

Stand-Off Hyperspectral Raman Imaging



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INTRODUCTION

Stand-off Raman spectroscopy is a versatile tool in a range of fields of application, such as safety investigations (detection of explosives at safe distances) or geosciences (planetary exploration). During the project "OPTIX" (FP7) we showed that the detection of small amounts of explosives and hazardous chemicals at distance of 100 m is possible even through opaque containers. Here, we present a different approach to remote Raman sensing emplyoing hyperspectral Raman spectroscopy. The classical grating as a dispersion element is exchanged in favor of a liquid crystal tunable filter (LCTF), which allows direct imaging of a selected Raman shift onto the intensified CCD (iCCD). This maintains a high degree of local information and allows for higher troughput, as whole areas can be imaged at once. IN this poster we show our first prototype as well as first measurement results on a reference sample consisting of different polymers. Chemometrics are then applied to extract chemical information from the large dataset.

INSTRUMENTATION



The setup for stand-off hyperspectral Raman spectroscopy consists of a **frequency doubled Nd:YAG** (operating at **532 nm**) laser with a pulse length of 4.4 ns and a repetition frequency of 10 Hz as light source. The beam is widened by a beam expander to a diameter of approximately **50 mm**. The backscattered light is collected using a **6 inch** Schmidt-Cassegrain **telescope** (Celestron C6), after which a **tunable LC-filter** (VariSpec VISR) selects a spectral position, which is detected with a **PIMAX 4 1024RF iCCD** camera. The camera gate width was set to **5 ns**. The laser and camera are synchronized to achieve maximal signal with a relative delay of **129 ns**. The laser pulse energy was adjusted to **20 mJ per** pulse, which results in a energy density of 1.6 mJ/cm². The sample was positioned in **12 m** distance to the telescope. To collect spectra of the sample the LCTF is tuned to a specific Raman shift, then **30 on-chip accumulations** are performed before the next spectral position is investigated. The spectral resolution was set to **5 cm⁻¹** and 501 steps (**600 - 3100 cm⁻¹**) were collected. This takes approximately 30 minutes in total.

FIRST MEASUREMENTS WITH A TEST SAMPLE



Foto of the widened laser beam hitting the test sample. The beam has a diameter of approximately 50 mm. The backplate is made of Teflon, the other parts are polypropylene (PP), polyethylene (PE) and Nylon 6 (N6).



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CHEMOMETRIC DATA ANALYSIS





Reference spectra for all polymers in the test sample with intensity distribution at the marked positions.

A test sample was built using a 4 mm thick **Teflon** plate as foundation. Small **PP**, **PE** and **Nylon 6** plates were cut and glued to the Teflon plate, using as little glue as possible to avoid spectral interferences. Reference spectra of the different polymer plates were obtained using a confocal Raman microscope (Horiba LabRAM 800 HR). Then the sample was put at 12 m distance to the telescope and hyperspectrally Raman imaged.

The obtained dataset was evaluated using **ImageLab** by Epina GmbH. First, a spike detection and removal was performed. The nylon plate exhibits flourescence, which was also observed in the microscope Raman spectra. This resulted in an overall higher intensity for the nylon plate, which was corrected by emplyoing a **baseline correction** (Lieber algorithm, order 4, 5 iterations). On the characteristic bands of teflon the intensity distribution mirrors the intensity of the laser spot on the sample.



K-means clusters of PE (red), PP (blue), Nylon 6 (green) and Teflon (cyan). Background pixels are depicted in black.

K-means clustering was done on the dataset. To reduce calculating time a pixel mask was employed excluding background pixel, which where not illuminated. The data was standardised and 4 clusters were assumed. The 4 different polymers were classified sufficiently well, except the PP and PE clusters, the reason being their very similar Raman spectra.

CONCLUSION & OUTLOOK



Comparison of averaged spectra obtained with the stand-off hyperspectral Raman imaging system with reference microscope Raman spectra for Teflon, PP, PE and Nylon 6.

A stand-off hyperspectral Raman imaging setup was built using a tunable liquid crystal filter as dispersive element and a 1024x1024 px gated iCCD camera as detector. A test sample consisting of 4 different polymers was constructed and imaged at a distance of 12 m in respect to the collection optic. The averaged spectra of the polymers are in good accordance to the reference spectra obtained via a Raman microscope. K-means clustering was performed as a example of how chemometrics can be used to classify the different polymers in the sample. Further work will include optimising accuisition parameters as well as miniaturisation of the setup in order to make it mobile.

Financial support was provided by the Austrian Science Fund (FWF) under the programme Translational-Research-Programme n° 265: stand-off Raman spectroscopy.

Der Wissenschaftsfonds.