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Numerical Simulation of Impact of the Spark Discharge Parameters and Electrode Material on the Intensity of Spectral Lines in the Emission Spectral Analysis

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Numerical modeling was used to calculate influence of discharge power and material of a sample and electrodes on sensitivity of emission spectral analysis with spark discharge in air using lines of atoms, single- and doubly charged ions. Mathematical model incorporates thermodynamic calculation of plasma composition at LTE conditions, mass transfer of electrode vapor and calculation of temperature considering inelastic collisions of electrons with particles. Calculations show that electron concentration in current channel varies in 4 times only whereas power density and evaporation rate vary over one order of magnitude and temperature varies from 11000 to 19000 K. Line intensity of doubly charged ions have a maximum and decreases in 3-10 times at twofold variation of evaporation rate. That defines narrow range of parameters for maximal sensitivity of analysis that is the case at analysis of carbon using the line CIII 229.687 nm. In general the model provides a means for selection of optimal conditions for sensitivity and reproducibility of analysis. Comparison with experiment show that calculated and measured temperatures and electron concentrations are in a good agreement. The model gives also more deep insight into the interconnection between power density, concentration of vapors and parameters of LIB plasma at LTE stage.

Keywords: emission spectral analysis, spark plasma parameters, numerical simulation, intensity of spectral lines, electrode materials