The tortuous issues of data analysis in LIBS Imaging

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The imaging capability of laser-induced breakdown spectroscopy (LIBS) represents an attractive way of development for the technique, with innumerable applications in various fields, such as geology, industry, and biology. In LIBS imaging, laser-induced plasma are generated continuously while scanning the sample surface over the region of interest. This approach has many advantages such as multi-elemental capability, ease in use, and operation at atmospheric pressure. This is furthermore the only all-optical technique providing space-resolved elemental information with ppm-scale sensitivity and μ m-range resolution. Another asset of the technique lies in its high acquisition speed (up to kHz) which, combined with its full compatibility with optical microscopy, provides LIBS unique features compared to other elemental imaging methods such as laser ablation inductively coupled plasma mass spectrometry or synchrotron X-ray fluorescence.

However, there are major issues inherent to this technology related to the data analysis. Indeed, the high complexity of the spectrum data and the huge size of the generated datasets make this step long and unwieldy. The size of these datasets varies depending on spatial resolution but hundreds of megabytes to multiple gigabytes of data produced for one sample are no exception. Besides, each spectrum is recorded from single laser shot and can thus be rather noisy. The large number of spectra to process combined with their complexity and their noisy nature, induce recurrent issues that may questioned the quality of the imaging outputs (incorrect extraction due to spectral interference, possible loss of information, and so on). In this presentation, we will detail, using real case examples, the various obstacles generally encountered in this data analysis step. Different methods, allowing elemental images to be constructed from the spectrum dataset will be then proposed, from "basic" line intensity extraction to the use of advanced chemometrics.