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Contributions of Shifted Excitation Raman Difference Spectroscopy to Agri-Photonics – Pathway towards Smart Farming

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Abstract

Shifted excitation Raman difference spectroscopy (SERDS) provides molecule-specific information and can effectively address interferences from fluorescence and daylight. We applied SERDS using an in-house developed 785 nm dual-wavelength diode laser as excitation light source for soil investigations. Results from laboratory-based measurements as well as on-site field trials conducted with an in-house developed portable SERDS system demonstrate the capability for spatially-resolved qualitative and quantitative analysis of relevant soil parameters, including organic carbon and carbonates, thus providing important contribution to precision agriculture.

1 Introduction

The concept of precision agriculture [1] gains significant attention in modern agricultural practice. To derive informed treatment decisions for site-specific farming, e.g., with respect to fertilization, liming or irrigation, detailed information regarding the current soil composition is of crucial importance. Existing complex, expensive, and time-consuming standard laboratory analyses could ideally be complemented by fast and non-destructive optical methods that show great promise as innovative approach for soil characterization. Its ability to obtain molecule-specific information from soil makes Raman spectroscopy a well-suited candidate for such a task. However, due to the weakness of the Raman effect, the technique suffers from dominant background interferences, that can originate, e.g., from fluorescence or ambient daylight.

In this contribution, we apply shifted excitation Raman difference spectroscopy (SERDS) [2] as an effective tool to address such challenges. The technique uses a physical approach with two slightly shifted laser wavelengths that are used to record two Raman spectra. While Raman signals directly follow the applied wavelength shift, background interferences remain unaffected. Subtraction of the two recorded spectra thus provides a neat way of separating Raman signals from unwanted disturbing interferences.

We present initial SERDS investigation on collected soil samples using a customized laboratory setup. Subsequently, a portable SERDS instrument was developed and realized. This system was then applied for on-site soil investigations directly on an agricultural field in Northeast Germany to evaluate its capability for qualitative and quantitative analysis.

2 Materials and Methods

For all presented investigations, an in-house developed monolithic dual-wavelength diode laser with two emission lines around 785 nm [3] is applied as excitation light source for SERDS.

2.1 SERDS Laboratory setup

In preparation for on-site soil analysis, initial SERDS laboratory investigations were performed using 150 soil samples that were collected from an agricultural field in Germany. To address soil heterogeneity at the micrometer scale, a measurement spot size of 100 µm was chosen. The heterogeneity at the millimeter scale was addressed by applying a 100-point raster scan approach where each sample was probed in a 10×10-point grid within an area of approximately 1 cm^2. Further information can be found in our previous publications [4, 5].

2.2 Portable SERDS instrument

The transfer of SERDS from the laboratory environment towards the field setting is achieved by means of an in-house realized rugged and portable SERDS system [6] that was specifically designed for soil analysis. Similar to the above-mentioned laboratory setup and for comparison, also the portable instrument applies a measurement spot size of approximately 100 µm. For the on-site study on an agricultural field in Germany, twenty-five positions on the soil surface down to depths of 10 cm along a length of 480 m were exemplarily selected and at each position 10 different points were probed to address soil heterogeneity [7]. Additionally, soil samples were collected from the measurement positions for subsequent analysis with the SERDS laboratory setup to validate the results obtained on-site.

3 Results and Discussion

3.1 SERDS laboratory measurements

Results demonstrate the detection of organic carbon and 13 soil minerals, including silicates, carbonates, titanium dioxides, and phosphate. Moreover, a successful prediction of the contents of organic matter [4] and carbonate [5] as important soil parameters could be realized by means of partial least squares regression (PLSR). Overall, the outcomes of the laboratory study show the ability of SERDS for qualitative (detection of soil constituents) and quantitative (prediction of organic matter and carbonate contents) soil investigations. In the next step, our approach was transferred from the laboratory towards the field environment by applying an in-house developed portable SERDS instrument.

3.2 On-site soil investigations

On-site investigations on the above-mentioned field were exemplarily carried out at selected points along a distance of 480 m. As an example, Raman spectra of one measurement position recorded at the two slightly shifted excitation wavelengths are displayed in Figure 1. It becomes evident that the characteristic Raman signals are superimposed on a strong background contribution. In this case, only the strong Raman signals of quartz (465 cm^{-1}) and the sapphire window contained in the Raman probe head (418 cm^{-1}) are hardly visible. Applying SERDS efficiently separates the Raman signals from the interfering backgrounds thus enabling the calcium carbonate polymorph aragonite (1084 cm^{-1}) and organic carbon (1350 cm^{-1} and 1590 cm^{-1}) to be detected and identified. Furthermore, two additional Raman signals originating from the sapphire window are present at 577 cm^{-1} and 749 cm^{-1}.

In terms of qualitative soil analysis, the detection of organic carbon and in total 9 soil minerals, e.g., silicates, carbonates, titanium dioxides, and phosphate was demonstrated thus confirming the results of the investigations using the SERDS laboratory setup. The measurements conducted at 25 selected points along a distance of 480 m revealed a spatially heterogeneous distribution of carbonaceous matter and carbonates across the field. As depicted in Figure 2, elevated concentrations of both constituents are located in a region covering distances of 250-350 m from the first probed point on the field.

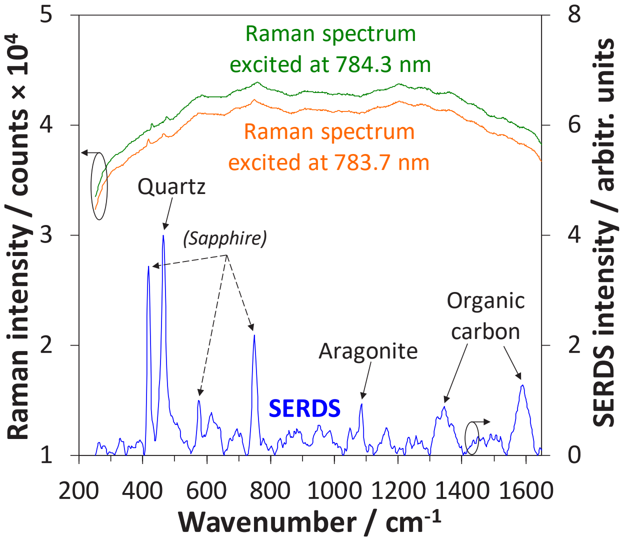

Fig. 1 Average of 50 Raman spectra excited at 783.7 nm and 784.3 nm using integration times of 50 ms for each Raman spectrum obtained on-site at a selected measurement position on an agricultural field in Germany (top curves), and reconstructed SERDS spectrum (bottom curve).

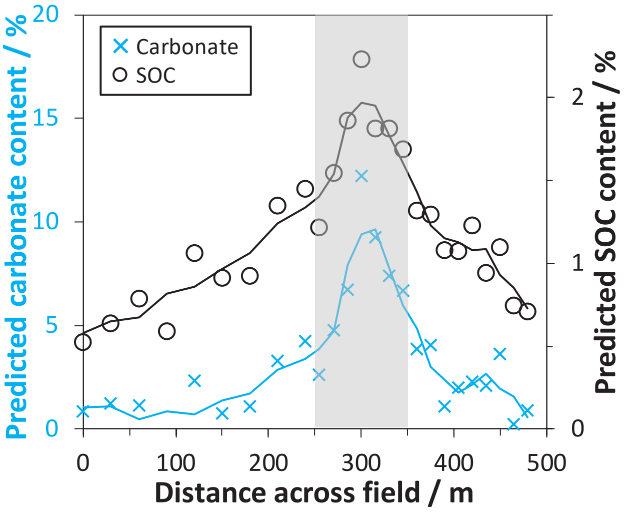

Fig. 2 Contents of carbonate and soil organic carbon (SOC) predicted by PLSR from SERDS spectra measured on-site with the portable SERDS instrument plotted in dependence of the measurement position across the field. Solid lines represent 3-point moving averages to guide the eye. The gray area indicates a range of elevated carbonate and SOC concentrations.

Moreover, a successful prediction of the contents of organic carbon (coefficient of determination: $R^2 = 0.89$, root mean square error of cross-validation: RMSECV = 0.3 %) and carbonate ($R^2 = 0.86$, RMSECV = 2.5 %) as important soil parameters could be realized. The achieved prediction performance is comparable to the SERDS laboratory analysis conducted on samples collected from the 25 probed locations on the field [7].

4 Conclusion

The outcomes of our study demonstrate the capability of portable SERDS for qualitative as well as quantitative on-site soil investigations directly on an agricultural field. This approach could significantly contribute to precision agriculture by providing spatially-resolved molecule-specific information about the soil composition.

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