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PII: S0584-8547(14)00202-X
DOI: doi: 10.1016/j.sab.2014.08.027
Reference: SAB 4779

To appear in: *Spectrochimica Acta Part B: Atomic Spectroscopy*

Received date: 26 December 2013
Accepted date: 8 August 2014

Please cite this article as: P. Pořízka, A. Demidov, J. Kaiser, J. Keivanian, I. Gornushkin, U. Panne, J. Riedel, Laser-Induced Breakdown Spectroscopy for *in-situ* Qualitative and Quantitative Analysis of Mineral Ores, *Spectrochimica Acta Part B: Atomic Spectroscopy* (2014), doi: 10.1016/j.sab.2014.08.027

Laser-Induced Breakdown Spectroscopy for *in-situ* Qualitative and Quantitative Analysis of Mineral Ores

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Abstract

In this work, the potential of Laser-Induced Breakdown Spectroscopy (LIBS) for discrimination and analysis of geological materials was examined. The research was focused on classification of mineral ores using their LIBS spectra prior to quantitative determination of copper. Quantitative analysis is not a trivial task in LIBS measurement because intensities of emission lines in laser-induced plasmas (LIP) are strongly affected by the mineral matrix (matrix effect). To circumvent this effect, typically matrix matched standards are used to obtain matrix dependent calibration curves. If the sample set consists of a mixture of different matrices, even in this approach, the corresponding matrix has to be known *prior* to the downstream data analysis. For this categorization, the multielemental character of LIBS spectra can be of help. In this contribution, a principal component analysis (PCA) was employed on the measured data set to discriminate individual rocks as individual matrices against each other according to their overall elemental composition. 27 igneous rock samples were analyzed in the form of fine dust, classified and subsequently quantitatively analyzed. Two different LIBS setups in two laboratories were used to prove the reproducibility of classification and quantification. A superposition of partial calibration plots constructed from the individual clustered data displayed a large improvement in precision and accuracy compared to the calibration plot constructed from all ore samples. The classification of mineral samples with complex matrices can thus be recommended prior to calibration analysis.

Key words: Laser-induced breakdown spectroscopy; LIBS; Chemometrics; Principal Component Analysis; geochemical analysis

Introduction

With a steadily increasing consumption of mineral resources, it is crucial to optimize the exploration of new ore deposits and the mining process itself with reliable and rapid analytical methods for identification of minerals. However, reliable *in-situ* identification of minerals can be very challenging. Currently in-field identification of minerals is typically based on visual examination of their physical properties by an experienced geologist, which, however, can result in false positives [1]. More advanced laboratory-based techniques, such as X-ray fluorescence (XRF) and inductively coupled plasma optical emission or mass spectrometry (ICP-OES/MS)