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LIBS and Raman image fusion: An original approach based on the use of chemometric methodologies

Laser-induced breakdown spectroscopy (LIBS) imaging is an increasingly popular and powerful technique across many scientific fields. LIBS imaging allows for the detection of atomic elements in complex samples, providing crucial spectral and spatial information. Key advantages of this method include minimal sample preparation, high acquisition speeds of up to 1 kHz, high spatial resolution (on the micron scale), and sensitivity in the ppm range. Another significant benefit of current LIBS systems is the ability to perform additional spectroscopic analyses, such as Raman measurements, on the same platform.

Traditionally, LIBS imaging data has been analyzed using univariate approaches, focusing on maps at specific LIBS wavelengths. However, this method limits the extraction of the full range of information available in the spectra, hindering a comprehensive understanding of the relationship between spatial and spectral data. Chemometrics and multivariate analysis, particularly spectral unmixing, can address this limitation.

This presentation aims to demonstrate the potential of simultaneously analyzing LIBS and Raman imaging data from the same sample using the Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) unmixing method [1]. To showcase the value of this integrated analysis, we apply it to a complex polymetallic mineral containing carbonates, silicates, and sulfides. We will show that by using a data analysis pipeline previously validated by our group, we can extract the pure chemical contributions of these heterogeneous minerals. While the presented protocol is effective for analyzing LIBS and Raman data separately, it is far more insightful when both datasets from the same sample are analyzed together, revealing new insights that would be missed without this integrated approach.

References

[1] A. Nardecchia, A. de Juan, V. Motto-Ros, C. Fabre and L. Duponchel, Spectrochimica Acta B, 198 (2022).