction order, d is the groove spacing, λ is the light's wavelength, α the incident angle of light and β the diffracted angle of light leaving the grating. [11]

While setting up our spectrometer it was important to determine that we were indeed observing the first order and not the zeroth order as for the zeroth order (m = 0), α and β are equal and opposite, resulting in the light simply being reflected meaning no diffraction was taking place.

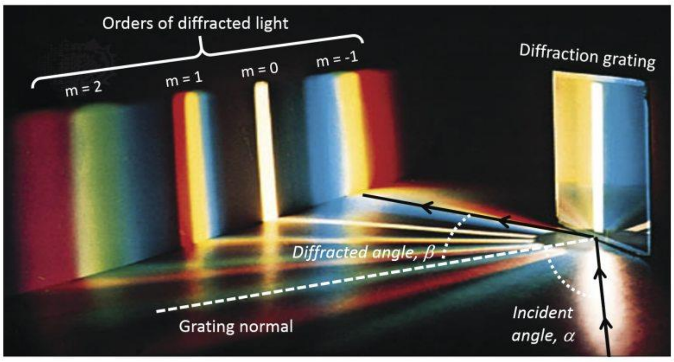


Fig.4.3: Polychromatic light diffracted from a grating. [11]

4.2.2 Choosing the Appropriate Groove Density

As discussed above, the groove frequency of the grating helps in determining the spectrometer's wavelength coverage and is also a major factor in the spectral resolution. The wavelength coverage of a spectrometer is inversely proportional to the dispersion of the grating due to its fixed geometry. However, the greater the dispersion, the greater the resolving power of the spectrometer. The higher groove density grating spreads the light over a larger area of the detector; increasing the spectral resolution as seen in Fig.4.2. The simple rule of thumb is when the number of grooves is doubled, the resolution is roughly doubled. [10] Inversely, decreasing the groove frequency decreases the dispersion and increases wavelength coverage at the cost of spectral resolution.

However, for any given spectrometer configuration based on reflection gratings it is furthermore possible to tune the wavelength range by rotating the grating. This is, however, not possible with spectrometers based on transmission gratings. This is due to the fact that the orders of a transmission grating do not rotate when the grating is rotated much like light going through a window. [13] Many spectrometers come equipped with the ability to rotate the grating instead of the fixed position grating implemented in our build. This way the user can span different wavelength ranges by rotating the grating in order to find and observe spectra they are interested in.

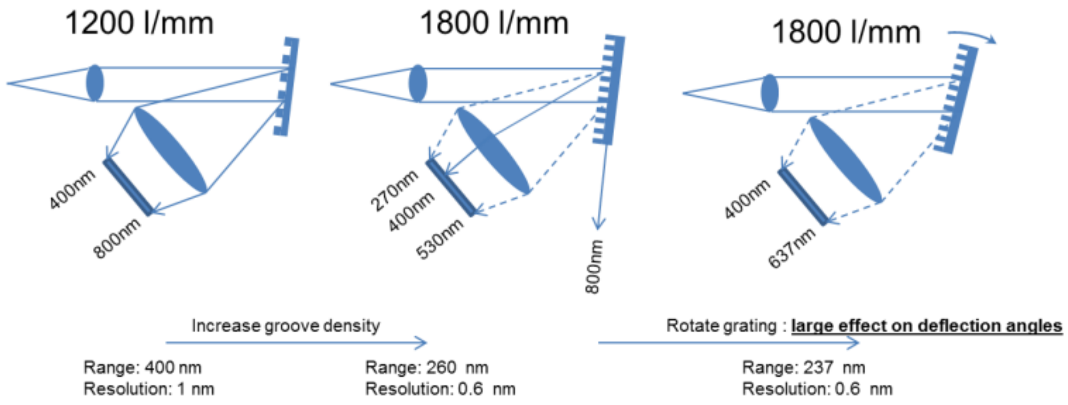


Fig.4.4: Example of reflection grating based spectrometer and the effect of changing the grating density and rotation. [13]

Figure 4.4 illustrates how the resolution and wavelength range can be changed by changing the grating frequency and orientation. This aspect of tilting the grating was pivotal in reducing the size of our final build as it meant that we could achieve our target wavelength range while minimizing our total footprint of the spectrometer itself.

4.3 Collimating and Focus Optics

Collimating lenses/mirrors are optics that make the light rays, that enter the spectrometer setup, parallel. These collimating optics are placed in the setup with their focal planes aligning with the entrance slit to collimate the light. The light leaving the collimator is therefore a thin, parallel beam, which ensures that all the light from the slit strikes the diffracting element at the same angle of incidence. This is necessary as we want to form a sharp image. As one of our main goals of this project is to shrink and miniaturize our setup to handheld size, we can intuitively understand that it is in our best interest to use a collimating lens with a small focal length to reduce the size of our spectrometer.

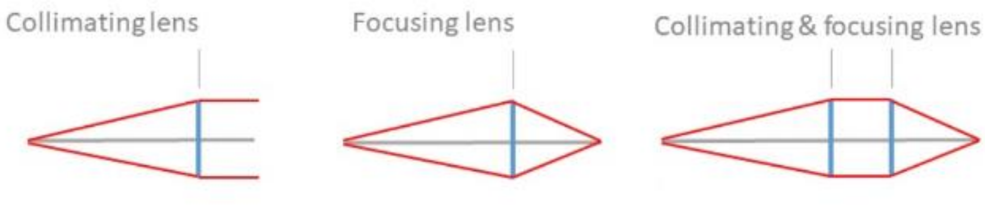


Fig.4.5: Collimating and Focusing Lenses [14]

The role of the focusing optics in a spectrometer setup is, as the name would suggest, to focus the light reflected from the diffraction grating onto the detector. In order to get the sharpest image possible, the detector is located on the focal plane of the focusing mirror/lens. The distance between the focusing optic and the detector is termed the spectrometer focal length. The longer the spectrometer focal length the better the spectral resolution. A longer focal length provides increased spectral resolution due to wider separation of light, however, will also increase the size of the system. Fig.4.5 highlights the difference in the resolving of peaks using different focal lengths. It is of utmost importance that we selected appropriate focal lengths to achieve a handheld size while upholding the spectral resolution goals we set out to achieve.

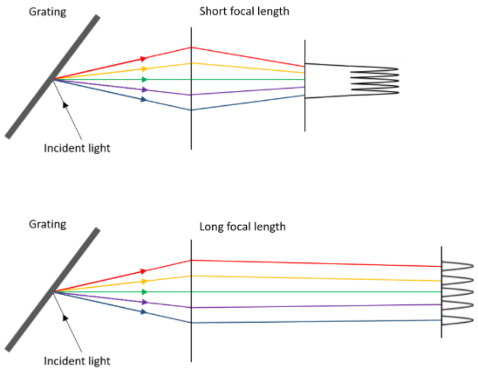


Fig.4.6: Dispersion of light using a short focal length (top), and a long focal length (bottom). [15]

4.3 Detector

In modern spectrometers, linear detector and CCD arrays have enabled the development of fixed grating spectrometers. When the pixels across the CCD are hit by the incident light, each pixel represents a part of the spectrum that the electronics can translate and display with a given intensity using a software programme. This development has made it possible to construct spectrometers without any moving parts, considerably reducing the size and power consumption. [16] Compact multi-element detectors have enabled the development of a new class of low-cost, compact spectrometers.

The spectral range of any spectrometer setup can be determined by the position of the grating for a given focal length and detector width. In particular, the greater the spectral dispersion is the smaller the spectral coverage falling on the active area of the detector will be. This is easy to understand since the detector has a fixed number of pixels and total width. For high spectral dispersion, each pixel will have a small range of wavelength values associated to it, and the spectral coverage will be equal to that value times the number of pixels in a single row of the detector. This can be seen in both Fig.4.2 and Fig.4.6, where for a detector with a fixed length, a higher dispersion would decrease the spectral range of our spectrometer but in turn increase the spectral resolution over this short range.

Spatial resolution is a measurement of how detailed objects are in an image based on pixels. Whereas, spectral resolution is the amount of spectral detail in a image based on the number and width of spectral lines. For a simple understanding of spatial resolution, imagine walking down a long hall towards a painting. As you get closer, your eyes start recognizing features because everything is sharper. For any type of sensor, this means the spatial resolution is becoming finer. Spatial resolution is the detail in pixels of an image. High spatial resolution means more detail and a smaller grid cell size. Whereas lower spatial resolution means less detail and larger pixel size. [17]

As we now see, the size of the pixels in the detector also has an influence on the effective resolution of a spectrograph. According to sampling theories such as Nyquist sampling of stellar profiles [18], the sampling frequency should be at least greater than three times the highest frequency contained in the signal in the context of spectrographs. This means that there must be at least three pixels per spectral resolution element, as indicated by 7 , otherwise it is the size of the detector pixels that will define the resolution of the spectrograph, not diffraction or the slit width.

To maintain focus and to not spend too much time on this section, we will not discuss the noise properties of detectors here, but such consideration is essential in computing signal, S/N ratio, and whether a particular detector is appropriate to a measurement. Therefore, when choosing the detector to use within our spectrometer build, a small pixel size with a long detector length or large pixel count are desirable commodities.

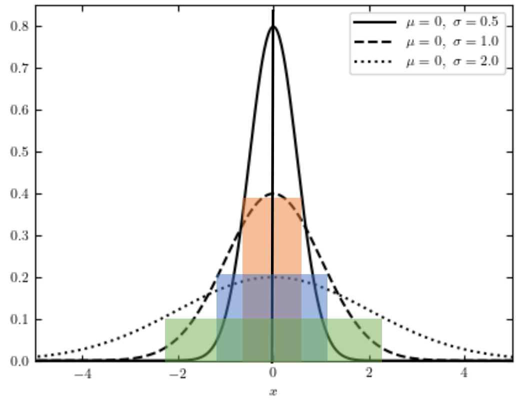


Fig.4.7: Sampling theory of profiles. Three profiles are shown. The coloured boxes indicate the size of the three-pixel span required to sample each profile.

5 Key Parameters

When designing the spectrometer builds that we will discuss in this report, it was important to have end goals and constraints in mind. First, it was important to state the measurement problem which in our case was to view spectra within the visible light range. Secondly, we must determine the desired wavelength range, dispersion, resolution and resolving power. Thirdly, determine the size we wanted the setup to be. Finally, we would then devise optical components that would meet the constraints set.

The reality is that after each step, it is likely that there will be some mismatch with constraints and goals. Perhaps resolution will be too high. Perhaps wavelength range will be too narrow. We then had to loop back to adjust some constraints in light of others. It is this dynamic back and forth among goals, parameters, and invention that makes a recipe for spectrometer design incredibly tedious. In this section, we will cover the key parameters and constraints considered when constructing our spectrometer and why they must all be compromised to maintain a low cost and compact size.

Two of the most important properties of a spectrograph are the dispersion, which sets the wavelength range of the spectrum, and the spectral resolution, which sets the size of the smallest spectral features that can be studied in the spectrum.

5.1 Dispersion and Wavelength Range

The primary purpose of a diffraction grating is to disperse light spatially by wavelength. A beam of polychromatic light incident on a grating will be separated into its component colours upon diffraction from the grating, with each colour diffracted along a different direction. Dispersion is a measure of the separation, either angular or spatial, between diffracted light of different wavelengths. Angular dispersion expresses the spectral range per unit angle, and linear dispersion expresses the spectral range per unit length. [18]

Recalling the grating equation, given by Equation 2, we can obtain an expression for the angular dispersion by differentiating the grating equation with respect to wavelength, noting that α, the angle of incidence, is a constant. [18]

$$D = \frac{d\beta}{d\lambda} = \frac{m}{d\cos\beta} \tag{3}$$

As the groove frequency (the inverse of groove spacing, d) increases, the angular dispersion increases. This in essence means that the angular separation between wavelengths increases for a given order m. Thus, we can establish that the angular dispersion of a spectrum is greater for higher orders of the spectrum and smaller values of the grating spacing.

However, we use will use a linear scale to express dispersion at the detector rather than an angle. Hence, linear dispersion is defined as the rate of change of wavelength along the spectrum per unit linear distance on the detector face.

$$\frac{d\lambda}{dx} = \frac{d\cos\beta}{m\,F_{focus}} \tag{4}$$

where F_{focus} is the focal length of the spectrometer focusing optic. [18]

Generally, the linear dispersion is expressed in units of nm/mm or Å/mm. For example, if a spectrometer has a linear dispersion of 10 Å/mm and the detector being used has a size of 20 mm in the dispersion direction, then the wavelength range of the resulting spectrum will be 200 Å. [18]

5.2 Resolving Power

The spectral resolution or spectral resolving power, R, of a spectrometer is defined as the ability to distinguish between two wavelengths separated by a small amount, Δλ. Spectral resolution is usually quoted in terms of the dimensionless quantity: [18] [19]

$$R = \frac{\lambda}{\Delta\lambda} \tag{5}$$

For example, to resolve the sodium doublet, shown in Fig.4.1, where peaks lie at 589nm and 589.6nm, the resolving power would have to be:

$$R = \frac{\lambda}{\Delta\lambda} = \frac{0.6\,nm}{589.6\,nm} \approx 1000$$

Resolving power measurements are the convoluted result of all optical elements in the system, including the locations and dimensions of the entrance slit and detector, the quality of these optics, the aberrations in the images, and the magnification of the images.

5.3 Spectral Resolution

The terms resolving power and resolution are sometimes interchanged. While resolving power is a dimensionless quantity, resolution has spectral units, usually nanometres. One of the most important characteristics of a spectrometer is the spectral resolution. The spectral resolution of a system determines the maximum number of spectral peaks that the spectrometer can resolve. For example, if a spectrometer with a wavelength range of 200nm had a spectral resolution of 1nm, the system would be capable of resolving a maximum of 200 individual wavelength peaks across a spectrum. The level of spectral resolution required is dependent on the sample and what information the user is aiming to obtain from the spectrum. The main factors that determine the spectral resolution achievable are, as previously discussed, slit width, diffraction grating groove density, spectrometer focal length, and detector pixel size.

After the data is collected from the sample, the spectral resolution is measured at the full width half maximum (FWHM) of the peak of interest. One very common mistake when calculating spectral resolution is to overlook the fact that in order to determine the FWHM of a peak, a minimum of three pixels is required, therefore the spectral resolution is equal to three times the pixel resolution (Δλ/pixel). [20]

5.4 Free Spectral Range

Free spectral range is the maximum spectral bandwidth that can be obtained in a specified order without spectral interference from adjacent orders. [21]For any grating instrument configuration, the light of wavelength λ diffracted in the m = 1 order will coincide with the light of wavelength λ/2

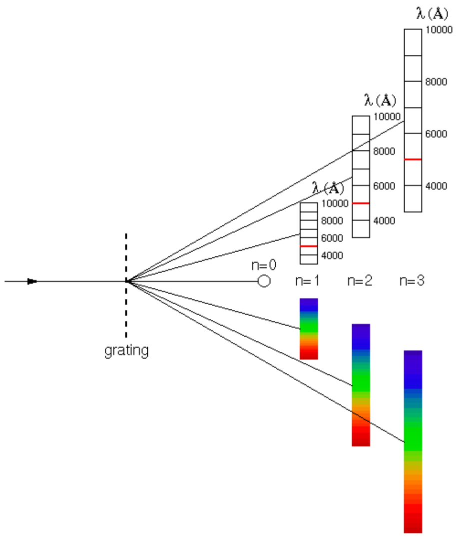


Fig.5.1 Schematic showing the overlap between the first, second and third spectral orders produced by a diffraction grating. [21]

diffracted in the m = 2 order, etc. In this example, the red light (600 nm) in the first spectral order will overlap the ultraviolet light (300 nm) in the second order. A detector sensitive at both wavelengths would see both simultaneously. This superposition of wavelengths, which would lead to ambiguous spectroscopic data. [21] This will not be a problem for our builds as our detector only is sensitive to the visible spectrum. As grating spacing decreases, the free spectral range increases. It decreases with higher orders.

We can derive an expression for the free spectral range in a given order by noting that two wavelengths in adjacent orders, λ_1 and λ_2, that fall on top of each other must satisfy the relation; $n\lambda_1 = (n+1)\lambda_2$. Setting λ_2 as the minimum wavelength present in each, then the free spectral range, FSR, is given by: [22]

$$\mathrm{FSR} = \lambda_1 - \lambda_2 = \frac{\lambda_2}{n} \tag{6}$$

6 Design Process

Now we will delve into the design process and stages which were ventured through before settling on a final design for our spectrometer. Before we started designing, we had to devise a list of parameters or constraints in which we would like our final build to reflect.

1. **Wavelength Range** – The Visible Range – an operational range of 50-100nm should suffice.
2. **Spectral resolution** – 1-2nm in order to surpass other DIY builds seen in my research.
3. **Cost** – less than commercially available micro-spectrometers – aim for < €500.
4. **Size** – aim to be a handheld and portable size - < 15cm x 15cm x 10cm.

At this stage in the build only measurement goals and environmental constraints were at focus. This way we could concentrate on what the finished product would be without being restricted by instrumental constraints.

6.1 Before We Build

As to make this stage as straight forward as possible, A Czerny-Turner configuration was chosen for this first design. The Czerny-Turner is the most common configuration for spectrometers due to its ability to be made compact while still maintaining the necessary resolution to perform high-level spectroscopy. In addition, only a few optical components are required: a set of confocal mirrors, a reflective diffraction grating, an entrance slit and a detector. Detection was realized by a CMOS ThorLabs camera.

6.1.1 Calibration of Components

Before we used the components within our setups, it was vital that we ensure that they are of the specification we believe them to be. Calibration was an essential step for finding the focal lengths of our mirrors and calibrating our variable slit.

To measure the focal lengths of our mirrors, we employed a simple technique. This was accomplished by focusing an image of a distant window on a screen using our mirror whose focal length was to be determined. A sharp image of the window was then formed at the focus of the concave mirror. Therefore, the distance of the screen from the mirror was equal to the focal length of the mirror.

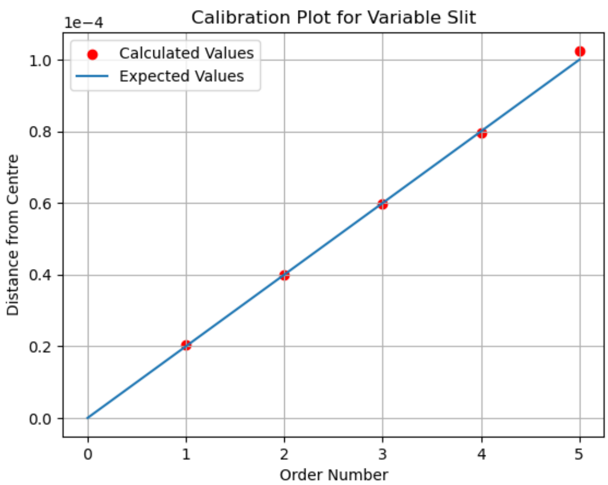


Fig.6.1 Calibration plot for slit width, L = 113.5cm, λ = 632nm. Expected values were values read off the slit scale and calculated values were found using Equation 8 for each order of m.

It was essential also that before any measurements were taken that the slit width of the variable slit in our setup was calibrated. We achieved this by analysing the diffraction pattern that formed when we shone a 632nm red laser through the slit at different slit widths and checking if our calculations aligned with the calculated values using the formula below:

$$d = \frac{\lambda \times L}{m \times z} \tag{7}$$

where d is the slit width, z is distance from the centre to first minima and L is the distance from the slit to the screen. The formula above is dependent on the small angles approximation therefore L>>z.

6.2 Building on the Optical Bench

6.2.1 Components

Now with our components calibrated, it was time to begin constructing our first spectrometer. The plan was to first build a spectrometer on the bench with confocal concave mirrors with large focal lengths and then later aim to reduce the size of the setup to fulfil our goals. A table of the components used is listed below.

Table 6.1 Optical and electronic components used in first spectrometer build.

Component	Description
Entrance Slit	Variable Slit set to 20µm
Collimating Mirror	Concave mirror, f = 180 mm, Diameter = 50mm
Diffraction Grating	Flat Grating, 1200/mm
Focusing Mirror	Concave mirror, f = 180 mm, Diameter = 50mm
Detector	CS165CU/M - Zelux® 1.6 MP Color CMOS Camera, M6 Taps, 1440 x 1080 Pixel (1.6 MP) Sensor with 3.45 µm Square Pixels

A 1440 ×1080 pixels CMOS detector was chosen to record the spatial profile. The scale of each pixel was 3.45µm × 3.45µm, and the length of the receiving surface of the detector was 4.968mm. The grating constant was chosen as 1200 lines/mm, and the width of the slit was varied.

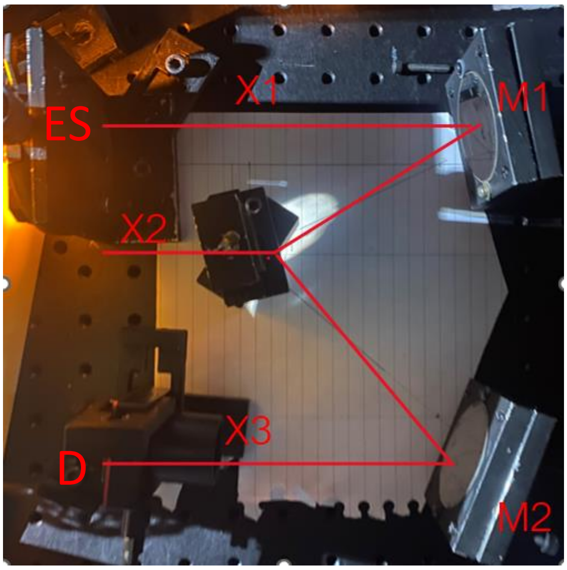


Fig.6.2 Setup for First Spectrometer build.

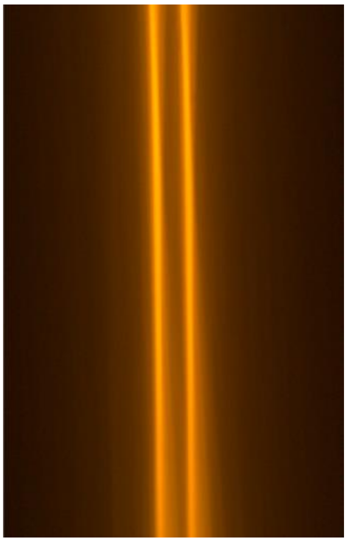
As explained in previous sections, the confocal mirrors were positioned with the collimating mirror's focal plane aligning with the entrance slit and the focusing mirror with its focal plane falling on the detector face. Both X1 and X3 were 180mm. However, after optimization, X1 increased to 185 mm and X3 was reduced to 175 mm, other parameters like detector size and pixel width, and mirror focal length were unchanged. As we can see from Fig.6.2, the grating was indeed tilted in order to have our desired wavelength range fall on the detector as explained in Section 4.2.

In order to ensure our optical axis fell on the centre of our mirrors and passed through the centre of the slit, a 632nm red laser was used to align our components as optimally as possible. This was an important step as having our components aligned properly was vital to ensuring the best resolution was achieved.

6.2.2 Specifications

In sodium's spectrum, there are two wavelengths of light that are quite famous, and they are jointly known as the "Sodium Doublet." When electrons fall from the 3p to the 3s orbital, they can either emit light with a wavelength of 589.0 nm or 589.6 nm. These wavelengths of light are remarkably close and provide us with a perfect opportunity to test our spectrometers resolving power.

So, by attempting to analyse and resolve the sodium doublet we could in turn determine the specifications of our build and thus adjust constraints if we fall short of our initial goals.



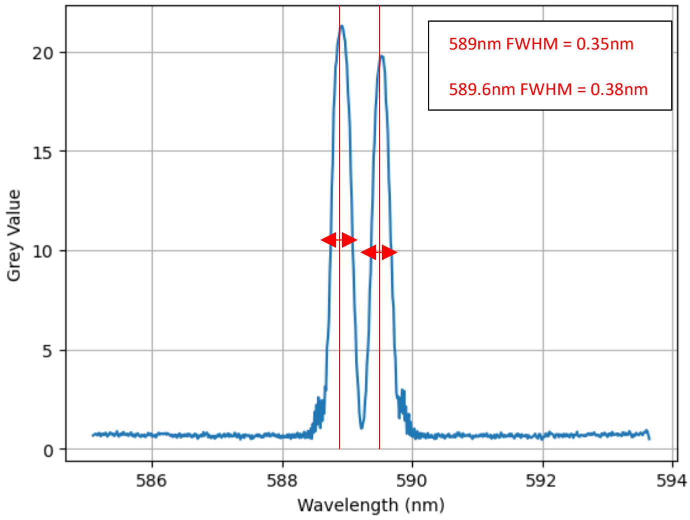


Fig.6.3 Resolved Sodium Doublet using First Spectrometer setup. (Image has been cropped and does not show full wavelength range) (Slit width - 20µm)

It can be seen from Fig.6.3, the sodium doublet can be easily distinguished and is clearly resolved. Our images were obtained by connecting the spectrometer to a computer where a ThorLabs software was used to visualise and capture our spectra. The images were then processed using a software called ImageJ, where the plot profiles of the images could be analysed, and the data transferred to Python to be plotted. Resolving this doublet means our spectrometer build has a resolving power > 1000. The FWHM of the peaks can also be determined to give a value of the spectral resolution. As the grating was not in a fixed position and was able to be rotated it was possible to then observe different parts of the visible light spectrum at 13.5nm intervals.

However, as previously stated in our goals, this 13.5nm was too narrow of a range and not in line with what we aim to achieve. The estimated values for Wavelength Range and Dispersion were gathered using Equation 4 and the length of the detector. Errors on values are calculated using the approx. value of nm/pixel and each value is given by the half of the smallest possible measurement which is a half of pixel on each side of our peak in each case.

Table 6.2 Specifications for first spectrometer build.

Specification	Description
Wavelength Range	13.5nm
Calculated Wavelength Range	14.1nm
Resolving Power	>1000
Spectral Resolution	0.35 ± 0.01nm @ 589nm
Dispersion	2.70 ± 0.01nm/mm
Calculated Dispersion	2.85nm/mm

7 Miniaturized Design

Our next port of call was to improve this design in line with our initial goals. The above build had an excellent resolution which surpassed our initial resolution requirement. However, it had a very narrow operational wavelength range of just 13.5nm and was too big in size. So, in our next design we aimed to address these problems and miniaturize our design and widen our spectral range.

7.1 Change of Optics

7.1.1 Decreased Focal Length

Therefore, to address the size and range issues of our previous design, it was clear that the focal lengths of the collimating and focusing mirror must be changed. As previously discussed, the longer the spectrometer focal length the better the spectral resolution. A longer focal length provides increased spectral resolution due to wider separation of light as highlighted in Fig.4.5. Therefore, by implementing optics of a smaller focal length we will have a smaller cone of light falling on the detector active area, increasing our operational wavelength range. This will in turn decrease our spectral resolution. But, having significantly surpassing our goals in this regard with our previous build, we can afford to loosen the reins on the 0.35 ± 0.01nm we have attained at 589nm.

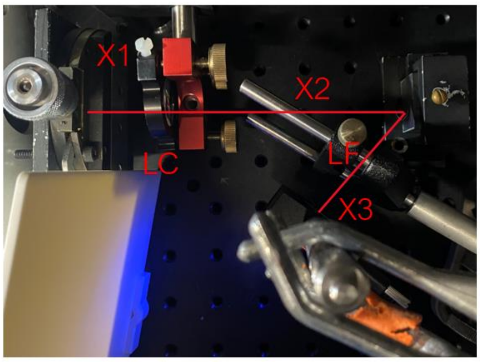
7.1.2 Mirrors to Lenses

Unfortunately, as fate would have it, there was a shortage of smaller focal length mirrors available during the time of construction of this project. Due to time restrictions and other factors, we had to adapt our design in order to accommodate this. We opted to switch out our long focal length mirror for smaller focal length lenses. However, there are factors to consider when making this change such as the configuration, the light path and the changing of refractive index due to different wavelengths of light. This same phenomenon is also responsible for chromatic aberration. When white light is passed through a simple convex lens, several focal points arise in close proximity that correspond to the minor refractive index differences of the component wavelengths. This effect tends to produce coloured halos surrounding the images of objects which can be seen within our images. Correction of this aberration is usually accomplished using combinations of two or more lens elements composed of materials having different dispersive properties, such as an achromatic lens.[22]

7.2 Construction

7.2.1 Components

As stated above, due to the change from mirrors to lenses within our optical bench it was necessary to change our configuration. The new design can be seen below in Fig.7.1. The construction stage of



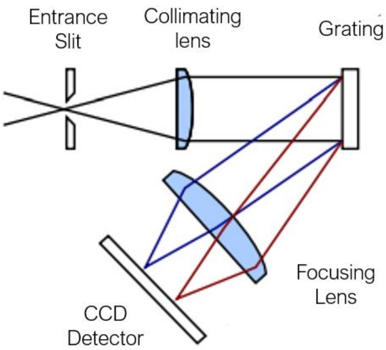


Fig.7.1 Closeup and Schematic of the Miniaturized Spectrometer

this version was exponentially more tedious than the last. This was due to the decreased size of the system. Therefore, the lengths between components were extremely challenging to optimize and hone in. It was also important to have the lenses perpendicular to the optical axis otherwise the light would not be refracted properly, and aberrations would occur.

Table 7.1 Optical and electronic components used in miniature spectrometer build.

Component	Description
Entrance Slit	Variable Slit set to 20µm
Collimating Mirror	Convex lens, f = 25 mm, Diameter = 18mm
Diffraction Grating	Flat Grating, 1200/mm
Focusing Mirror	Convex lens, f = 25 mm, Diameter = 18mm
Detector	CS165CU/M - Zelux® 1.6 MP Color CMOS Camera, M6 Taps, 1440 x 1080 Pixel (1.6 MP) Sensor with 3.45 µm Square Pixels

7.2.2 Specifications

As can be read in Table 7.1, the slit, diffraction grating, and detector remained unchanged. It is evident that the substitution of the optics has significantly increased the spectral range of our spectrometer. It has worsened the resolution as was to be expected. However, we remain within our initial constraints and are one step closer to our final product.

Table 7.2 Optical and electronic components used in miniature spectrometer build.

Specification	Description
Wavelength Range	160.0nm
Calculated Wavelength Range	159.8nm
Resolving Power	>289.5
Spectral Resolution	0.82 ± 0.11nm/mm
Dispersion	32.2 nm/mm
Calculated Dispersion	32.2 nm/mm

7.3 Captured Spectra

As our spectral range and spectral resolution had reached their initial goals, we could now observe the spectral emission lines of multiple sources. This way we can compare the different builds and work out if we are ready to finalise our design and fix our components in place. We have chosen Sodium, Mercury, and Neon as our three spectral lamps to observe.

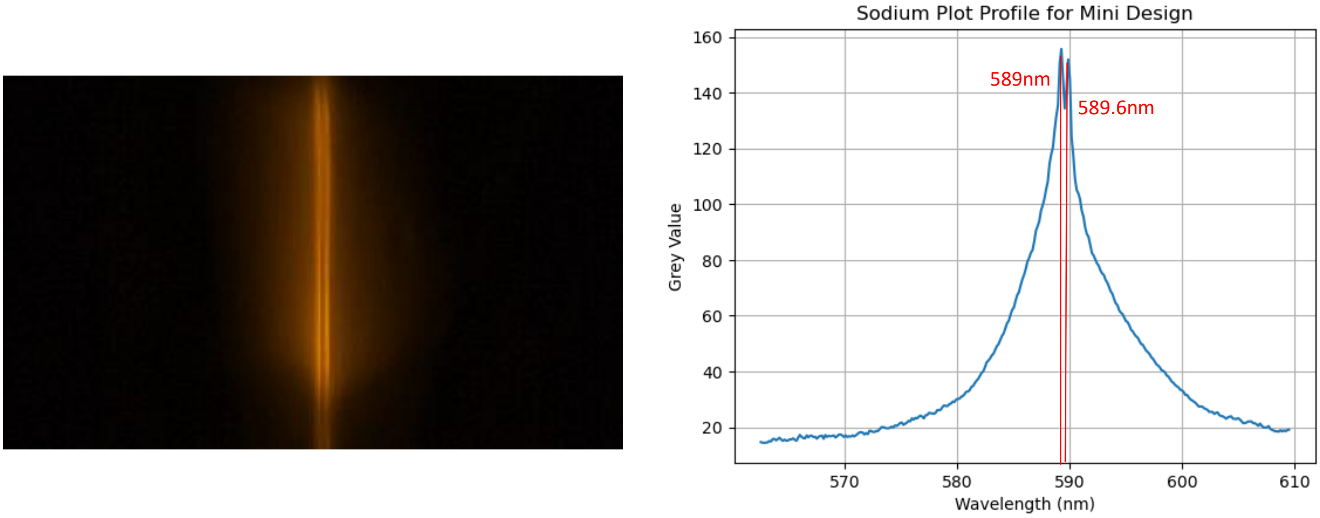


Fig.7.2 Sodium Doublet found using Miniature Spectrometer setup. (Plot and Image have both been cropped and do not show full spectral range)

From the images and plot profiles found using the miniature spectrometer build, we can see that our initial constraints have been followed and our goals have been achieved. We were able to produce a spectral resolution of 0.82±0.1nm which is below our 2nm limit. We were also able to maintain a wide spectral range of 160nm which can be seen in full use in the image and plot profile for Neon. The Mercury lamp was useful for resolving the doublet and finding our resolving power for our miniature build. However, unlike our initial build, our mini spectrometer was not able to resolve the notorious sodium doublet. This was expected however, and our resolving power and spectral resolution are still respectable and comply with our goals.

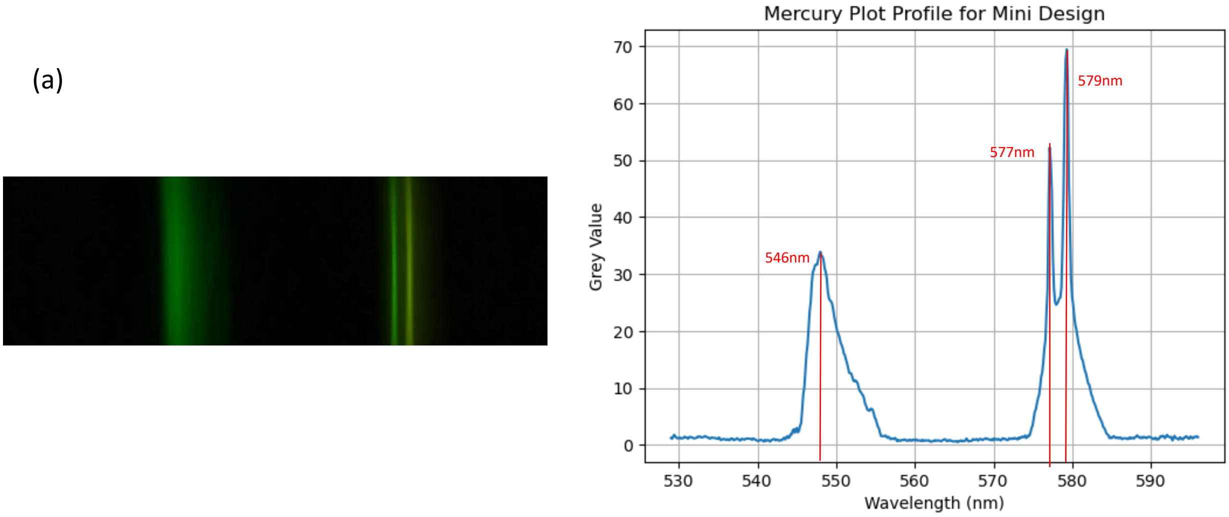
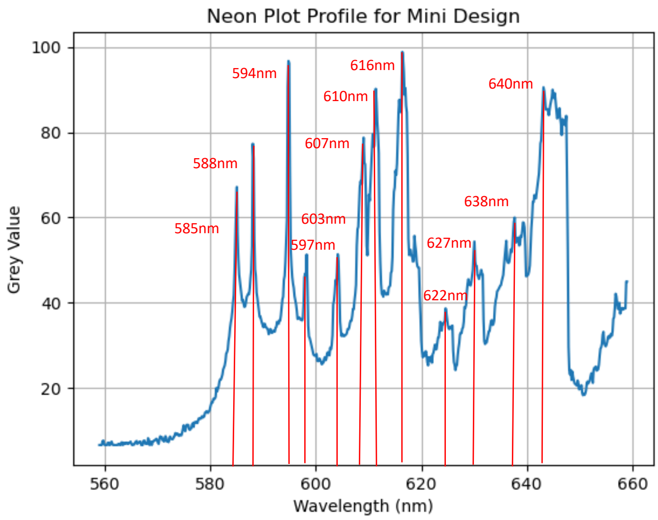


Fig.7.3 Mercury (a) and Neon (b) Emission Spectra found using Miniature Spectrometer setup. (Plot and Image have both been cropped and do not show full spectral range)

(b)



8 3D Printing

This stage in the project was pivotal as all pieces designed for the final build had to be of the correct dimensions to ensure decent throughput and alignment of our components. Any miscalculations in the design process would cause the lenses or detector to not be central on the optical axis causing a loss of focus or aberrations. The final design used the same components as the miniaturized build. All printed pieces were designed using AutoCad's Fusion 360 and then superglued in place to ensure they would not move when the spectrometer itself was being transported.

8.1 Design Stage

When designing the final configuration of our spectrometer, it was at this point that we could minimize the size of the total system. As the distance between the collimating lens and the slit, and the distance between the focusing lens and the detector were fixed, the minimization occurred in the distance between the grating and our two lenses. By minimizing this distant, we were able to fit our total system in a case of size 10cm x 9cm x 6cm.

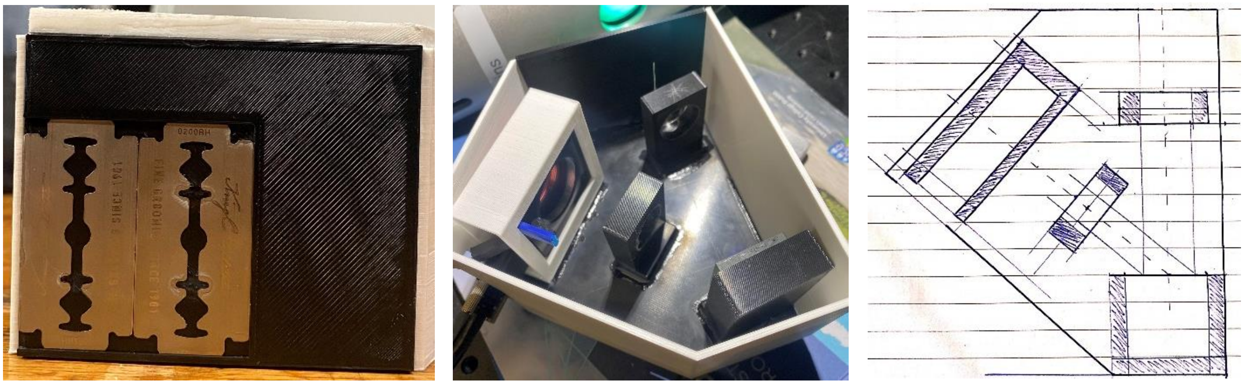


Fig.8.1: (a) a closeup of the slit design. (b) a view of the finished design (c) sketch of the final design

8.1.1 Designing the Slit

As variable slits are complex and often bulky systems, it was then decided that a fixed width slit would be used for our final build. The construction of this was done by designing and printing a model of an entrance slit of dimensions 2mm x 1mm (HxL). As a part of the design of this entrance slit piece, a thin slot was implemented to insert two razorblades over the larger slit. These razorblades were aligned over the centre of the slit, parallel to each other and the slit itself. A singular piece a paper was clamped between them while they were glued in place and removed once the glue was dried to ensure a small enough slit was produced. Using the same process as described in Section 6.1.1 to measure the slit width which was found to be 60µm.

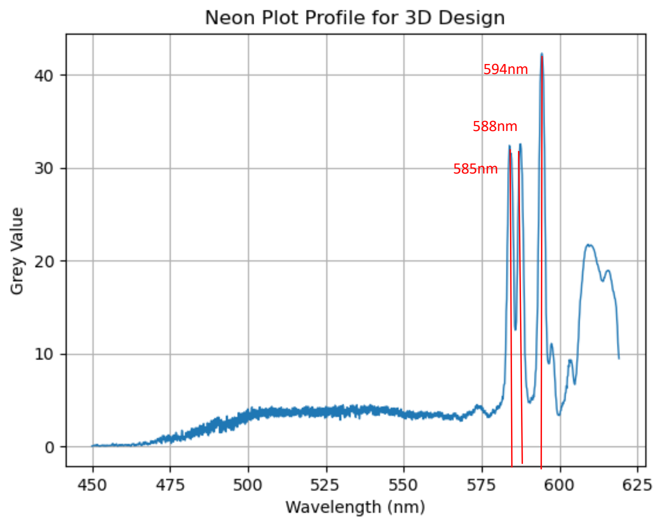
8.1.2 Design the Detector Mount, Grating Mount and Lens Mount.

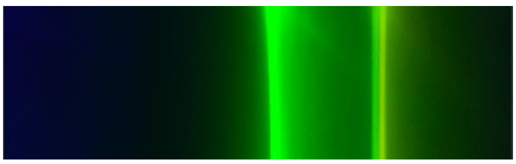
The design process for the detector mount, grating mount and lens mount was rather straightforward. Dimensions for our components were measured using callipers and then mounts were designed and printed to their exact dimensions. A file was then used to get the mounts to fit snugly around our components which meant no adhesive was needed due to the tight fit meaning friction was our main force keeping our pieces in alignment.

9 Assessment of Final Build

9.1 Spectra Captured with Final Build.

When constructing the final build, it was difficult to ensure the exact perfect alignment of all components was maintained. It was not possible to adjust the alignment of the lenses on the vertical axis and the same applies to the detector. It was also not possible to adjust the alignment of our components after they had been glued down. This unfortunately led to a loss of resolution in our final build as did our increased slit width.





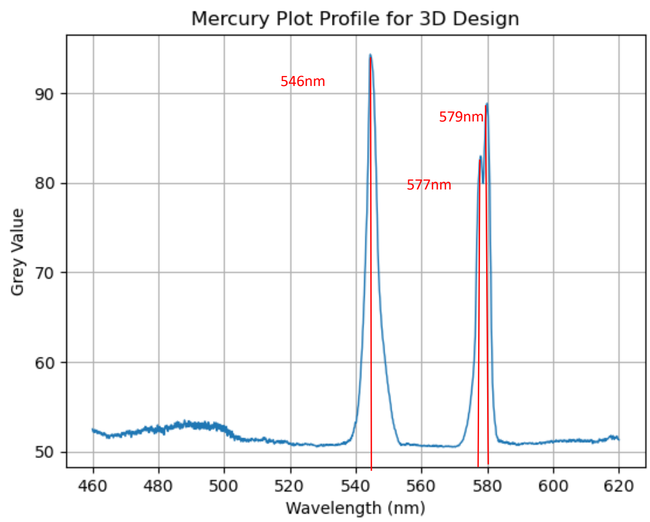


Fig.9.1 Mercury (a) and Neon (b) Emission Spectra found using Miniature Spectrometer setup.

As our components were all now fixed in place, our final wavelength range fell between 420nm and 620nm. This was chosen with the Mercury spectral lines in mind. We were also able to observe some of the Neon emission lines with our final build. From Fig.9.1 we can see that our resolving power did suffer and was barely able to distinguish the Mercury doublet which lie 2nm apart. This loss in resolving power can be traced back to our slit width which was fixed at 60µm rather than 20µm used in the mini-spectrometer build. However, even with this loss in resolving power, all our initial goals and constraints were achieved by our final build. A spectral resolution of 1.9nm was observed at 594nm in the Neon plot. This remains below our 2nm threshold which we held for our resolution. Our spectral range remained unaffected during construction and was measured at an impressive 160nm between 420nm and 620nm.

Table.9.1 Comparison of Miniature Build and the final 3D Build for various peaks of Neon and Mercury

Peak Position Literature (nm) [24]	Peak Position Measured (nm)	Build 2 (±0.11nm)	Build 3 (±0.11nm)	FWHM (nm)	Build 2 (±0.11nm)	Build 3 (±0.11nm)
Mercury 546.0nm		547.0nm	546.5nm		4.95nm	3.3nm
Mercury 576.9nm		577.0nm	577.7nm		0.94nm	-
Mercury 579.0nm		579.1nm	579.9nm		0.82nm	-
Neon 585.2nm		585.0nm	584.1nm		-	2.5nm
Neon 588.2nm		588.2nm	587.7nm		1.4nm	1.9nm
Neon 594.4nm		594.5nm	594.8nm		1.9nm	2.4nm

10 Conclusion

We can conclude that it is possible to construct a miniature low-cost spectrometer that matches the spectral resolution and sensitivity demands for atomic line emission spectroscopy using 3D printing. However, this project only opens the door for future advancements and adaptations to our design. For instance, the 60µm slit width could be drastically improved to improve resolving power and spectral resolution. Beam blocks could also be implemented within the system in to block any stray light that may incident on the detector face. Also, perhaps if the lens used were replaced with short focal length mirrors the chromatic aberration may be corrected which can be seen in our images quite clearly. This in turn would improve our build. A rotatable grating would also improve our build and allow us to span the whole visible spectrum instead of our fixed spectral range.

However, our build did in fact perform well above its price range. Our total build cost less than €500. This cost could be further improved by implementing a much cheaper detector as our detector accounted for 84% of our cost. A replacement such as the "Raspberry Pi Camera Module 3 Wide" [25] has smaller pixel width and a larger pixel count and active area length for $35. It also comes in a smaller size than our detector which was the driving force in determining our total build height. Alas, compared to the "Ocean Optics Stainless Steel Miniature Spectrometer" [26], our build is a fraction of it's €3800 price and fairs well compared to its 1.5nm resolution. The low price of our design is optimal for the application in schools, thus possibly securing hands-on experience for many students in spectroscopy.

Smaller, lower-cost spectrometers and optical benches like our build are ideal for integrating into other analytical devices. They are also perfect for performing quick and accurate measurements and can be easily transported and even used outside of a laboratory setting. This was not possible for larger, higher cost spectrometers of the past.

In conclusion, the development of a low-cost miniature 3D printed spectrometer could represent a significant advancement in the field of spectroscopy, with the potential to have a profound impact on a range of scientific and industrial and educational applications.

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