

Revealing hidden structures in chemical maps using self-organized mapping

High resolution chemical mapping is one of the advantages of modern LIBS systems. However, the combination of large number of shots with the precision of utilized spectrograph can lead to a dataset with an enormous count of variables. Even worse, the heterogeneity of the sample surface chemical composition can make usage of conventional methods remarkably useless. Therefore, we investigated an automatic multivariate method called Self-Organized Mapping (SOM) to reveal information prior to the conventional analysis. This information can be used for identification of elemental associations, elemental isolations or for reduction of the original dataset to a feasible number of representatives.

Experiment setup

The sample under investigation is a sandstone-hosted uranium ore, which contained detectable abundances of Si, Zr, U, Nb, Fe, and Ti. The measurement was conducted on the orthogonal double-pulse LIBS setup. Wavelength of the ablation and reheating laser were 532 nm and 1064 nm, pulse energies were 30 mJ and 80 mJ and pulse duration were 12 ns and 8 ns respectively. Laser spot size was 50 μm , spatial resolution 100 μm . Spectra were captured by echelle spectrometer coupled to ICCD detector. Gate delay was set to 1.5 μs , gate width to 20 μs .

Results

We have trained a SOM network of 900 neurons organized in a 30×30 rectangular grid. Figures 1-6 shows the sum of neuron weights on wavelengths representing individual elements under investigation (circles represent individual neurons of the network), namely: U, Zr, Si, Fe, Nb, Ti. Comparison of Figure 1 and Figure 2 indicates strong association of uranium and zircon. Figures 2 and 3 shows that zircon and silicon are rather isolated, this means that the sandstone (described by high abundance of Si) is bearing mineral phase of hydrozircon (combination of Zr and U). Investigation of Figures 4 and 5 imply that Fe and Nb are present on the surface, where a low amount of both Si and Zr were detected; this could be explained by assigning a mineral phase to this combination (for example ilmenite). Last observation is deduced from Figure 6, it is shown that titanium is isolated, found only in a small subset of the data and in a high abundance.

Supplementary material

The principle of the SOM method and a detailed explanation of the data treatment can be found in J. Klus, *et al.*, Spectrochim. Acta B **131**, 66-73 (2017).

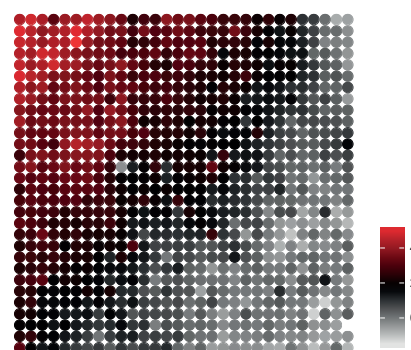


Fig. 1: U II 409.013 nm.



Fig. 2: Zr II 349.621 nm.

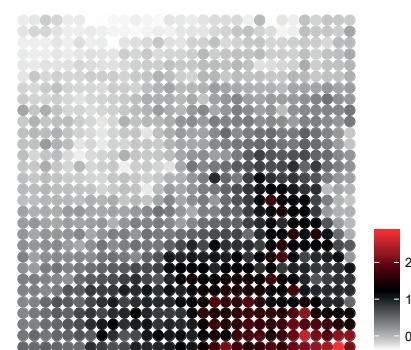


Fig. 3: Si I 251.431 nm.

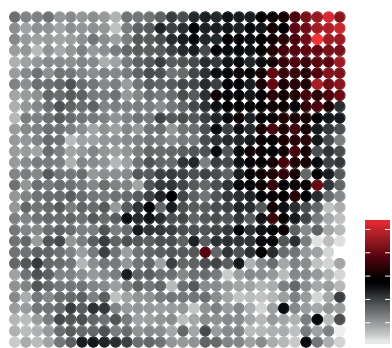


Fig. 4: Fe I 358.120 nm.

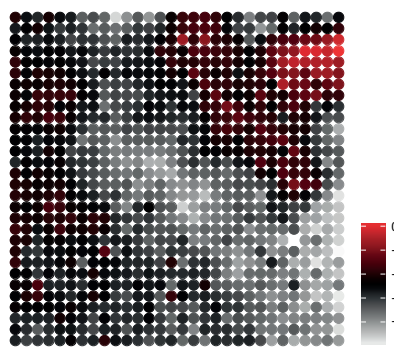


Fig. 5: Nb II 255.139 nm.

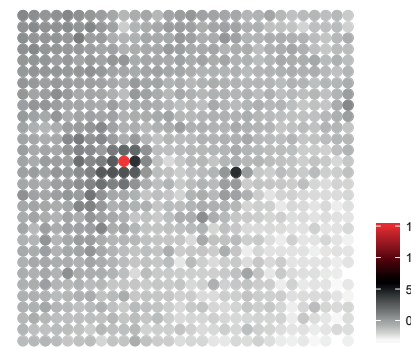
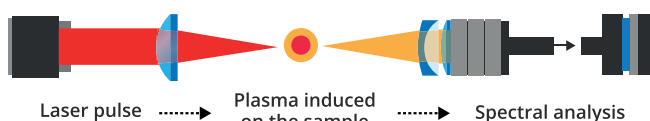


Fig. 6: Ti II 325.424 nm.

LIBS measurement with the Sci-Trace

Laser-Induced Breakdown Spectroscopy (LIBS) is a modern and flexible analytical technique. It is a combination of laser ablation and atomic emission spectroscopy. Pulsed laser rejects a small part (down to few nanograms) of analyzed material and creates a microplasma.



Spectral analysis of the laser-induced plasma radiation provides a qualitative and quantitative data about the chemical composition of the analysed sample.

It is possible to analyze solid, liquid or gaseous samples without any special sample preparation in a matter of seconds.

LIBS is sensitive to the majority of chemical elements, including light elements, with limits of detections as low as about 1-10² ppm.

Measurements from this application list were performed utilizing the **Sci-Trace** - configurable analytical instrument specialized on the LIBS technique.

Sci-Trace is designed by scientists for scientists and can be configured to meet the requirements not only of novice or experienced LIBS researchers but also of any analytical laboratory user. Sci-Trace is easily extendable with a number of specialized modules, therefore it is always ready for experimentator`s diverse ideas.

Sci-Trace includes advanced spectra processing software: the **AtomAnalyzer**.

