Stand-off hyperspectral imaging – towards mobile, high throughput remote chemical identification and quantification using chemometrics

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Stand-off Raman spectroscopy is a versatile tool for a variety of applications, such as safety investigations, forensics or geosciences. 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 employing hyperspectral Raman spectroscopy. The classical grating as a dispersion element is exchanged in favor of a liquid crystal tunable filter (LCTF), which allows for direct imaging of a selected Raman shift onto the intensified CCD (iCCD). This maintains a high degree of local information and allows for higher throughput, as whole areas can be imaged at once. Measurements with our first prototype, still equipped with a water-cooled, flashlamp-pumped excitation laser, as well as first measurements with a diode pumped, air cooled, small laser are shown. The capability of remote chemical analysis incorporating chemometrics on a reference sample consisting of different polymers will be presented.

Stand-off Raman spectroscopy, where the instrumentation is physically separated from the sample under investigation, can be extremely advantageous for analysis of dangerous, fragile or inaccessible samples. It is mostly used in safety applications, i.e. detection of explosives [1] or geosciences, where the remote detection of minerals on planetary surfaces is desirable [2].

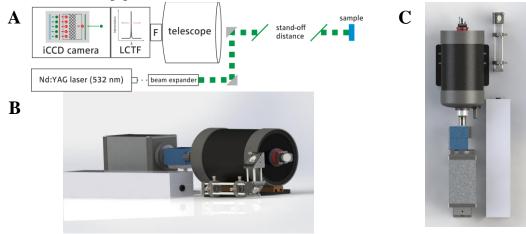


Figure 1. (A) Experimental configuration illustrating the laser, the telescope as the collection optic, the Rayleigh filter [F], the LCTF as the dispersive element and the camera. (B) and (C) depict rendered CAD drawings of the experimental setup.

Usually, a pulsed laser point is targeted on the surface of interest, the backscattered photons are collected using different forms of telescopes and directed towards a spectrometer. However, when large surface areas must be scanned, it is advantageous widening the laser spot and using a square detection array to directly image the area under surveillance. Different kinds of filter can be used to discriminate different Raman shifts, i.e. acousto-optical filters [3] or, as in this study, LCTFs [4].

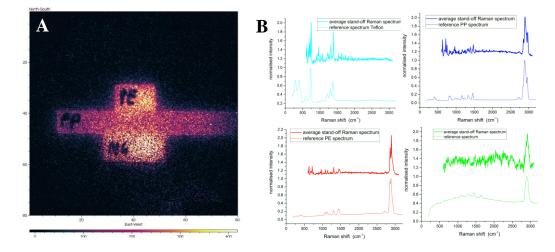


Figure 2. (A) Intensity distribution at 2900 cm⁻¹ (B) Collection of figures comparing spectra obtained by binning 10 pixels on a specific part of the image representing the respective polymer and spectra obtained with a Raman microscope (Horiba LabRAM 800 HR).

The presented prototype can collect Raman spectra from a sample at several meters' distance (15 m for this study), which are directly loaded into Epina ImageLab [5], a chemometric analysis program for imaging purposes. A test sample consisting of four different polymers was measured and different chemometric methods were applied to increase signal-to-noise ratios and to classify the results.

Furthermore, a compact, air-cooled, diode-pumped laser with high repetition rates (~10 kHz) was tested to facilitate a mobile prototype with minimal electrical as well as physical requirements. The results are compared to a stationary, water-cooled and flashlamp-pumped laser.

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