Hyperspectral imaging for in-situ applications
Methods to improve the classification of materials using hyperspectral imaging

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Faculty of Science, Technology and Media
Doctoral Thesis in Computer and Electrical Engineering
Mid Sweden University
Sundsvall, 2024-01-25
Akademisk avhandling som med tillstånd av Mittuniversitetet i Sundsvall framläggs till offentlig för avläggande av Doktorsexamen i elektronik den 25 jan 2024, klockan 09:00 i sal O102, Mittuniversitetet Sundsvall. Seminariet kommer att hållas på engelska.

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Printed by Mid Sweden University, Sundsvall
ISSN 1652-893X

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For my son, Mikaal
ABSTRACT

This thesis addresses several research questions related to in-situ hyperspectral imaging systems, proposes measurement methods for more accurate imaging, and examines the impact of the methods on material classification.

First, the thesis investigates the possibility of successfully calibrating a hyperspectral imaging system using a low-cost PTFE reference. A hyperspectral imaging system and practical calibration procedure using an inexpensive calibration reference are introduced. This reference enables accurate measurement of a material’s reflectance spectra independent of lighting and the camera’s spectral distribution of intensity and sensitivity. The study presents experiments conducted on winter roads covered with water, snow, and ice. The results show the robustness of the calibration and the suitability of the system for classifying materials.

The thesis further focuses on increasing the dynamic range (DR) of line scanning hyperspectral cameras. A method that relies on the use of multiple exposures is proposed to increase DR, benefiting applications such as plastic detection and polymer sorting. Experiments show that the proposed method can increase the DR for hyperspectral SWIR imaging from 43 dB to 73 dB. Material classification experiments reveal significant accuracy improvements with multiple exposures for large dynamic ranges.

The thesis also examines the effect of variations in relative humidity. It shows that even minor changes in humidity can significantly affect measurements. Frequent calibration and pruning of active wavelength bands are proposed as solutions to reduce the classification error rate for polymers from 20% to less than 1%.

The thesis also investigates the classification of colored materials by combining visible and infrared imaging. The clas-
Abstract

Sification algorithm shows high overall accuracy, close to 99.9\% for one test case, which also shows the potential of this approach.

Finally, the use of infrared hyperspectral imaging combined with Convolutional Neural Networks (CNN) for the classification of black polymers is evaluated. CNN outperforms all traditional classification algorithms, further demonstrating the potential of the proposed method. Further research on larger and more diversified material samples is recommended.
SAMMANFATTNING

Denna avhandling tar upp flera forskningsfrågor som rör in-situ hyperspektrala avbildningssystem, föreslår mätmetoder för mer exakt bildupptagning och undersöker metodernas inverkan på klassificering av material.

Först undersöker avhandlingen möjligheten att framgångsrikt kalibrera ett hyperspektralt avbildningssystem som använder en lågkostnads-PTFE referens. Ett hyperspektralt bildsystem och en praktisk kalibreringsprocedure som använder en billig kalibreringsreferens introduceras. Denna referens möjliggör exakt mätning av materialets reflektionsspektra oberoende av ljusets och kamerans spektra fördelning av intensitet och känslighet. Studien omfattar experiment på vintervägars beläggning av vatten, snö och is. Resultaten visar på robusthet i kalibreringen samt systemets lämplighet för klassificering av material.

Avhandlingen fokuserar vidare på att öka det dynamiska området (DR) för linjeavbildande hyperspektrala kameror. En metod för multipla exponeringar föreslås att öka DR, vilket gynnar applikationer som plastdetektering och polymersortering. Försök visar på att föreslagen metod kan höja DR för multispektral SWIR-avbildning från 43 dB till 73 dB. Experiment med klassificering av material avslöjar betydande noggrannhetsförbättringar med multipla exponeringar för stort dynamiskt område.

Avhandlingen undersöker också effekten av variationer i relativ fuktighet. Den visar att även mindre fuktighetsförändringar kan påverka mätningarna väsentligt. Frekventa kalibreringar och beskärning av aktiva våglängdsband är föreslagna lösningar som minskar klassificeringsfelet från 20 % till mindre än 1 % vid klassificering av polymener.

Avhandlingen undersöker också klassificering av färgat material genom att kombinera synlig och infraröd avbildning. Klassificeringsalgoritmen visar på hög övergripande nogrann-
Sammanfattning

het, nära 99,9 % för ett testfall, vilket också visar på potentialen i detta tillvägagångssätt.

Slutligen utvärderas användningen av infraröd hyperspekttral avbildning i kombination med Convolutional Neural Networks (CNN) för klassificering av svarta polymerer. CNN överträffar alla traditionella klassificeringsalgoritmer, vilket också lyfter fram potentialen med föreslagen metod. Ytterligare forskning på större och mer diversifierade materialprover rekommenderas.
ACKNOWLEDGEMENTS

I am deeply thankful to my Ph.D. supervisor for his unwavering support and guidance and for accepting me as a doctoral student under his mentorship. Throughout the course of my Ph.D. journey, his insights and encouragement have been pivotal in shaping the direction of my research.

I am profoundly grateful to my parents for their unwavering and unconditional support throughout my academic journey. Their encouragement, sacrifice, and belief in my potential have been a driving force behind my achievements.

I also want to give a special mention to my wonderful wife, Cecilia. She is the reason I made not one, but two memorable tours to Mexico during this research work. And while these trips may have delayed the completion of this thesis, I would not trade those experiences for all the on-time submissions in the world. Thank you, Cecilia, for bringing some adventure to my academic endeavors and for reminding me that sometimes detours make the best stories—even if they are written in the margins of my thesis timeline.

Lastly, I want to thank everyone who was present during my Ph.D. research for creating such a wonderful working atmosphere within the department.
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Paper I
Calibration of a Hyper-Spectral Imaging System Using a Low-Cost Reference

Paper II
Extending Effective Dynamic Range of Hyperspectral Line Cameras for Short Wave Infrared Imaging

Paper III
Impact of water vapour on polymer classification using in-situ short-wave infrared hyperspectral imaging

Paper IV
Improved classification of multi-color polymers using hyperspectral imaging
Shaikh, M.S.; Thörnberg, B., Accepted for publication in Journal of Spectral Imaging (JSI), 2023.121

Paper V
Classifying Black Polymers Using Convolutional Neural Networks and Short-wave-Infrared Hyperspectral Imaging
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Chapter 1

INTRODUCTION

Spectral imaging is a technique in which spectral information is presented as the third dimension of a two-dimensional spatial image, often referred to as “spectral cube”. This concept was first introduced in 1985 in the context of remote sensing for Earth exploration [Goe+85]. Spectral imaging has many applications across various scientific and engineering disciplines, including but not limited to satellite-based remote sensing [TB11] [CBP03] [CBF06], agricultural studies [COL+08] [Mis+17] [Asa+18], defense applications [TC10], medical diagnostics [Hao+21], and food quality assessment [Mar+15] [Lu+00]. Generally, the spectrum of light emitted from a light source and diffusely reflected in the surface of various materials is analyzed. The illumination can be ambient light from the sun or an artificial source of illumination, such as xenon lamps, halogen lamps, or LEDs. The diffused reflection of the light contains unique spectral signatures depending on the material composition of the reflecting surface [Stu97]. Consequently, spectral imaging allows for the recording of unique spectral signatures in two dimensions, such that a trained classifier can be used to determine the surface material at each individual pixel [JCT15].

Spectral imaging is generally classified into three categories: Multi-Spectral Imaging (MSI), Hyper-Spectral Imaging (HSI), and Ultra-Spectral Imaging. This abstract categorization is based on factors such as spectral resolution, the number of spectral bands, and the intervals between these bands. MSI, for instance, typically employs up to 10 distinct bands, which need not necessarily be contiguous. HSI, on the other hand, offers the capability to capture data across a spectrum encompassing hundreds of bands. In practical implementation, spectral imaging sensors collect data as a series of images, each corresponding to a specific narrow segment of the electromagnetic spectrum, referred to as a spectral band. These individual images are subsequently combined to generate a three-dimensional hyper-spectral data cube denoted as $I(x, y, \lambda)$. In this context, $I$ represents the intensity (or
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digital value), while $x$ and $y$ denote the spatial dimensions of the scene. $\lambda$ represents the spectral dimension, signifying a range of wavelengths. The effectiveness of these sensors is often assessed in terms of spectral resolution, which defines the width of each band of the spectrum captured.

1.1 Problem motivation

HSI introduces a remarkable technological leap that can detect the unseeable, revealing the intricate composition of materials in extraordinary detail. This cutting-edge approach, merging the power of imaging and spectroscopy, transcends conventional visual analysis. By capturing the unique spectral fingerprints of objects, HSI offers a wealth of information beyond what the human eye can perceive. Its applications span a wide spectrum, from remote sensing to medical diagnostics.

The significance of HSI lies in its unparalleled ability to classify materials based on their distinct spectral signatures. In fields such as agriculture, it assists in identifying healthy crops and detecting diseases by analyzing plant reflectance patterns [Wan+22]. In the realm of defense, it aids in target identification and camouflage detection [HS22] through precise material discrimination. Medical diagnostics benefit from HSI’s capacity to detect subtle tissue abnormalities, enabling early detection of diseases. Moreover, in food inspection, it helps ensure quality and safety by identifying contaminants and variations in products.

In various sectors, the positive societal impact of HSI is profound. Satellite-based remote sensing, empowered by HSI, enhances our understanding of global environmental changes, supporting sustainable resource management. In the agricultural sector, it increases crop yield and minimizes pesticide usage through precise disease detection [Tud+21]. In medical diagnostics, early disease identification translates to improved patient outcomes and reduced healthcare costs. The food industry benefits from heightened quality control, ensuring
safer consumption. These applications collectively foster a healthier, safer, and more sustainable society.

In relation to mounting concerns about polymer pollution, HSI is emerging as a game-changer in polymer recycling. It has the potential to further improve sorting processes by distinguishing between different types of polymers with exceptional accuracy. While current methods struggle with color diversity in plastic compositions [Pau+19a] [Bro+96a], improved HSI methods can potentially resolve this issue, enabling effective separation and recycling.

Despite numerous advancements in the field of HSI, there remains a need for continued efforts to enhance measurement techniques to further improve material classification. Presently, several methods are employed for conducting hyperspectral measurements, yet their potential repercussions on classification outcomes remain underexplored. By improving measurement methods, there exists the potential to improve material classification results, which would benefit multiple industries and also have a positive impact on society.

1.2 Research problems

In-situ hyperspectral measurements, and thereby their use for material classification, are subject to the influence of various factors. These factors are related to the specific environment in which the imaging occurs, the components comprising the imaging system, and the particular application cases for the technology.

Changes in relative humidity, temperature, and ambient lighting stand out as notable examples of factors related to the imaging site environment. A comprehensive understanding of the impact of these factors on hyperspectral measurements, and by extension material classification, is still lacking. The extent to which these environmental variables affect the accuracy of hyperspectral measurements and, consequently, the precision of material classification needs to be quantified. This is integral for the advancement of imaging methodologies
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aimed at achieving greater precision in measurements and, in turn, improving the outcomes of material classification.

Within the imaging system itself, there exist factors that contribute to inaccuracies in hyperspectral measurements, ultimately reducing the overall success rate of material classification. Notable examples of these factors are the limited sensitivity and dynamic range of cameras, the restricted wavelength range within which a single camera can operate, and the non-uniform distribution of camera sensitivity across the operating wavelengths of a device. Additionally, variations in the spectral distribution of halogen lamps, attributed to fluctuations in power supply and temperature, as well as aging, are noteworthy. Halogen lamps are commonly used as illumination sources due to their effective radiation in both the visible and infrared spectrum. These factors collectively contribute to a reduction in measurement quality and adversely impact the performance of material classification. Understanding and addressing these system-related factors is crucial for improving measurement precision and, consequently, material classification outcomes. To mitigate the effects of system-based factors, radiometric calibration is essentially used to ensure that captured images or data represent the true radiance or reflectance of objects being observed [Yan+17][PHG19], while relative radiometric calibration ensures consistent and accurate comparisons of recorded values without providing absolute radiometric units. When a spectral camera captures an image, it measures the amount of light present at various wavelengths. However, the camera’s pixels might not be equally sensitive to all wavelengths, and external factors such as the lighting conditions can also affect the measurements. Radiometric calibration involves adjusting the camera’s settings or correcting the captured data such that the resulting image accurately represents the true characteristics of the scene being captured. Calibration of true reflectance requires the use of one or more calibration standards, known as “calibration targets”. These calibration targets are typically made of a matte Lambertian reflecting surface, which reflects a near-identical intensity of light in all directions. The total reflection in all directions is typically close to 100 percent. In this context, a product called Spectralon(TM) is commonly employed to craft these calibration targets.
The specialized process of creating Spectralon\textsuperscript{TM}, which entails compressing polytetrafluoroethylene (PTFE) powder, results in an open-cell PTFE matrix with around 40\% void volume, thereby enhancing light scattering [WH81]. The cost of a Spectralon\textsuperscript{TM} calibration standard is approximately 2.2 EUR/cm\textsuperscript{2}. Depending on the specifics of the imaging setup, a relatively large calibration target may be required. Additionally, existing calibration methods do not allow the measured image, reference image, and dark current image captured with different exposure times [NLT13] [NA19] [Bol+12]. This is due to the fact that exposure time is completely ignored in the derivation of calibration algorithms. There is a need for easily repeatable in-situ calibrations using a reasonably priced calibration target that is not affected by humidity and temperature.

Apart from environmental and system-based factors, materials with certain spectral properties can sometimes make the HSI system record indistinguishable spectral signatures. HSI within SWIR wavelengths has been an effective method to classify/separate transparent or white polymers/materials, but the same is not true for colored polymers, especially darkly colored ones [Bro+96b] [Pau+19b] [DGM18]. A particular case in which this applies is the use of carbon black for material coloration. When it comes to black polymers, the effectiveness of SWIR hyperspectral imaging diminishes. The high absorption of SWIR rays by carbon black, in combination with low camera sensitivity and limited intensity of illumination sources, limits the ability of the imaging method to accurately distinguish between various black polymer samples. As a result, the detection and classification of black polymers using traditional SWIR spectroscopy entails significant challenges and limitations. However, a recent study [Xia+21] introduced a promising approach to address the limitations of vibrational spectroscopy within SWIR wavelengths for classifying black polymers. This study utilized Convolutional Neural Networks (CNN) to classify colored polymers, including black samples, with an impressive success rate of 98\%. If such high classification success rates can be achieved consistently across various datasets and samples, it can effectively resolve the long-standing bottleneck problem of polymer sorting. In contrast, [RPA17] refers to the use of NIR spectroscopy and
states that the Signal-to-Noise-Ratio (SNR) of this detector technology is too low to be used for the classification of black plastics. A possible assumption from this is that CNN and deep learning can potentially mitigate the limitations of low SNR. Consequently, there is a need to investigate further the utilization of CNN to classify black polymers and materials in general using SWIR HSI.

1.3 Research questions

This thesis aims to answer the following research questions (RQs):

- **RQ.1**: What are the major environmental factors that can reduce the performance of in-situ hyperspectral imaging systems?

- **RQ.2**: What are the major limitations of system components that can reduce the performance of in-situ hyperspectral imaging systems?

- **RQ.3**: How can we improve methods for image acquisition, processing, and system calibration such that the limitations and impacts found in RQ.1 and RQ.2 are mitigated?

- **RQ.4**: Can the use of deep learning artificial intelligence improve material classification by hyperspectral imaging systems?

- **RQ.5**: What have we learned from studying various applications for hyperspectral imaging?
1.4 Contributions

1.4.1 Calibration of hyperspectral imaging using system using low-cost reference

A method is proposed for calibrating hyperspectral imaging systems using a low-cost PTFE tile as a calibration target. The aim of this method is to accurately measure the true reflectance of objects while mitigating variations in the spectral distribution of the illumination source and camera sensitivities across the entire wavelength range of operation. By comparing the measured spectra of different winter asphalt conditions with their known spectra, it is shown that a calibration target with an accurate reflectance is not needed for the purpose of identifying materials by their spectral signatures. In contrast to existing calibration procedures, the proposed method allows for spectral measurements of materials, dark current, and the calibration target using different exposure times, thereby optimizing the SNR of measurements.

1.4.2 HDR imaging using hyperspectral line cameras

A tailored multi-exposure method is proposed for InGaAs-based hyperspectral line cameras. The main objective is to enhance the DR of hyperspectral imaging, thereby improving the SNR for low-intensity measurements while preventing saturation at high-intensity levels. What sets this proposed algorithm apart is the incorporation of DC modeling, a crucial consideration for InGaAs-based sensors. Furthermore, the algorithm integrates a specific criterion that establishes a minimum SNR requirement for all measurements. Any signal falling below this SNR threshold is deemed unreliable. The effectiveness of the algorithm is also demonstrated, particularly in scenarios where the dynamic range of the scene greatly exceeds that of the spectral camera. This improvement is notably observed in the classification success rate.
Chapter 1. Introduction

1.4.3 Analysis of the impact of water vapor on SWIR hyperspectral measurements

It is shown that vaporized water has an impact on hyperspectral measurements, even at pathlengths of hundreds of centimeters, especially in the case of large variations of Relative-Humidity (RH). The method proposed to overcome this source of uncertainty in measurements is to frequently calibrate the hyperspectral measurement setup such that the impact of varying air composition is reduced. It is also shown that RH-induced variations in measurement can drastically affect the classification of materials using an in-situ setup. However, it might be difficult to frequently switch materials for analysis with a calibration target in an industrial setting. An alternative method is proposed to prune the wavelengths that are susceptible to water vapor. The classification results show that even a significant change in humidity only has a minor impact on classification if the susceptible bands are pruned.

1.4.4 Improved classification of multi-color polymers

How the presence of color fillers affects the categorization of polymers is also investigated. It is shown that incorporating VIS wavelengths during the training and testing phases of machine learning models leads to improved classification outcomes. This improvement is particularly evident in the more accurate identification of colored polymers that are susceptible to misclassification.
1.4.5 Performance evaluation of CNN for classifying black polymers

The effectiveness of CNN to detect and categorize recyclable black polymers using Hyperspectral Imaging within the SWIR region was assessed. The classification of black polymers in the SWIR domain has presented a persistent challenge. To evaluate the effectiveness of CNN, a comparison was made with conventional machine learning algorithms. The results indicate that CNN improves upon the accuracy of these traditional algorithms in the classification of black polymers.

1.5 Thesis outline

The remainder of this thesis is organized as follows:

- Chapter 2 presents a brief theoretical overview of spectroscopy and spectral imaging.
- Chapter 3 describes the experiment setups used during this Ph.D. research.
- Chapter 4 presents a discussion of the results.
- Chapter 5 presents the final conclusions and recommendations for future research.
1.6 Authors’ contribution

The following is a table of the authors’ contribution to the publications included in this thesis.

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<td>I [Sha+21]</td>
<td>M. S. S.</td>
<td>Co-developed the method, performed experiments and collected data, data analysis and processing, wrote the article.</td>
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<tr>
<td></td>
<td>B. T.</td>
<td>Method development, project supervision, participated in writing the article, data analysis .</td>
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<tr>
<td></td>
<td>K. J.</td>
<td>Data analysis and processing.</td>
</tr>
<tr>
<td></td>
<td>J. C.</td>
<td>Participated in discussions on methods and the selection of calibration target</td>
</tr>
<tr>
<td>II [SJT22]</td>
<td>M. S. S.</td>
<td>Co-developed the method, conducted the experiments, collected and analyzed the data, wrote the article.</td>
</tr>
<tr>
<td></td>
<td>B. T.</td>
<td>Developed the method, supervised the project, participated in experimentation and data collection.</td>
</tr>
<tr>
<td></td>
<td>K. J.</td>
<td>Participated in data collection and experimentation, data analysis and processing.</td>
</tr>
<tr>
<td>III [ST22]</td>
<td>M. S. S.</td>
<td>Co-developed the method, performed experiments and collected data, data analysis and processing, wrote the article.</td>
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M. S. S. - Muhammad Saad Shaikh, B. T. - Benny Thörnberg, K. J. - Keyvan Jaferzadeh, J. C. - Johan Casselgren

Table 1.1: Publication contributions.
Chapter 2

THEORY OF
SPECTROSCOPY AND
SPECTRAL IMAGING

In the realm of analytical chemistry and materials science, vibrational spectroscopy and spectral imaging have emerged as powerful tools for characterizing and understanding the composition and properties of various substances. This chapter delves into the fundamentals and applications of these techniques, exploring their principles, methodologies, and the insights they offer into the molecular and structural aspects of matter.

2.1 Vibrational spectroscopy: an overview

Vibrational spectroscopy is a branch of spectroscopy that involves the study of the vibrations of molecules and solids. It is primarily divided into two main techniques:

2.1.1 Infrared spectroscopy

Infrared (IR) spectroscopy is a powerful analytical technique based on the interaction between infrared radiation and molecular vibrations. To understand how it works, a basic conception of the physics of molecular vibrations and energy absorption is required.

Molecules are made up of atoms that are connected by chemical bonds. These atoms are not stationary but vibrate continuously due to thermal motion. These vibrations can occur in several ways, with the most common being stretching and bending motions of chemical
bonds. When infrared radiation, in the form of photons, interacts with a molecule, it can induce changes in the molecule’s vibrational energy levels [Len13]. For a vibration to be IR active (observable by IR spectroscopy), there must be a change in the molecule’s dipole moment during the vibration. This change in dipole moment results in the absorption of energy from the incident photons.

An IR radiation source illuminates the sample. When the incident photons match the energy required to induce a vibrational transition in the molecules, they are absorbed. The amount of energy absorbed corresponds to the vibrational energy level of the molecule. The reflected light is then analyzed, and the absorbed energy is recorded as an absorption spectrum.

2.1.2 Raman spectroscopy

Raman spectroscopy is based on the inelastic scattering of photons when they interact with molecules. Unlike IR spectroscopy, which relies on the absorption of energy, Raman spectroscopy involves the scattering of incident light. To understand the underlying physics, it is necessary to explore the nature of the Raman effect.

When photons interact with a molecule, most are elastically scattered (Rayleigh scattering), meaning they retain their original energy and frequency. However, a small fraction of the scattered photons undergo inelastic scattering, resulting in a change in their energy (frequency). This phenomenon is known as the Raman effect [Len13].

A monochromatic light source (usually a laser) is directed onto the sample. Most incident photons are elastically scattered (Rayleigh scattering), but a small portion undergo Raman scattering. The energy difference (frequency shift) between the incident and scattered photons corresponds to the energy of the molecular vibrations. A Raman spectrometer analyzes the scattered light, producing a Raman spectrum that reveals the vibrational modes of the molecules in the sample. The energy of the scattered photons changes due to the interaction with molecular vibrations. When a photon interacts with
a vibrating molecule, it can either gain or lose energy, depending on whether the molecule is in a higher or lower vibrational energy state. These energy changes are manifested as shifts in the frequency of the scattered photons.

Raman spectroscopy is highly useful for characterizing crystalline materials, polymers, and complex biological samples. It provides detailed information about molecular vibrations and can be used to differentiate between different chemical species, making it a valuable analytical tool in various fields, including chemistry, biology, and materials science.

2.2 Spectral imaging: an overview

Spectral imaging is a powerful technique that enables the capture and analysis of data across various wavelengths within a scene. In this section, a brief overview of spectral imaging methods, photo-detectors, and dispersion elements is provided.

2.2.1 Imaging methods:

*Whisk-broom method*

The whisk-broom imaging mode, also known as the point-scanning method, has a long use history. It was originally employed by the Earth Resources Technology Satellites and later applied in instruments like the Airborne Visible/Infrared Imaging Spectrometer.

Whisk-broom sensors utilize rotating mirrors to scan the landscape from side to side, perpendicular to the direction of the sensor platform, as shown in Fig. 2.1. These rotating mirrors redirect the reflected light to a single point or just a few sensor detectors grouped together. This method involves scanning a single point along two spatial dimensions by moving either the sample or the detector. The reflected light is then dispersed by a prism and captured by a linear array detector.
This process enables the acquisition of spectral image data cubes by scanning the surface and dispersing the wavelength domain [Uto+14].

![Diagram of a whisk-broom hyperspectral camera](image)

**Figure 2.1**: A general scheme for a whisk-broom hyperspectral camera

Whisk-broom imaging can be time-consuming because it requires scanning both the horizontal and vertical dimensions. This comprehensive scanning approach ensures detailed spectral data but may extend the time for data acquisition. To address the challenges of time and complexity, an alternative scanning method with a high acquisition rate and accuracy is used, known as the spectral confocal laser-scanning method. This approach involves illuminating and capturing images through confocal or conjugate pinholes, which restrict the in-focus optical section thickness. Multiple lasers and wavelength dispersive spectrophotometers are incorporated to obtain spectral information.
2.2.1. Imaging methods:

An advantage of the whisk-broom imaging method is that it typically involves fewer sensor detectors, which reduces the number of calibrations required compared to other types of sensors. Many commercial spectral confocal scanning instruments apply the whisk-broom imaging mode due to its ability to balance the need for detailed spectral data with efficient acquisition.

Push-broom method

The push-broom method, also referred to as line scanning, has been employed by Earth observation satellite systems. Unlike the whisk-broom method, which captures one pixel at a time, the push-broom method can simultaneously acquire spatial and spectral data. It generates unique images with one spatial dimension and other spectral dimensions in a single scan using a matrix detector [Hyv+11].

Push-broom imaging captures a slit image from the surface, dispersing it onto a two-dimensional photo detector. Spatial data is represented along one axis, while wavelength data is represented along the second axis. The spectral image data cube is then constructed by moving the camera or the surface in the direction of another spatial axis, as shown in Fig.2.2.

Push-broom scanners collect more light than whisk-broom scanners due to the longer exposure times on the detector, resulting in a comparatively higher spectral resolution [Mey+11]. However, synchronization is crucial, as either the camera or the object must move to acquire each line of the image during scanning.

Staring method

The staring imaging method, often referred to as the band sequential method, is a distinctive approach of spectral scanning. It is different from the more conventional push-broom and whisk-broom methods due to its unique system of data acquisition. In the case of staring imaging, the system captures a single-band 2D grayscale image that
Figure 2.2: A general scheme for a push-broom hyperspectral camera
2.2.1. Imaging methods:

encompasses complete spatial information in a single shot. This makes it highly suitable for applications that require a high level of spatial detail in conjunction with spectral analysis.

One of the key differentiators of staring imaging is its use of filters, such as fixed bandpass filters, linear variable filters, variable interference filters, or tunable filters. These filters are strategically positioned in front of a matrix detector within the imaging system. As incoming light passes through the optical system, these filters play a critical role in the spectral selection process. They allow only a narrowband segment of the electromagnetic spectrum to reach the focal plane of the detector. Typically, a matrix CCD sensor serves as the detector, capable of capturing images with high spatial resolution [Yu+22].

The process of spectral data acquisition in staring imaging is inherently unique. At any given moment, the system captures a 2D image at a specific wavelength, as shown in Fig.2.3. The complete spectral image cube is constructed by systematically tuning the output wavelength of the filter over time [Gup11]. This dynamic approach allows for the efficient acquisition of spectral information across various wavelengths, providing valuable insights into the composition and characteristics of the imaged scene.

Furthermore, the staring method excels in dynamic range preservation. It accommodates different exposure settings at various wavelengths, ensuring that high-intensity and low-intensity spectral features can be captured accurately and without data saturation. This unique characteristic makes staring imaging particularly well-suited for fields such as remote sensing, astronomy, and environmental monitoring, where detailed spectral analysis is paramount for scientific and analytical purposes.

**Snapshot method**

The snapshot method is also known as the single-shot method. Unlike other methods discussed, such as the whisk-broom, push-broom,
Figure 2.3: A general scheme for the staring imaging method
2.2.1. Imaging methods:

Figure 2.4: A general scheme for the snapshot hyperspectral imaging method

and staring methods, which involve scanning in either the spatial or spectral dimension, the snapshot method eliminates the need for any form of scanning [GTL14].

The primary advantage of the snapshot mode is its ability to capture both spatial and spectral information in a single exposure. This is made possible by directly imaging remapped and dispersed image zones onto a CCD detector, enabling the simultaneous acquisition of spatial and spectral data without the time-consuming scanning process [Wei+96].

However, the method does come with inherent limitations. The spatial and spectral resolutions are bound by the total number of pixels available on the CCD camera. In essence, the number of voxels, representing 3D data points, cannot exceed the pixel count of the CCD. Consequently, there exists a trade-off between spatial and spectral sampling. However, the spectral imaging approach can be adjusted according to specific requirement. Users can opt to enhance spatial sampling at the expense of spectral resolution or vice versa [GKT09]. Fig.2.4 shows a general scheme for the snapshot hyperspectral imaging method.
Chapter 2. Theory of spectroscopy and spectral imaging

2.2.2 Imaging detectors

For the visible range, two detector types are most common: CCD detector and Focal Plane Arrays (FPA) constructed from silicon. Standard CCD detectors exhibit relatively low quantum efficiency in the blue and ultraviolet spectral regions due to silicon’s high absorption coefficient of these wavelengths [Nor15]. Better performance is achieved through thinned back-illuminated and cooled CCD detectors [Rog04; Dia+08]. For wavelengths in the ultraviolet range, high quantum efficiency detectors made from aluminum gallium nitride (AlGaN) can be used [Lon+02]. Despite their low sensitivity and resolution compared to modern solid-state FPA, low-cost lead oxide-lead sulfide (PbO-PbS) vidicons have been widely used for the VIS-SWIR range [Cas+99].

Infrared FPAs cover a broad range of spectral regions from 1 μm to 25 μm and are based on different materials, including platinum silicide (PtSi), indium antimonide (InSb), InGaAs, and mercury cadmium telluride (MCT) [Fin+14; Gao+21]. PtSi detectors, known for their affordability and compatibility with silicon technology, offer an economical choice, but they exhibit relatively low quantum efficiency. InSb detectors, sensitive in the 1–5 μm spectral range, need to be cooled to around 80 °K [Nor15]. InGaAs and MCT detectors were initially developed for high-end technologies and military applications but have gained popularity in commercial applications following declassification [Tra]. Standard InGaAs detectors, grown on indium phosphide (InP) substrates, offer sensitivity in the 0.85–1.7 μm spectral range [HM08]. MCT detectors, which cover the entire infrared region (1–20 μm), can have their spectral cut-off finely tuned by adjusting the Hg:Cd ratio in the semiconductor composition [Tra; DSR04]. However, MCT detectors operating above 3 μm must be cooled to the temperature of liquid nitrogen, making them the most expensive detectors available [AF03]. Nonetheless, they exhibit exceptional performance. Recent advancements have extended the capabilities of InGaAs and SWIR-MCT detectors into the visible light range, enabling coverage of the 0.4–1.7/2.5 μm spectral range with a single array, albeit with lower quantum efficiency compared to CCD detectors [Mar+05; Chu05].
In summary, the choice of imaging detector in spectral analysis depends on the specific spectral range of interest, desired sensitivity, and budget constraints. Detector technologies have evolved to accommodate various applications, from everyday visible light imaging to specialized infrared spectroscopy, offering a wealth of options for capturing spectral data across the electromagnetic spectrum.

### 2.2.3 Optical filters and dispersion devices

The ability to separate wavelengths effectively is fundamental in the field of spectral imaging. The choice of devices for this purpose often depends on the specific application. Various categories of devices have been developed, each with its own advantages and considerations. The primary categories of devices used for wavelength separation are optical filters, prism-grating-prisms (PGP), and electronically tunable elements like Liquid Crystal Tunable Filters (LCTF) and Acousto-Optic Tunable Filters (AOTF) [Vag07].

Spectral imaging systems frequently utilize optical filters to achieve wavelength separation. Mechanical scanning devices use a rotating wheel that holds interference filters in front of the detector to filter incoming radiation. While this approach is effective, mechanical scanning devices have limitations. They can accommodate only a limited number of filters, and the rotation of the filter wheel often introduces vibrations that can disrupt image registration. Additionally, their tuning speed tends to be relatively slow, and they may lack portability [Bal+03].

LCTF [Tra] and AOTF [Gup09] operate based on a number of different principles but share certain advantages. They contain no moving parts, ensuring mechanical robustness, and offer high tuning speeds along with a compact design [MHT94; Sah+18]. LCTFs and AOTFs can be tuned electronically to cover a wide spectral range from the visible to the mid-infrared. However, a range of modules may be required to span a broad spectrum fully. LCTFs may exhibit reduced sensitivity in the blue light region, although this can be
compensated for through longer exposure times [Str+01]. AOTFs offer wavelength-independent tunability but may introduce some image shifting [Ber06].

PGP dispersing devices leverage transmission holographic gratings with high diffraction efficiency, often comprising several hundred bands. This technology offers true hyperspectral capabilities, enabling precise spectral separation [Aik01]. Unlike spectral imaging systems equipped with optical or electronically tunable filters, PGP devices record the spectral and one spatial dimension, while temporally sampling the second spatial dimension. However, for immobile targets, PGP devices necessitate scanning the entire object to collect data before generating an image, making real-time imaging challenging.

The choice of optical filters and dispersion devices in spectral imaging depends on the application requirements. Mechanical scanning devices, while effective, come with limitations in terms of filter count, vibrations, and speed. LCTFs and AOTFs offer high-speed, versatile tuning capabilities, and PGP devices provide true hyperspectral capabilities but may require scanning for immobile targets.

2.3 In-situ versus remote hyperspectral imaging

Hyperspectral imaging, a potent technique for spectral analysis, can be broadly classified into two categories: in-situ (on-site) and remote sensing (from a distance). Remote sensing is generally performed using satellites or aircraft/drones. In-situ hyperspectral imaging involves the direct capture of data at the target location, allowing for precise validation of ground truth and flexibility in data acquisition parameters. Researchers have real-time access to information and increased control over experimental conditions. However, this method is limited by its inability to cover extensive areas efficiently and the resources required for on-site data collection.

On the other hand, remote hyperspectral imaging provides a more comprehensive view by capturing data from a distance. This approach
2.3. In-situ versus remote hyperspectral imaging

is particularly beneficial for large-scale environmental monitoring, agriculture, and assessing inaccessible or hazardous regions. Despite its advantages in terms of wide coverage area and cost-efficiency, remote sensing faces challenges related to limited ground truth validation and susceptibility to atmospheric conditions, potentially affecting data accuracy.

Comparatively, in-situ imaging excels in precision and direct validation but struggles with scalability. Remote sensing, while offering a macroscopic perspective, may compromise fine details and data accuracy. Hybrid approaches, which integrate both in-situ and remote hyperspectral data, aim to optimize the advantages of each method. By combining the precision of in-situ measurements with the extensive coverage of remote sensing, researchers can attain a more nuanced and comprehensive understanding of the target environment. However, these hybrid approaches come with logistical complexities and the need for sophisticated data integration techniques to reconcile differences in spatial and spectral resolutions.
In this study, hyperspectral imaging was conducted using two push-broom cameras: the Specim Fx17 and the Specim Fx10, each offering distinct features and capabilities. The Specim Fx17 is equipped with an InGaAs detector, making it particularly well suited for applications that require sensitivity in the NIR and SWIR ranges. On the other hand, the Specim Fx10 employs a CMOS detector, providing advantages such as high-speed data acquisition and excellent spatial resolution. This camera is designed to cover a broad spectral range, extending from VIS to NIR. Both cameras incorporate a PGP element for efficient light dispersion.

This chapter presents details of the experiment setups used to acquire spectral data and the sample preparation methods from the selected test cases. Infrared vibrational spectroscopy was applied to different test cases for material analysis.

3.1 Experiment Setup #1:

The experiment setup shown in Fig.3.1 was used for conducting all spectral measurements in Papers I-III. The camera was placed at a height of 85 cm between two halogen lamps, all oriented in a downward direction at an angle of approximately 45 degrees relative to the ground plane. This specific angle was chosen with the aim to reduce specular reflections from the examined surface while ensuring a sufficient signal from the diffused reflections. This same experiment setup was used for obtaining measurements from both the calibration reference and test samples.
Figure 3.1: Experiment Setup #1: (a) schematic depiction of the Setup (b) photo of the Setup.

3.2 Experiment Setup #2:

Experiment Setup #2, shown in Fig.3.2, was used to conduct spectral measurements relevant to Papers IV and V. This setup, functioning as a scanner, was constructed using aluminum profiles. Positioned at the top of the frame were two hyperspectral cameras, facing downward in orthogonal alignment. At the base of this framework, a linear stage was integrated, facilitating the precise movement of a polycarbonate sheet perpendicular to the camera’s scanning paths.

In preparation for the experiment, a layer of aluminum foil paper was affixed to the polycarbonate sheet, serving as the background against which the polymer samples would be examined. Aluminum foil was chosen for its opaqueness, distinctive spectral characteristics that differentiate it from the polymers, and its resilience to common environmental variables, such as humidity and temperature fluctuations.

To ensure integration, both the cameras and the linear stage were linked to a laptop computer via an ethernet switch and a motor controller. For illumination of the polymer samples, four halogen lamps were installed at the rear of the frame, set at an angle of 40° in
3.3 Calibration

Calibration of the spectral camera is a critical process in the field of spectral imaging, aimed at ensuring the accuracy and reliability of data captured by the camera. Calibration involves adjusting the spectral camera system to a known reference standard, facilitating the conversion of sensor measurements into physically meaningful units. This is essential for accurate interpretation and comparison of spectral data across different scenes and sensors.

Calibration is necessary due to various factors that can introduce errors in the collected data. These factors include variations in sensor sensitivity, atmospheric conditions, and other instrumental artifacts. By calibrating the spectral camera, such discrepancies can be corrected, leading to more accurate and consistent measurements.

Radiometric calibration focuses on converting sensor measurements into radiance or reflectance values. This is achieved by us-
Chapter 3. Methodology

ing calibrated reference panels, known light sources, or integrating spheres to establish a reliable relationship between recorded sensor values and physical properties of the observed scene.

Relative reflectance refers to the comparison of reflectance values between different areas or features of an image rather than providing absolute reflectance values. In the context of spectral camera calibration, relative reflectance is often calculated after relative radiometric calibration. It enables comparison of the reflectance of the analyzed surface versus a calibration target, providing insights into variations in material composition or other relevant parameters.

3.4 HDR imaging

High Dynamic Range (HDR) imaging is a technique that captures and processes a broader range of luminance levels than traditional imaging methods. In conventional photography, DR is limited, often resulting in either blown-out highlights (saturated pixels) or underexposed shadows. HDR imaging overcomes this limitation by combining multiple exposures of the same scene, each taken at different exposure settings. These exposures, ranging from underexposed to overexposed, are then merged using specialized software to produce a final image with enhanced detail in both the shadow and highlight areas. This process allows HDR images to more accurately represent the full spectrum of light intensities present in a scene, providing a visually striking and realistic depiction of the subject. HDR imaging finds applications in various fields, from photography and cinematography to computer graphics and medical imaging, where capturing a wide range of luminance is crucial for accurate representation. In this research a multi-exposure method is proposed for HDR imaging using a SWIR hyperspectral line camera [SJT22].
3.5 Illumination

Setup #1 employed two AC-powered halogen lamps connected to a variable voltage transformer, allowing adjustments from 0 V to 220 V. This variation in voltage changed both the average intensity and spectral distribution of the emitted light [Sha+21]. While the illumination was intense and served its purpose effectively, flickering was observed at very low exposure times, rendering it unsuitable for exposure times around 100-500 microseconds. In general, halogen lamps are known for their generous radiation in both the VIS and IR regions.

To address the flickering issue at low exposure times, Setup #2 introduced DC-powered halogen lamps. Throughout the research, ambient light was intentionally removed as a potential factor, given that the dominant illumination source at the experimental site was exclusively the halogen lamps. This held true for all experiments conducted during the research, with the exception of those detailed in Paper II ([SJT22]). For the experiments in Paper II, frequent calibrations were used to mitigate the influence of ambient light changes at the site.

3.6 Samples preparations:

Over the course of this research, test samples were selected from different application areas of hyperspectral imaging. In this section, a brief overview of the preparation of test samples is presented.

3.6.1 Winter road condition

In Paper I, winter road conditions was taken as a test application case for the evaluation of a PTFE tile as a calibration target. During experimentation, Setup #1 was used to conduct measurements of the calibration target and different asphalt conditions, namely snowy,
icy, wet and dry. The measurements were conducted outdoor at temperatures between –2 °C and –6 °C in darkness at night. The stray light from distant street lamps could have added a small amount of background bias to the measurements. However, the only dominant sources of illumination at the time of the experiments were the halogen lamps shown in Fig.3.1.

### 3.6.2 Food waste with polymers

Paper II showcased the detection of polymers in food waste as a test application. The sampling location was the storage hall of the HEMAB gasification plant. Food waste arrives at the facility via trucks and is unloaded into the storage hall for gasification and food fertilization. This waste primarily consists of leftover food from households. The waste arrives in recyclable paper bags, but often contains various types of undesirable polymers, likely originating from food packaging and grocery bags.

The polymer samples were initially sorted and placed within the camera’s field of view (FOV). Polymers of diverse color, material, and condition were deliberately selected to enhance the variety of samples. In the case of food waste, half of the samples comprised relatively intact food items, hand-picked from the waste and positioned in the imaging area. The other half consisted of more decomposed food items, making it impossible to identify individual components. These samples also included biodegradable paper bags.

Throughout the sample preparation and imaging processes, particular attention was paid to black polymers. Black polymers were treated as a distinct category of material, with images and samples captured separately to those of other polymers. This was necessary because black polymers are particularly difficult to detect due to their low reflectivity.
3.6.3 Polymer samples

Papers II-V used recyclable polymer samples to showcase polymer classification as the test case application. Samples were composed of six different types of recyclable plastics. These recyclable plastics were categorized by their recycling numbers from 1 to 7. The first 6 types were used in this study. Table 3.1 presents the details of the plastics used with their polymer names, recycling numbers and abbreviations.
Papers II-III utilized colored polymer samples to showcase polymer classification as a test case application. However, the impact of color on the polymers’ spectra was not studied in these papers. Paper IV included comparatively more colored polymers in the test samples and the influence of color on the polymers’ spectra was studied. Paper V also utilized all six categories of polymers presented in Table 3.1 but included only black-colored polymers.
This chapter presents a summary of the results related to each RQ and extends the discussion from the attached papers.

4.1 Environmental factors that can degrade measurement accuracy and subsequent material classification

4.1.1 Changes in lighting at imaging site

With regard to RQ.1, RQ.2 and RQ.3, Paper 1 presents a hyper-spectral imaging system and practical calibration procedure using a low-cost calibration reference made of PTFE. The imaging system included a hyperspectral camera and an active source of illumination with a variable spectral distribution of intensity. The change in light profile at the imaging site can be considered an environmental factor (ambient light) or system-based factor (variations in illumination source). The calibration reference was used to measure the relative reflectance of any material surface independent of the spectral distribution of light and camera sensitivity.

Winter road conditions were taken as a test application case, and several spectral measurements of snow, icy asphalt, dry asphalt, and wet asphalt were taken at different exposure times using different illumination spectra. The results from these recorded measurements match closely with the known signatures of snow, ice, and wet asphalt presented in previous studies [Sat+03] [CSL07].
During experimentation, it was learned that minor alterations in the experimental setup during the measurement of test samples and the calibration references can significantly influence measurements. Subsequent investigations were conducted to assess the resilience of the PTFE calibration reference to fluctuations in humidity and temperature. The findings indicate that the calibration reference exhibits robustness against such environmental variations.

Graphs of the measured relative reflectance for different road conditions supported the conclusion that measurements were independent of illumination. Principal component analysis (PCA) of the acquired spectral data for road conditions showed well-separated data clusters, demonstrating the system’s suitability for material classification independent of illumination.

4.1.2 Change in RH at imaging site

With regard to RQ.1, Paper III shows that vaporized water has an impact even at pathlengths of hundreds of centimeters, especially in the case of large variations of RH. The method proposed to overcome this source of uncertainty in measurements is to apply frequent calibrations of the hyperspectral measurement setup, such that the impact of the varying composition of the air is suppressed.

The spectral signature of a 3D-printed object made of polylactic acid (PLA) was used as a test case. It was found that the uncertainty of measurement, computed as a coefficient of variation, could be reduced from 5% to 1% in the most error-prone wavelength region. It was also shown that the RH-induced variations at measurement can drastically affect the classification of materials at an in-situ measurement site. Polymer-type identification was selected as the test application case for material classification. The measurement variations due to the change in relative humidity are shown to result in a 20% classification error at its minimum. In the context of RQ.3, with repeated calibrations, the classification error was reduced to less than 1%.

However, it may be difficult to switch analyzed material frequently
4.1.3. Other potential environmental factors

with a calibration reference in an industrial process. A second alternative method was proposed to prune the wavelengths that are susceptible to water vapor. The classification results showed that even a significant change in humidity has a minor impact on the classification if the susceptible bands are pruned. This method is shown to work well for the selected test case of polymer classification.

4.1.3 Other potential environmental factors

Variations in temperature and precipitation at the imaging site can also cause inaccuracies in the hyperspectral measurements. The impact of these factors is not studied in this research.

Temperature variations can influence the spectral signatures of materials, particularly those that are sensitive to temperature shifts. This thermal effect can alter the reflective properties of surfaces, leading to variations in the recorded spectra. Additionally, temperature changes may impact the performance of the imaging equipment itself, introducing noise or calibration drift that can affect the overall quality of the spectral measurements.

Precipitation, such as rain or snow, can further complicate spectral measurements. Rainfall, for example, can alter the reflective characteristics of surfaces by introducing moisture, affecting the absorption and scattering of light. Snow, on the other hand, may alter the surface’s physical structure, potentially leading to changes in reflectance properties.

Both temperature and precipitation can pose challenges to accurate spectral measurements in outdoor environments. To mitigate these impacts, careful consideration of environmental conditions and appropriate calibration techniques may be necessary.
Chapter 4. Discussion and comments on the results

4.2 Impact of system-related factors on measurement and classification accuracy

4.2.1 Limited DR of imaging sensors

Many applications of spectral imaging require a spectral camera in SWIR with a high DR to capture all the meaningful spectral details in a scene. However, the technological limitations and high cost of spectral cameras result in them having lower DR than the scenes they are required to capture.

With regard to RQ.2 and RQ.3, Paper II proposes a multi-exposure method to increase the DR of hyperspectral imaging using a line camera. In Paper II, spectral measurements of materials were conducted for scenarios in which the DR of a scene was greater than the DR of a line camera. To demonstrate the problem and test the proposed multi-exposure method, plastic detection in food waste and polymer sorting were chosen as the test application cases. The DRs of the hyperspectral camera and the test samples were calculated experimentally. A multi-exposure method is proposed to create HDR images of food waste and polymer samples. Using the proposed method, the DR of the SWIR imaging system was increased from 43 dB to 73 dB, with the lowest allowable signal-to-noise ratio (SNR) set to 20 dB. PCA was performed on both HDR and non-HDR image data from each test case to prepare the training and testing data sets.

Finally, two support vector machine (SVM) classifiers were trained for each test case to compare the classification performance of the proposed multi-exposure HDR method against the single-exposure non-HDR method. The HDR method was found to outperform the non-HDR method in both test cases, with classification accuracies of 98% and 90% respectively, for the food waste classification, and 95% and 35% for the polymer classification.
4.2.2 Limitations in wavelength range for hyperspectral cameras

Hyperspectral cameras are powerful tools designed to capture a vast range of wavelengths within the electromagnetic spectrum, allowing for detailed and precise imaging across various applications. However, each hyperspectral camera is engineered with a specific range of wavelengths it can detect. This limitation is primarily due to the design of the camera’s sensors and filters, which are optimized to capture data within a certain wavelength range. While some hyperspectral cameras may cover a broad range, others are more specialized and focused on a narrower spectrum. These limitations in wavelength range can impact the camera’s versatility, as it may not be suitable for certain applications requiring data outside its specified range. One such application can be the classification of colored materials using hyperspectral imaging.

Hyperspectral imaging in the SWIR range has gained popularity due to its precision, speed, and non-destructive nature. However, it comes with limitations. The method’s accuracy significantly decreases when it comes to classifying colored polymers. In the context of RQ.2 and RQ.3, as presented in Paper IV, a proposal was made to enhance the classification of colored polymers by incorporating VIS wavelengths. Colored polymer samples were specifically chosen based on their chemical compositions, and their spectral characteristics were examined.

Two noteworthy cases were observed in red and transparent LDPEs, where the spectral profiles in the SWIR region underwent significant changes, making them closely resemble the spectra of PPs. Two SVM classifier models were trained using the polymers’ spectra in both the SWIR and SWIR plus VIS ranges, respectively. The first classifier exhibited a 25% misclassification rate for the identified LDPEs, while the second classifier achieved a remarkable 2% error rate for the same LDPE samples.

In general, the classifiers demonstrated high accuracy levels, with overall classification rates of 99.1% and 99.9%, respectively. This
exceptional overall classification accuracy can largely be attributed to the use of small and relatively uncomplicated plastic samples in the experimentation process.

4.2.3 Illumination source

The efficacy of spectral imaging is closely linked to the characteristics of the illumination source, and potential issues in this regard can significantly impact the quality and reliability of the acquired data. Variations in the intensity and spectral distribution of the illumination source can introduce distortions, affecting the accuracy of recorded spectral signatures. Uneven illumination across different wavelengths may lead to inconsistencies in the recorded spectra, impacting the overall reliability of the data. Additionally, issues such as flickering or fluctuations in the light source, especially at low exposure times, can introduce noise and artifacts into the spectral images. It is crucial to carefully address and mitigate these potential issues through proper calibration, selection of stable light sources, and consideration of the specific requirements of the spectral imaging system to ensure accurate and meaningful results.

The AC-powered light source employed in Setup #1 exhibited inefficiency and generated excessive heat, posing a threat to sensitive samples. Notably, during the experiments detailed in Paper I, it was observed that the heat generated by the light source caused snow and thin ice to melt, presenting challenges in accurately measuring samples from winter road surfaces. High-intensity illumination and short exposures were required to achieve a higher DR and record signals with optimal SNR, but this was hindered by the tendency of the AC-powered source to flicker at low exposure times. In response to these challenges, we transitioned from an AC-powered to a more stable DC-powered illumination system in Setup #2. This change aimed to address the issues related to heat generation and flickering, ultimately enhancing the reliability and precision of measurements, but at the cost of much longer exposure times, hence lower DR and SNR, especially for low-reflective materials. Both AC- and DC-powered
sources lacked the capability for modulation [Cas+16], hindering
effective suppression of ambient light.

4.3 Evaluation of CNN for black polymer classification

Hyperspectral imaging in the SWIR range has become a popular
method in the polymer industry for sorting without causing damage
and for quick analysis. Although this generally works well, it has
difficulties distinguishing black polymers due to the strong absorption
of SWIR radiation by carbon black, a common component in such
materials. However, a recent study has shown that CNN can achieve
remarkably high accuracy in classifying black polymers.

In pursuit of an answer to RQ.4, in Paper V, we employed 1D
CNN to classify specific recyclable black polymers. We compared
the CNN’s performance with traditional classification algorithms
such as SVM, k-Nearest neighbors, and Multi-layer perceptron neural
networks. Surprisingly, CNN surpassed all conventional methods,
demonstrating their potential of solving the persistent challenge of
classifying black polymers using SWIR hyperspectral imaging.

It is essential to note that all the experiments, including those
reported in the previous studies, were conducted under controlled
laboratory conditions with limited sample sizes. Given the superior
performance of CNN in our comparative analysis, we strongly recom-
mend further investigations into their effectiveness with real-world
black polymer samples. These studies could potentially revolutionize
polymer sorting processes and improve recycling efficiency.

4.4 Ethical considerations for hyperspectral imaging

Hyperspectral imaging for material classification is a powerful and ver-
satile technology with numerous applications, ranging from environ-
mental monitoring to agriculture and mineral exploration. However,
it also raises ethical considerations that warrant careful examination.
One primary concern is the potential for invasiveness and privacy infringement. Hyperspectral imaging can capture highly detailed and specific information about the composition of objects or areas, which could be used to reveal sensitive information about individuals or their properties without their consent.

Moreover, the collection and use of hyperspectral data must be subject to strict regulations to prevent abuse and protect individual rights. This includes the need for clear guidelines on data ownership, consent, and data sharing. The responsible use of hyperspectral imaging in areas like agriculture or forestry must consider the potential environmental impacts and sustainability concerns, ensuring that the technology does not inadvertently harm ecosystems or communities.

Hyperspectral imaging also holds the potential for positive ethical impact in the realm of circular economy and recycling. By enabling more precise identification and separation of materials in waste streams, hyperspectral imaging can significantly enhance recycling processes. This advancement can contribute to reducing the environmental burden associated with improper waste disposal practices, such as dumping in developing countries or resorting to waste incineration for thermal power generation. With hyperspectral technology, there is an opportunity to create more sustainable waste management systems, fostering responsible recycling practices that align with environmental and ethical considerations. This not only mitigates the negative impact on ecosystems and communities but also aligns with global efforts to create a more sustainable and equitable approach to waste management.

Ultimately, as hyperspectral imaging technology continues to advance, it is essential for governments, organizations, and researchers to uphold ethical principles, respecting individual privacy, safeguarding against misuse, and prioritizing fairness and social responsibility in its applications. Ethical considerations should be integrated into the development, deployment, and regulation of hyperspectral imaging to harness its benefits while minimizing potential risks and ethical dilemmas.
5.1 Conclusions

This chapter presents the conclusions related to the RQs formulated in Chapter #1:

5.1.1 RQ.1

What are the major environmental factors that can reduce the performance of in-situ hyperspectral imaging systems?

- Paper I shows that the change in spectral distribution of light at an imaging site can profoundly affect the measurement and material classification.
- Variations in ambient illumination were compensated for in Paper II by frequently repeated calibrations.
- Paper III shows that SWIR hyperspectral imaging in in-situ applications is affected by water vapor even if the pathlength of light through air is only hundreds of centimeters.
- The error induced in spectral measurements by RH change is shown to degrade the classifier’s performance drastically.

5.1.2 RQ.2

What are the major limitations of system components that can reduce the performance of in-situ hyperspectral imaging systems?
• Paper I shows how much the hyperspectral measurement can vary with the change in active illumination at the imaging site. This illumination change can be due to the physical change in the experiment setup, variations in supply voltage of the light source, or aging of the light source.

• Paper II shows that with a DR that is lower than that of the scene, the hyperspectral camera cannot measure the material spectra adequately.

• Paper IV shows that for particular applications, one camera cannot measure the spectra in all required spectral bands due to the limited spectral bandwidth of the camera detector.

• Paper V shows that spectral profiles from low-reflective materials display very low SNR, caused by the low sensitivity of the camera.

5.1.3 RQ.3

How can we improve methods for image acquisition, processing, and system calibration such that limitations and impacts found in RQ.1 and RQ.2 are mitigated?

• Paper I shows that the material spectra can be measured with precision, independently of the spectral distribution of the illumination source and the irregular sensitivity of the hyperspectral camera, using a low-cost PTFE calibration reference.

• It was also shown that the PTFE calibration has a spectral distribution of reflectance independent of environmental factors such as humidity and temperature.

• In Paper II proposes a multi-exposure method for hyperspectral line cameras with the aim to increase the DR of hyperspectral imaging.
5.1.4 RQ.4

- Use of the multi-exposure method was shown to improve the DR of SWIR imaging from 43 to 73 dB.
- Finally, the use of the proposed multi-exposure method was shown to result in the improvement of the classification success rate from 90 to 98% and 35 to 95% for the selected test application cases.
- Frequent calibration of the imaging system or pruning of the wavelength bands that are susceptible to water vapor were shown to improve the classification of plastic materials at sites where large variations in RH can be observed.
- Paper IV demonstrates that the addition of VIS wavelengths with SWIR by utilizing an additional camera improved the success rate for the classification of colored materials.

5.1.4 RQ.4

Can the use of deep learning artificial intelligence improve material classification by hyperspectral imaging systems?

- As per the comparative analysis presented in Paper V, CNN performance was outstanding compared to the other machine learning algorithms.
- However, it was shown that the classification success rate drops as the variety of test samples increases.
- More investigation is required to find a definite answer to this question.

5.1.5 RQ.5

What have we learned from studying various applications for hyperspectral imaging?
• A calibration standard with accurate reflectance close to 100 percent is not needed if the purpose is to identify materials by their spectral signatures.

• Small changes to the imaging setup can affect the hyperspectral measurements considerably.

• We found SWIR hyperspectral imaging very reliable in identifying winter road condition. The technology can be used with confidence in relevant applications.

• With the advancements in machine learning and optical sensing, effectiveness of hyperspectral imaging can be increased with the aim to resolve bottleneck problems in material classification.

5.2 Future work

The research conducted thus far, as detailed in the presented papers, primarily focused on controlled lab environments with clean and non-degraded samples, excluding the specific experiments outlined in Paper II. However, for a more comprehensive assessment of the applicability of the proposed methods and the impact of degrading factors on measurements and material classification, it is imperative to extend the research to real-world scenarios. The inclusion of diverse, impure, and decomposed materials in the experiments will provide a more realistic and challenging environment, allowing for a thorough evaluation of the robustness and effectiveness of the proposed spectral imaging methods in practical applications.

In the initial experiments, the AC-powered illumination source exhibited inefficiency, excessive heat generation, and flickering at low exposure times, prompting the transition to a DC-powered source. While the DC-powered source proved more stable, a notable drawback was its lack of power. To further enhance the measurement and experimentation quality, future work should explore the availability and utilization of a significantly more powerful source that also offers modulatability. A more potent source with modulation capabilities
would not only address the limitations encountered in the previous experiments but also provide the necessary flexibility for effective ambient light cancellation [Cas+16], ensuring improved performance and reliability in a broader range of experimental conditions.

In the current research, the machine learning algorithms employed for material classification were primarily utilized to compare results with and without the integration of the proposed imaging methods. However, limited to no efforts were dedicated to the optimization of these algorithms, leaving room for further improvements in classification success rates. As part of future endeavors, focus will be placed on algorithm optimization to extract enhanced performance from the classification models. This optimization process will involve fine-tuning parameters, exploring algorithmic enhancements, and leveraging advancements in machine learning techniques. By investing in the optimization of machine learning algorithms, the research aims to achieve higher precision and accuracy in material classification, thereby maximizing the potential of the proposed hyperspectral imaging methods in practical applications.

For the experiments detailed in Papers IV and V, the implementation of Setup #2 involved constructing a scanning platform. Line scan cameras mounted overhead captured hyperspectral images, and the subsequent data processing and the training of the classifiers utilized every pixel individually. For future work, a more pragmatic methodology will be devised, entailing the initial generation of 2D images followed by image segmentation into group pixels representing the same material piece. The mean of all pixels associated with a material piece will then be computed. This averaged spectrum is anticipated to provide a more accurate representation of the material, effectively mitigating noise introduced by imaging artifacts, such as occlusion or irregular material shapes.
ACRONYMS

AlGaN
aluminum gallium nitride

AOTF
Acousto-Optic Tunable Filters

CCD
Charge-Coupled Device

CMOS
Complementary Metal-Oxide-Semiconductor

DC
Dark Current

DR
Dynamic Range

FOV
field of view

FPA
Focal Plane Arrays

HSI
Hyperspectral Imaging

InGaAs
Indium Gallium Arsenide

InP
indium phosphide
Acronyms

**InSb**
indium antimonide

**IR**
Infrared

**LCTF**
Liquid Crystal Tunable Filters

**MCT**
mercury cadmium telluride

**MSI**
Multispectral Imaging

**PbO-PbS**
lead oxide-lead sulfide

**PCA**
Principal Component Analysis

**PGP**
prism-grating-prisms

**PLA**
Polylactic Acid

**PTFE**
Polytetrafluoroethylene

**PtSi**
platinum silicide

**RH**
Relative-Humidity

**SNR**
Signal-to-Noise Ratio
Acronyms

SVM
   Support Vector Machines

SWIR
   Short-wave Infrared

VIS
   Visible
BIBLIOGRAPHY


[Bro+96a] W. van den Broek et al. "Plastic identification by remote sensing spectroscopic NIR imaging using kernel partial least squares (KPLS)". In: Chemometrics and Intelligent
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