Simple modeling of LIBS plasma parameters for extraterrestrial applications

P.B. Hansen, D.S. Vogt, S. Schröder, K. Rammelkamp, S. Kubitza, H.-W. Hübers

LIBS has been proven very useful for in-situ geochemical analysis on the Martian surface [1]. It has also been proposed for future missions to explore other bodies of the Solar System [e.g. 2]. For this reason, it has become more important to understand the capabilities and challenges of LIBS under atmospheric conditions that are different from Earth. There is also a high interest in calibration-free LIBS (CF-LIBS) due to the highly versatile measuring conditions in planetary exploration.

In this study, we have developed a method to assist the analysis of LIBS spectra acquired under different atmospheric conditions corresponding to different extraterrestrial mission scenarios. The method is developed from first principles and without resorting to measurements on calibration standards, similar to CF-LIBS [3]. Our approach follows from the same theory and assumptions as the standard approaches of CF-LIBS, such as the construction of Boltzmann plots, but many labor intensive steps are automated.

Assuming an optically thin plasma in local thermal equilibrium (LTE) with assumed distributions of electron density and temperature, a linear relationship exists between the intensities of the atomic emission lines and the elemental concentrations. Our approach is to set up a system of linear equations between the extracted integrated peak intensities, in a given spectrum, and the theoretically predicted peak-intensities by the Saha-Boltzmann equation.
From this system of equations, the concentrations are solved semi-analytically by minimizing the residuals between the peak-intensities. The minimization is repeated using different simply parameterized functions of the electron densities and temperatures, i.e. the plasma parameters.

We evaluate the applicability of the method to data acquired under different atmospheric conditions. Moreover, we investigate the consequences of different assumptions and distributions of the electron density and temperature to the results and discuss the limitations of the approach.

[1] Maurice et.al., Mars. J. Anal. At. Spectrom. (2016).

[2] Arp et.al., Spectrochimica Acta Part B: Atomic Spectroscopy. (2004).

[3] Tognoni et.al., Spectrochimica Acta Part B: Atomic Spectroscopy. (2009).