23ème Congrès de Chimiométrie, Université de Bretagne Occidentale, Brest, Juin 2022.

Data fusion in LIBS / PIL multimodal imaging: a strategy to facilitate spectral interpretation of complex samples

A. Nardecchia[1] V. Motto-Ros[2] L. Duponchel[1,*]

[1] Univ. Lille, CNRS, UMR 8516, LASIRE, Laboratoire de Spectroscopie pour Les Interactions, La Réactivité et L'Environnement, Lille, F-59000, France,

[2] Institut Lumière Matière, Université de Lyon, Villeurbanne, 69622, France.

(*) : ludovic.duponchel@univ-lille.fr

Keywords: Data fusion, hyperspectral imaging, LIBS, PIL.

Abstract

Laser-induced breakdown spectroscopy (LIBS) imaging is nowadays a very powerful technique for the elemental analysis of complex samples used in many different scientific fields [1-7]. This technique uses a pulse laser beam focused on the sample surface to generate a plasma that atomizes and excites the ablated matter. As a consequence, the excited atoms, ions and molecules release the excess of energy with electronic relaxations, and a characteristic emission spectrum for each element present in the matrix can be acquired using an optical microscope coupled with a spectrometer. In LIBS imaging, the sample surface is usually explored in a scanning configuration mode, acquiring one spectrum at a time for each spatial position of a predefined grid. LIBS technique shows many advantages, such as multi-elemental capabilities including light elements (<Mg), a high acquisition rate (up to 1000 spectra/s), high sensitivity (ppm and sometimes more), high dynamic range (major elements to traces can be observed), and compatibility with optical microscopy. In fact, it is now commonplace with LIBS to acquire large hyperspectral data sets containing millions of spectra acquired over a limited period of time and representative of a large sample area [8,9]. Another important aspect in the LIBS exploration of a sample is the possibility to obtain an additional plasma induced luminescence (PIL) [10] response using the same microscope (Figure 1).

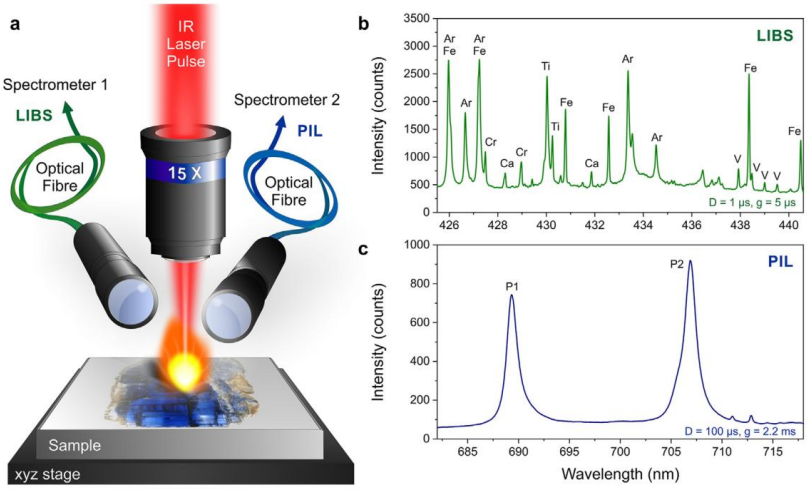

Figure 1: a) Experimental setup to acquire simultaneously LIBS and PIL spectra. b) Mean LIBS spectrum of a sample. c) Corresponding mean PIL spectrum.

Indeed, the plasma generated by the LIBS laser shot acts as an excitation source and produces the emission of a luminescence response for specific elements present on the sample surface [11]. Nevertheless, despite the relative simplicity of acquiring these additional PIL spectra, their interpretation remains uncertain [12]. We have at this date a rather limited knowledge on this phenomenon of luminescence in complex materials. The wide bandwidths (which can be seen in the mean spectrum in figure 1c) but also the low signal-to-noise ratio often observed in PIL make the task all the more difficult. The objective of this presentation will be to show that data fusion associated with a source separation method (such as MCR-ALS [13]) will facilitate the PIL spectral interpretation thanks to the information provided by LIBS. As multivariate curve resolution methods do not allow to work directly on several million spectra, this presentation will also be an opportunity to introduce an original data compression procedure able to preserve the relevant information of the original data set.

References

[1] L. Jolivet, M. Leprince, S. Moncayo, L. Sorbier, C.-P. Lienemann, V. Motto-Ros, Review of the recent advances and applications of LIBS-based imaging, Spectrochim. Acta B Atom Spectrosc. 151 (2019) 41e53, https://doi.org/10.1016/j.sab.2018.11.008

[2] V. Motto-Ros, S. Moncayo, F. Trichard, F. Pelascini, Investigation of signal extraction in the frame of laser induced breakdown spectroscopy imaging, Spectrochim. Acta B Atom Spectrosc. 155 (2019) 127e133, https://doi.org/10.1016/j.sab.2019.04.004

[3] T.A. Labutin, V.N. Lednev, A.A. Ilyin, A.M. Popov, Femtosecond laser-induced breakdown spectroscopy, J. Anal. At. Spectrom. 31 (1) (2016) 90e118, https://doi.org/10.1039/C5JA00301F

[4] R.R.V. Carvalho, J.A.O. Coelho, J.M. Santos, F.W.B. Aquino, R.L. Carneiro, E.R. Pereira-Filho, Laser-induced breakdown spectroscopy (LIBS) combined with hyperspectral imaging for the evaluation of printed circuit board composition, Talanta 134 (2015) 278e283, https://doi.org/10.1016/j.talanta.2014.11.019

[5] R. Gaudiuso, N. Melikechi, Z.A. Abdel-Salam, M.A. Harith, V. Palleschi, V. Motto-Ros, B. Busser, Laser-induced breakdown spectroscopy for human and animal health: a review, Spectrochim. Acta B Atom Spectrosc. 152 (2019) 123e148, https://doi.org/10.1016/j.sab.2018.11.006

[6] F. Trichard, F. Gaulier, J. Barbier, D. Espinat, B. Guichard, C.-P. Lienemann, L. Sorbier, P. Levitz, V. Motto-Ros, Imaging of alumina supports by laser-induced breakdown spectroscopy: a new tool to understand the diffusion of trace metal impurities, J. Catal. 363 (2018) 183e190, https://doi.org/10.1016/j.jcat.2018.04.013

[7] A. Nardecchia, C. Fabre, J. Cauzid, F. Pelascini, V. Motto-Ros, L. Duponchel, Detection of minor compounds in complex mineral samples from millions of spectra: a new data analysis strategy in LIBS imaging, Anal. Chim. Acta 1114 (2020) 66e73, https://doi.org/10.1016/j.aca.2020.04.005

[8] O. Caceres, F. Pelascini, V. Motto-Ros, S. Moncayo, F. Trichard, G. Panczer, A. Marín-Roldan, J.A. Cruz, I. Coronado, J. Martín-Chivelet, Megapixel multi-elemental imaging by laser-induced breakdown spectroscopy, a Technology with considerable potential for paleoclimate studies, Sci. Rep. 7 (1) (2017) 1e11, https://doi.org/10.1038/s41598-017-05437-3

[9] C. Fabre, D. Devismes, S. Moncayo, F. Pelascini, F. Trichard, A. Lecomte, B. Bousquet, J. Cauzid, V. Motto-Ros, Elemental imaging by laser-induced breakdown spectroscopy for the geological characterization of minerals, J. Anal. At. Spectrom. 33 (8) (2018) 1345e1353, https://doi.org/10.1039/C8JA00048D

[10] Gaft, L. Nagli, Y. Groisman, Plasma induced luminescence (PIL), Opt. Mater. 34 (2) (2011) 368e375, https://doi.org/10.1016/j.optmat.2011.05.024

[11] M. Gaft, Y. Raichlin, F. Pelascini, G. Panzer, V. Motto Ros, Imaging rare-earth elements in minerals by laser-induced plasma spectroscopy: molecular emission and plasma-induced luminescence, Spectrochim. Acta B Atom Spectrosc. 151 (2019) 12e19, https://doi.org/10.1016/j.sab.2018.11.003

[12] M. Gaft, R. Reisfeld, G. Panczer, Modern Luminescence Spectroscopy of Minerals and Materials, Springer Mineralogy; Springer International Publishing, Cham, 2015, https://doi.org/10.1007/978-3-319-24765-6

[13] J. Jaumot, R. Gargallo, A. de Juan, R. Tauler, A graphical user-friendly interface for MCR-ALS: a new tool for multivariate Curve resolution in matlab, Chemometr. Intell. Lab. Syst. 76 (1) (2005) 101e110, https://doi.org/10.1016/j.chemolab.2004.12.007