

STOCHASTIC-DETERMINATED DESIGN OF EXPERIMENT FOR LIBS SPECTROMETERS CALIBRATION

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Atomic emission spectral analysis, in most variants of its implementation, is characterized by comparatively low accuracy and reproducibility of the results. This is mainly due to the instability of the radiating plasma and the significant influence of the chemical nature of the matrix. From this follows the direct need for statistical processing of spectral data, incl. rather "sophisticated» [Kremers, Radziemsky, 2009]. For hardware quality management of the recorded spectrum, many instruments have several configurable parameters. Theoretically, it is not possible to predict the optimum set of values of these parameters. For the adjustment of spectral devices it is recommended to use the design of experiment [Kalinkin, 2002]. The most intensely negative effect of random processes is manifested in the case of laser inducted breakdown spectroscopy. LIBS devices, as a rule, have several parameters for excitation and registration of the spectrum, which have to be selected manually. A technique that simultaneously optimizes the spectrometer's settings and statistically describes the quantitative characteristics of the analysis is very much in demand in industrial and laboratory spectral analysis. Stochastic-determined design of experiment makes it possible to achieve these goals in a relatively small number of experiments (SDDE) with calibration samples of known composition [Fomin, 2016]. There is a problem of assigning spectral lines in samples of complex composition to one or another element. We have experimentally proved that the composition of the calibration samples can be one of the factors in the SDDE method. With this approach, it is simultaneously possible to select the optimal laser and spectrometer settings, as well as analytical lines of elements that are free from the influence of the matrix and other components of the sample.

References:

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