T2. Software package for optical emission spectrometry with arc discharge

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This work considers some mathematical models and algorithms, which are used in developing of expert system for automatic spectra processing in direct atom-emission analysis (AEA) of solid samples. The attraction of direct AEA consists of its universality and low price. Using visual interpretation, in a few minutes an experienced analyst can enumerate 50-70 elements in the samples with unknown element structure. The visual interpretation allows making qualitative analysis and semiquantitative analysis with 10-100 % of relative error. The visual interpretation together with the instrumental measurement and computer data processing can provide the results of quantitative analysis with 30 % of relative error.

The process automation of direct AEA is a complex and insufficiently formalized problem. The spectrograph computerization allows us using 30-100 of spectral lines. But there is no a software, which provides us with handling of this exhaustive data in the knowledge base, like the analyst does. Analyzing the visual interpretation properties we can conclude that this procedure can automatized using the expert system paradigm. Actually, the direct AEA includes all the characteristics the expert system asks, i.e.:

1. An analyst has to solve a lot of diagnostic problems arising in the sample classification.
2. The complete and adequate mathematical models have not been developed for the direct AEA yet. Therefore, there is no a steady-state theory in this field.
3. Changing to the instrumental measurement leads that the small number of analysts remain to be able to make the visual analysis.
4. Noise pollution is a natural feature of the direct AEA data since it operates with samples of heterogeneous composition.

Our report discusses a general scheme of the expert system and we try to give mathematical models and algorithms for some expert system components. In particular, we describe a methodology for fitting the optimal parameters of analysis based on multi-objective optimization. We also consider questions concerned with the calibration using methods of multivariate analysis such that the principal compound analysis and neuron networks. This report focuses on the formal mathematical method description illustrated with practical examples.