MASTER THESIS

Thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Engineering at the University of Applied Sciences Technikum Wien - Degree Program Master Embedded Systems

Examination of Low-cost Method for discriminating types of plastic via handheld spectrometer.

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Schlagworte: Schlagwort 1, Schlagwort 2, ...

Abstract

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Keywords: keyword 1, keyword 2, ...

Acknowledgements

First of all I would like to thank Elmyra for always pushing me to the top!

Contents

1. Introduction

3D-printing technology is developed further and is increasingly integrated into all kinds of manufacturing and fabrication processes, even in industrial applications. Combined with the demand for renewable and environmentally friendly solutions for manufacturing, quick and reliable recycling methods reduce the waste of plastics that are already produced. Contrary to the approach of developing new materials from renewable sources altogether. A big challenge that must be faced during the recycling process is sorting the waste materials. To ensure that the recycled materials are produced to a certain standard the sorting process has to meet a certain reliability criteria. Another important factor is efficiency, especially in industrial waste processing where large amounts of plastic waste are handled in a certain amount of time so the sorting process has to be able to keep up with these rates. The goal of this project is to combine both aspects, reliability and speed and investigate a low-cost method of visual discrimination of different kinds of plastics.

2. Theoretical Base

2.1. Basics of Spectroscopy

Spectroscopy is a fundamental analytical technique used to study the interaction between matter and electromagnetic radiation. This technique is pivotal in various scientific fields, including physics, chemistry, astronomy, and biology, due to its ability to provide detailed information about the composition, structure, and properties of matter.

2.1.1. Interaction of Light with Matter

When light interacts with matter, several processes can occur, including absorption, emission, reflection, and scattering. The specific outcome depends on the nature of the material and the wavelength of the incident light.

- **Absorption**: At certain wavelengths, photons can be absorbed by the material, causing transitions of electrons to higher energy states. The wavelengths at which absorption occurs are characteristic of the specific elements and molecular bonds within the material. This process can be described by Beer-Lambert Law, which relates the absorption of light to the properties of the material through which the light is traveling.
- **Emission**: After absorbing energy, atoms and molecules may return to their ground states by emitting photons. The wavelengths of these emitted photons are indicative of the energy levels of the emitting species. Emission spectroscopy, such as atomic emission spectroscopy (AES) and fluorescence spectroscopy, capitalizes on this principle.
- **Reflection and Scattering**: Light may also be reflected or scattered by materials. Reflection involves the bouncing of light off the surface, while scattering involves the redirection of light in different directions. Scattering can be elastic (Rayleigh scattering) or inelastic (Raman scattering), with the latter providing insights into molecular vibrations and rotational transitions.

2.1.2. Measurement of Wavelengths Using a Spectroscope

A spectroscope is an instrument designed to measure the spectrum of light. It works by dispersing light into its constituent wavelengths and detecting the intensity of light at each wavelength. The basic components of a spectroscope include:

- **Light Source**: Provides the initial beam of light, which can be broad-spectrum (e.g., a tungsten lamp) or monochromatic (e.g., a laser).
- **Sample Holder**: Where the material under study is placed. The light interacts with the sample, and its properties are altered based on the material's characteristics.
- **Dispersive Element**: This component, often a prism or diffraction grating, spatially separates light into its component wavelengths. A prism refracts light at different angles depending on the wavelength, while a diffraction grating uses interference to achieve dispersion.
- **Detector**: Captures the dispersed light and measures its intensity at different wavelengths. Common detectors include charge-coupled devices (CCDs), photomultiplier tubes (PMTs), and photodiodes.

The spectroscopic data is often represented as a spectrum, a plot of light intensity (or another quantity related to light) as a function of wavelength. The position and intensity of peaks within the spectrum provide critical information about the sample, such as its chemical composition, molecular structure, and physical properties.

2.1.3. Practical Applications

The applications of spectroscopy are vast and varied. In chemistry, it is used for qualitative and quantitative analysis of substances. In physics, it helps in studying the electronic structures of atoms and molecules. Astronomers use spectroscopy to determine the composition, temperature, density, and motion of celestial objects. In biology, it aids in understanding the structure of biomolecules and the dynamics of biological processes.

In conclusion, spectroscopy is an indispensable tool in scientific research, providing a window into the fundamental properties of matter through the analysis of light-matter interactions. The ability of a spectroscope to measure different wavelengths of light with high precision enables researchers to uncover detailed information about the materials under investigation, facilitating advances across multiple disciplines.

2.2. Methodology

To prove, test, and quantify the results of this project, multiple types of plastics are analyzed under different conditions. The methodology involves placing a sample of material in various lighting environments and conducting analyses to gather relevant data. To ensure that properties such as surface finish, shape, and size do not influence the measurements, all material samples are prepared in a standardized manner.

2.2.1. Samples

Given that this project focuses on recycling for 3D printing purposes, the materials selected as samples are those commonly available and actively used in 3D printing. The samples are manufactured using 3D printing technology. Each sample is standardized to a shape of a 5 cm x 5 cm square plate with rounded corners and a thickness of 5 mm.

2.2.2. Experimental Procedure

The experimental procedure consists of the following steps:

- **Sample Preparation**: All samples are prepared using the same 3D printing parameters to ensure uniformity in surface finish, shape, and size. This standardization is crucial to eliminate any variations that could affect the spectroscopic measurements.
- **Lighting Conditions**: Each sample is placed in different lighting environments to analyze how various light conditions impact the spectral characteristics of the material. The lighting conditions will include, but are not limited to, natural daylight, fluorescent lighting, and LED lighting.
- **Spectroscopic Analysis**: A spectroscope is used to measure the spectrum of light reflected, absorbed, and transmitted by the samples. The spectroscopic data are recorded and analyzed to identify the unique spectral signatures of each type of plastic under different lighting conditions.
- **Data Collection and Analysis**: The data collected from the spectroscopic measurements are processed to quantify the optical properties of the samples. This includes determining the wavelengths at which significant absorption, reflection, and transmission occur, and how these properties vary with different lighting conditions.
- **Comparison and Validation**: The results are compared against known standards and literature values to validate the accuracy and reliability of the measurements. Any discrepancies are analyzed to identify potential sources of error or variation in the experimental setup.

2.2.3. Standardization and Controls

To ensure the reliability and reproducibility of the results, several control measures are implemented:

- All samples are manufactured using the same batch of material to avoid any batch-to-batch variation.
- The 3D printer settings, including print speed, temperature, and layer height, are kept constant across all samples.
- The spectroscope is calibrated before each set of measurements to maintain consistency in the spectral data.

- Environmental factors, such as temperature and humidity, are monitored and controlled during the experiments to minimize their impact on the results.

By following this rigorous methodology, the project aims to provide a comprehensive analysis of the spectroscopic properties of different plastics used in 3D printing under various lighting conditions. This will facilitate the development of reliable and standardized methods for the recycling and reuse of 3D printing materials.

2.3. Raman Spectroscopy Method

Raman spectroscopy is a powerful analytical technique used to gain insights into the molecular composition and structure of materials. It is particularly useful for identifying organic and inorganic compounds, making it an ideal method for analyzing the plastic samples in this project.

2.3.1. Principle of Raman Spectroscopy

Raman spectroscopy is based on the inelastic scattering of monochromatic light, typically from a laser, by molecules in a sample. When the laser light interacts with the sample, most photons are elastically scattered (Rayleigh scattering), meaning they scatter without a change in energy. However, a small fraction of the photons are inelastically scattered (Raman scattering), resulting in a shift in energy corresponding to the vibrational modes of the molecules in the sample.

The Raman effect occurs due to the interaction of the incident light with the vibrational energy levels of the molecules. The energy difference between the incident and scattered photons provides a unique fingerprint for the molecular structure and composition of the sample.

2.3.2. Experimental Setup

The experimental setup for Raman spectroscopy involves the following key components:

- **Laser Source**: A monochromatic laser is used as the excitation source. Common laser wavelengths include 532 nm, 633 nm, and 785 nm. The choice of wavelength depends on the sample and the desired spectral resolution.
- **Sample Holder**: The sample is placed in a holder that allows the laser beam to be focused onto a specific area. The holder can be adjusted to accommodate different sample sizes and shapes.
- **Optics**: A series of lenses and mirrors are used to focus the laser beam onto the sample and to collect the scattered light. A notch or edge filter is used to block the elastically scattered light (Rayleigh scattering) and allow only the inelastically scattered light (Raman scattering) to reach the detector.

- **Detector**: The scattered light is dispersed by a spectrometer and detected by a charge-coupled device (CCD) detector. The CCD captures the Raman spectrum, which is a plot of intensity versus Raman shift (measured in wavenumbers, cm^{-1}).
- **Data Processing**: The raw spectral data are processed to correct for background noise and fluorescence. The resulting spectrum is analyzed to identify the characteristic Raman peaks corresponding to the molecular vibrations of the sample.

2.3.3. Procedure

The procedure for conducting Raman spectroscopy on the plastic samples includes the following steps:

- **Sample Preparation**: The plastic samples are cleaned to remove any surface contaminants that could interfere with the Raman signal. The standardized 5 cm x 5 cm square plates are used for consistency.
- **Laser Excitation**: The laser beam is focused onto the surface of the sample. Care is taken to avoid damaging the sample with excessive laser power.
- **Spectral Acquisition**: The scattered light is collected and directed into the spectrometer. The CCD detector records the intensity of the scattered light as a function of Raman shift.
- **Data Analysis**: The Raman spectrum is analyzed to identify the characteristic peaks. Each peak corresponds to a specific vibrational mode of the molecules in the sample, providing information about the chemical structure and composition.

2.3.4. Advantages of Raman Spectroscopy

Raman spectroscopy offers several advantages for the analysis of plastic materials:

- **Non-Destructive**: Raman spectroscopy is a non-destructive technique, allowing samples to be analyzed without causing any damage.
- **Minimal Sample Preparation**: Unlike some other spectroscopic techniques, Raman spectroscopy requires minimal sample preparation, making it convenient and efficient.
- **High Specificity**: The Raman spectra provide unique fingerprints for different molecular structures, allowing for precise identification of materials.
- **Compatibility with Water**: Raman spectroscopy is less affected by water, making it suitable for analyzing hydrated samples.

In conclusion, Raman spectroscopy is an invaluable tool for the detailed analysis of plastic samples in this project. By leveraging the unique vibrational signatures obtained through Raman scattering, this method provides a comprehensive understanding of the molecular composition and structure of 3D printing materials, aiding in the development of effective recycling strategies.

2.4. Near-Infrared Spectroscopy Method

Near-Infrared Spectroscopy (NIRS) is a non-destructive analytical technique widely used for characterizing the composition of various materials. It is particularly effective in identifying organic compounds, making it a valuable tool for analyzing the plastic samples in this project.

2.4.1. Principle of Near-Infrared Spectroscopy

NIRS operates on the principle of absorption spectroscopy in the near-infrared region of the electromagnetic spectrum, typically between 780 nm and 2500 nm. When near-infrared light interacts with a sample, specific wavelengths are absorbed by the molecular overtones and combinations of fundamental vibrations of the sample's constituent molecules. The absorption pattern, or spectrum, produced by these interactions provides a unique fingerprint that can be used to identify and quantify the different chemical components within the sample.

2.4.2. Experimental Setup

The experimental setup for NIRS includes the following components:

- **Light Source**: The near-infrared light source, often a tungsten-halogen lamp, provides the necessary illumination. The light emitted covers the near-infrared range, ensuring comprehensive analysis.
- **Sample Holder**: The sample is placed in a holder that can accommodate various sample types and sizes. For this project, plastic samples are prepared in standardized dimensions to ensure consistency.
- **Optics**: Lenses and mirrors direct the near-infrared light through the sample and onto the detector. The setup ensures that the light path is optimized for maximum interaction with the sample.
- **Detector**: The transmitted or reflected light from the sample is captured by a detector, typically an InGaAs (Indium Gallium Arsenide) detector, which is sensitive to near-infrared wavelengths. The detector converts the light into an electrical signal that corresponds to the intensity of the absorbed wavelengths.

- **Data Processing**: The electrical signal is processed to generate a near-infrared spectrum, representing the absorbance of different wavelengths by the sample. This spectrum is analyzed to identify and quantify the molecular components.

2.4.3. Procedure

The procedure for conducting NIRS on plastic samples involves the following steps:

1. **Sample Preparation**: The plastic samples are cleaned to remove any surface contaminants that could interfere with the NIR signal. The samples are standardized to 5 cm x 5 cm square plates with a thickness of 5 mm to ensure consistency.
2. **Light Interaction**: The near-infrared light is directed onto the sample. The light that is either transmitted through or reflected off the sample is collected for analysis.
3. **Spectral Acquisition**: The detector captures the transmitted or reflected light and converts it into an electrical signal. This signal represents the intensity of light at various wavelengths.
4. **Data Analysis**: The resulting spectrum is analyzed to identify characteristic absorption peaks. Each peak corresponds to specific molecular vibrations, providing detailed information about the chemical composition of the sample.

2.4.4. Advantages of Near-Infrared Spectroscopy

NIRS offers several significant advantages for the analysis of plastic materials:

- **Non-Destructive**: NIRS is able to analyse materials and samples in a non-destructive manner which allows the samples to be used indefinitely or reuse the materials in another way.
- **Minimal Sample Preparation**: NIRS requires very little preparation of samples which makes it even more suitable for analysing 3D-printed materials. The process of 3D-printing, especially FDM usually does not lead to a smooth surface finish. Even if the 3D printer is set up in a proffesionall manner the surface can show signs of roughness or depending on the orientation of the printed object produce layer lines.
- **Rapid Analysis**: Depending on the exact setup NIRS allows for rapid measurements and analysis of materials which in turn prommises a high efficiency of mechanisms that rely on it.
- **High Penetration Depth**: Near-infrared light can penetrate deeper into samples compared to other spectroscopic methods, allowing for bulk analysis.
- **Compatibility with Various States**: NIRS is suitable for analyzing samples in different states, including solids, liquids, and gels, making it a versatile analytical tool.

In conclusion, Near-Infrared Spectroscopy is a vital technique for this project's detailed analysis of plastic samples. By capturing the unique absorption patterns in the near-infrared region, NIRS provides a comprehensive understanding of the molecular composition and structure of materials used in 3D printing. This understanding is crucial for developing effective recycling strategies and supporting sustainable practices in the field of 3D printing and materials science.

2.5. 3D-Printing

Since the main use case for this project is focused on 3D-printable materials and a great number of parts for this project are 3D-printed this section will explain the basics of this technology.

2.5.1. 3D-printing technologies

3D printing is known as an additive production method which means instead of removing material from an oversized blank of material like in classical machining the material is applied bit by bit to form the desired shape. One of the most widely used methods is called Fused Deposition Modeling (FDM). In this method, a spool of filament is pushed through a heated nozzle. the position and height of the nozzle is controlled by several motors. Layer by layer the desired shape is produced on the building plate.

3. Experimental Setup

The Spectrometer setup is based on an open-source project which utilises a low-cost handheld spectroscope. [1] The PySpectroscope project is a program and an associated hardware design created for hobbyists to test homemade lasers and perform fluorescence spectroscopy. The setup consists of a camera which is equipped with an appropriate lens. The camera is fixed to a base which aligns it with the handheld spectroscope which is also fixed to the base. This assembly is pointed at a sample holder which is oriented to hold the 3D-printed samples at a 45° angle. Lastly, a light source is fixed to an appropriate mount and pointed at the sample holder so that the light that is reflected off the sample shines directly into the spectroscope. The Experiment setup was then fixed inside a plastic container which can be sealed with a lid to ensure no external light can interfere with the measurement. The whole setup is described in the graphic below and the physical setup is shown in the picture.

3.1. Components

As part of this project all mounts for the physical components were designed and 3D-printed specific to this application.

3.1.1. Spectroscope base and camera mount

The Spectroscope used in this project is a TE-313[2] Diffraction Grating Spectroscope that is specifically designed for Educational Science use as seen in figure 3.3. It can be used as a handheld spectroscope to showcase different effects and changes in the spectral behaviour of light. When a camera is fixed to the spectroscope and the intensity of the different light levels is measured it turns into a spectrometer which creates useful data.

The spectroscope needed to be fixed in a way that allows the user to rotate it along its cylindrical axis so that it can be orientated at the correct angle. When the correct position is reached the spectroscope can be fixed with a screw on top. The Camera needs to be mounted directly in line with the inner circular view window of the spectroscope. To achieve that, the spectroscope mount and the camera mount are fixed together on a 5mm thick copper plate to ensure a sturdy base.

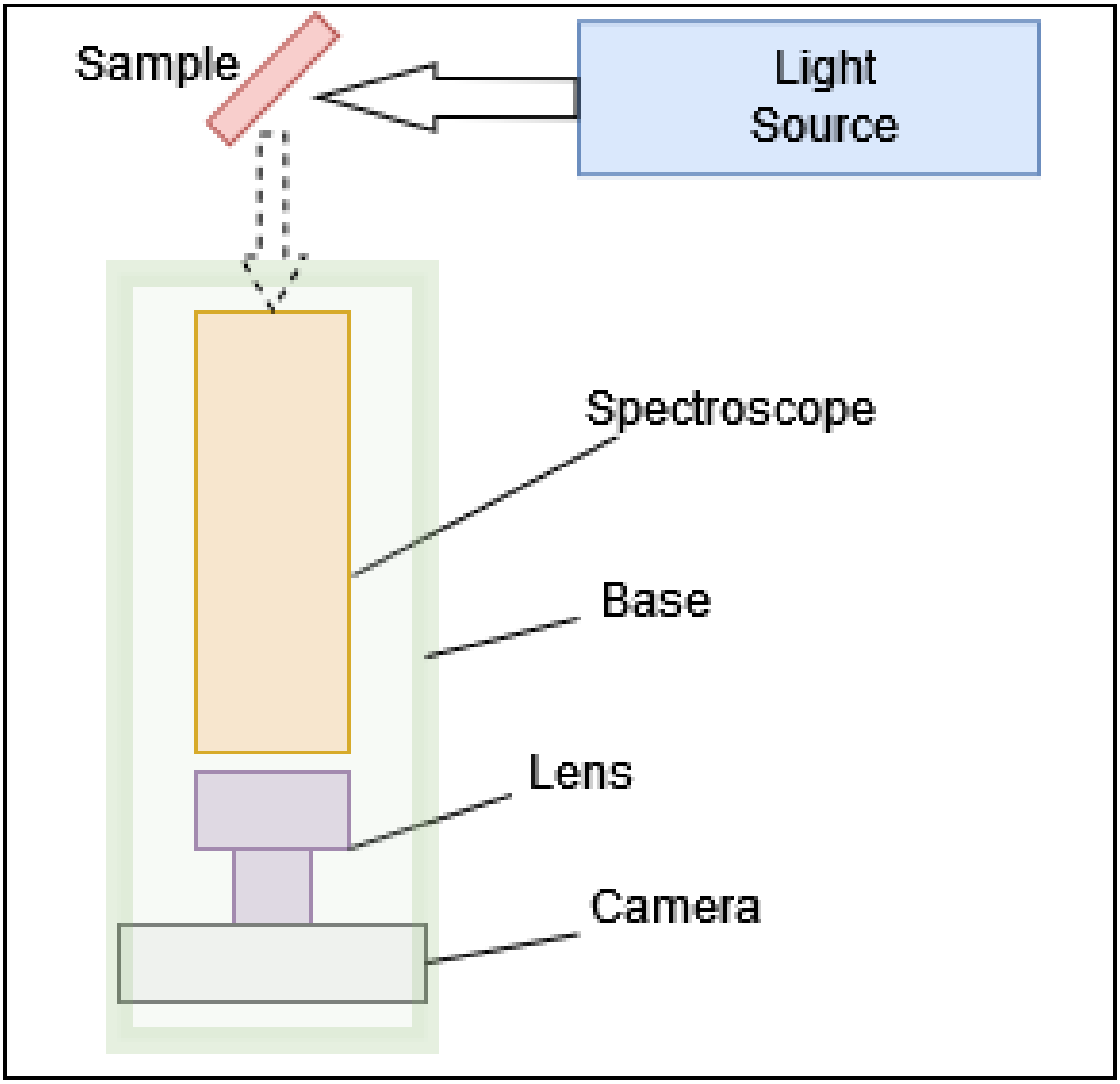

Figure 3.1.: Diagram of spectrometer setup

Figure 3.2.: Picture of spectroscope setup

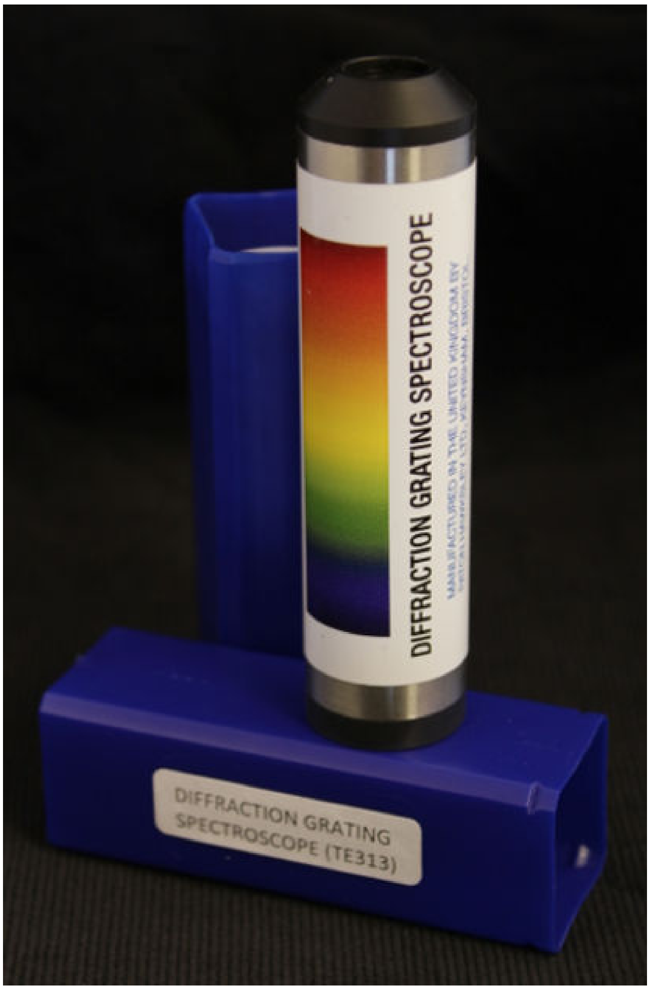

Figure 3.3.: Diffracting Spectroscope [2]

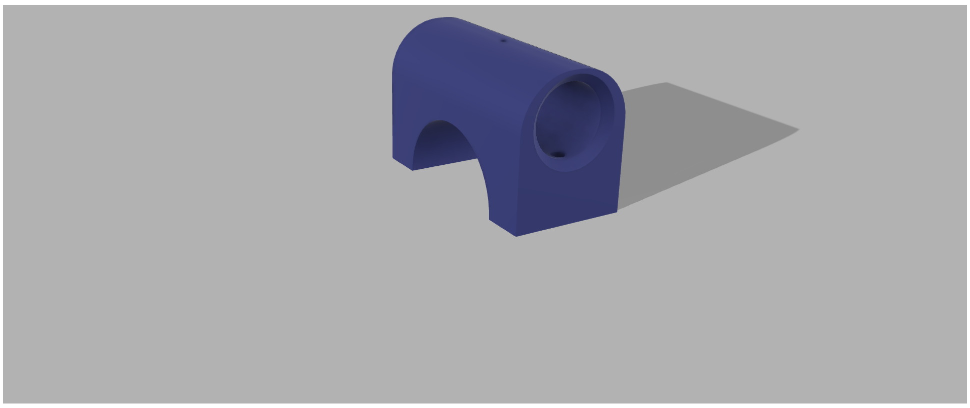

Figure 3.4.: Spectroscope Mount 3D-Design

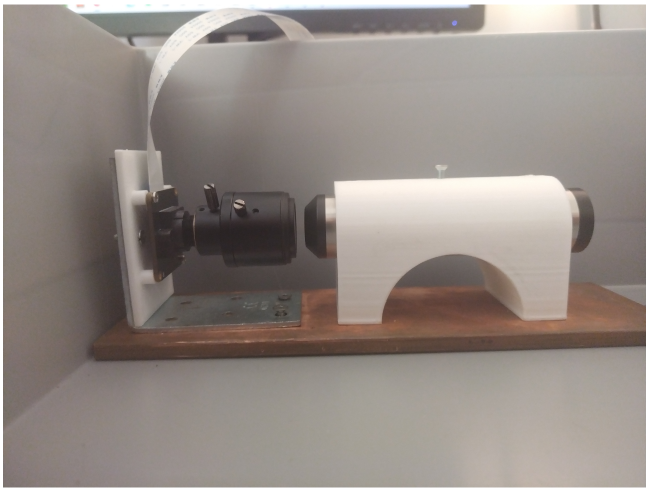

Figure 3.5.: Spectroscope mount

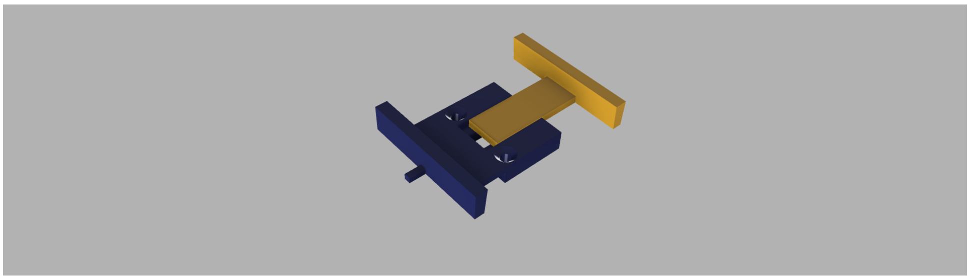

Figure 3.6.: Sample holder 3D-Design

3.1.2. Sample holder

The sample holder is also a 3D-printed part. Because of this, it had to be designed to minimise the amount of plastic that can be seen from the front so that the material of the sample holder does not interfere with the measurement of the actual sample.

3.1.3. Light Source mount

3.1.4. 4-in-1 Flashlight with Focus Function for Plastic Spectroscopy

The light source employed in this project is a high-performance, single-mode LED flashlight featuring four light modes: red, green, blue, and white. This versatile flashlight is ideal for spectroscopic measurements of various plastic materials, providing a focused beam capable of covering distances over 120 meters. Its different light modes are critical for testing material response to various wavelengths.

Red and Green Light for Material Characterization

In plastic spectroscopy, the red and green light modes are used to observe the optical and molecular responses of different polymers to these specific wavelengths. The varying absorption and reflection characteristics of plastics under red and green light can reveal important information about their chemical structure. This is particularly relevant in distinguishing between types of plastics with similar visible-light properties but different infrared or near-infrared responses. These modes allow for selective excitation of certain bonds or surface features, enabling precise analysis of material properties without causing sample degradation.

Blue Light for Fluorescent and Reflective Plastic Analysis

The blue light mode is particularly effective in fluorescence and reflectivity analysis of certain plastic materials. Many polymers exhibit fluorescence under blue light, which can be used to identify specific additives or coatings. By illuminating the plastic samples with blue light, the resulting fluorescence or reflective behavior can be captured and analyzed. This method is especially useful for identifying trace materials or detecting surface treatments, where blue light excites certain molecular bonds to emit measurable light for further spectroscopic analysis.

Waterproof and Shockproof Design for Field and Lab Use

The flashlight's waterproof and shockproof design ensures its durability in both laboratory and field settings. Whether the experiment is conducted in controlled lab environments or in outdoor conditions, the rugged construction guarantees reliable performance. Its resistance to environmental factors like water and mechanical shock makes it suitable for extended experimental use in conditions that might otherwise affect more delicate equipment, ensuring uninterrupted spectroscopic measurements of plastic samples.

White Light for Baseline and Calibration Measurements

The white light mode serves as a general-purpose light source, particularly useful for baseline measurements and calibration in spectroscopic analysis. Its broad-spectrum emission enables uniform illumination of plastic samples, providing a reliable reference point for comparative analysis across different wavelengths. This mode is especially valuable for aligning the experimental setup and ensuring consistency in the illumination of all plastic samples under investigation. The flashlight operates with either three AAA batteries or a 18650 rechargeable battery, offering flexibility in long-term experiments.

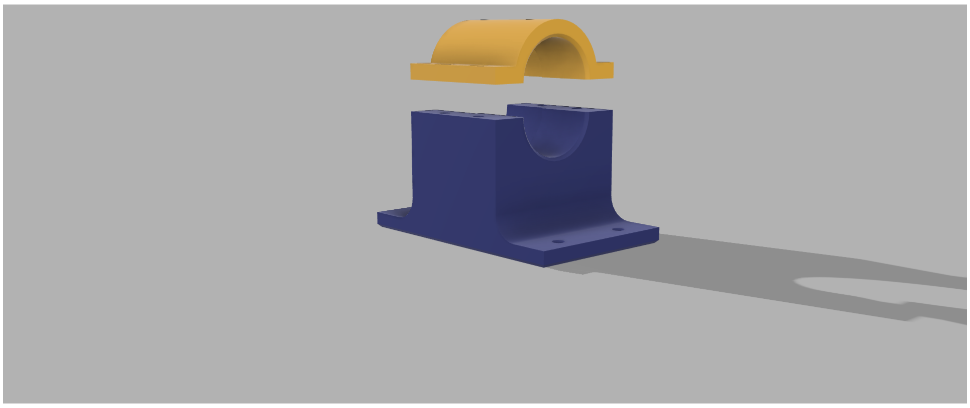

Figure 3.7.: Light source holder 3D-Design

3.2. Materials used

Since the project is focused on differentiating materials used for 3D printing, the selected samples were chosen to be widely available and commonly used by FDM-3D printers.

3.2.1. Material: Polylactic Acid - PLA

PLA is arguably the most user friendly 3D-printing Material. It is easily available and relatively cheap. [3] It does not require special precautions other than the right printing nozzle and bed temperature.

3.2.2. Material: Polyethylene Terephthalate Glycol - PETG

3.2.3. Material: Acrylonitrile Butadiene Styrene - ABS

3.2.4. Material: Acrylonitrile Styrene Acrylate- ASA

Name	Melting Temperature / °C	Colour	Manufacturer	
PLA	180-200	black		
PETG	200	black		
ABS	240	black		
ASA	230	black		

Table 3.1.: Caption

3.3. Measurement

Included in the PySpectrometer Project [1]was a software package that was designed to create measurements and usable data points from the Handheld Spectroscope. The package was designed for the use of a RaspberrPi microcomputer in 2020 for a now outdated platform. The project is not currently supported. The software side was designed to work in tandem with the hardware, providing real-time data acquisition, signal processing, and analysis through proprietary software. However, during the course of the project, it was discovered that the original software platform was no longer supported by the original creator. This led to a critical challenge, as the software was essential for operating the spectrometer and processing the spectral data. To overcome this issue, the software component had to be substituted by an alternative solution. A web-based platform was selected to replace the proprietary software, allowing data to be processed and analyzed externally. This alternative solution, while functional, introduced some limitations, such as reduced real-time processing capability and less integration with the hardware control system. Despite these drawbacks, the measurement process was able to continue, and the collected spectral data was processed successfully through the external platform, ensuring the project could proceed as planned. Future work may involve developing a custom software solution that is fully compatible with the hardware and capable of addressing the limitations posed by the current web-based platform.

All Samples were measured multiple times using different lights from the source to ensure comprehensive data collection.

4. Analysis and Interpretation of Results

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List of Abbreviations

FDM Fused Deposition Modeling

A. How To

Adding appendixes is as simple is everything else . . . trust me!