DEVELOPMENT AND APPLICATION OF NEW DATA PROCESSING ALGORITHMS FOR THE SOFTWARE OF MODERN ATOMIC EMISSION SPECTROMETERS exemplified by STEEL AND ALLOY characterization [[1]](#footnote-1)\*)

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The analytical AES procedure enables the choice and accounting of spectrum excitation system parameters, recording systems, set of spectral lines, etc. For each spectrometer there is an individual set of calibration curves got by research of standard samples with certified values of impurity index. Recorded spectral line intensity depends inter alia on plasma background radiation (independent of a particular element impurity concentration), dynamic range of CCD-arrays and, the so-called, “third” elements [1-4]. It is necessary to systematically recalibrate emission spectrometers (to adjust the calibration curves) in the course of their operation.

Modern spectral analysis software is not capable of calculating exactly the plasma background radiation at the spectral line of the analyte. This necessitates, among other things, to calibrate the spectrometer for a large number of samples. To consider the radiation is particularly important in the case of the analyte low concentration.

We have developed a unique method which allows us to calculate exactly the plasma background radiation at the spectral line of the analyte. This, in turn, provides an opportunity to export calibration curves into the low concentration areas of the devices of the same type using only two samples. The spectra of these samples are used to determine the two linear conversion coefficients of the intensities under measure.

We have compared the developed recalibration algorithm (with the plasma background radiation accurate records) with the traditional recalibration algorithm (without the plasma background radiation accurate records). It is illustrated by the determination of carbon concentration at low concentration range (0,005–0,05%) for low- and medium-alloy steels by GSO set, on 4 different “SPAS” spectrometer modifications. All the developed algorithm-based calibration curves are close to linear.

The developed algorithm allows us to significantly reduce standard deviation while testing low impurity level samples, as well as to greatly improve the metrological characteristics of the existing techniques. Above all, it enables the usage of only two standard samples instead of several dozen ones when performing calibration.

References

1. Mosichev V.I., Nikolaev G.I., Kalinin B.D. Metally i splavy. Analiz i issledovanie. Metody atomnoi spektroskopii. Atomno-emissionnyi, atomno-absorbtsionnyi i rentgenofluorestsentnyi analiz [Metals and alloys. Analysis and research. Atomic spectroscopy methods. Atomic emission, atomic-absorption and X-ray fluorescent analysis]. St. Petersburg, Professional Publ., 2006. 716 p. [in Russian].
2. Zaidel’ A.N., Ostrovskaya G.V., Ostrovskii Yu.I. Technique and practice of spectroscopy. Nauka, Moscow, 1972. P. 375 [in Russian].
3. Mustafaev A.S., Tsyganov A.B., Dobrolezh B.V., “Linear CCD-sensors based multiprocessor photometer system for spectral analysis”, Zapiski Gornogo instituta, Vol. 187, pp. 98-100, 2010 [in Russian].
4. Sukhomlinov V.S., Mustafaev A.S., Popova A.N., Koubaji H. Accounting for the effects of third elements in the emission spectral analysis and construction of global analytical techniques. Journal of Physics: Conference Series, 1384, [012054]. <https://doi.org/10.1088/1742-6596/1384/1/012054>

1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLVIII/Pt/ru/GH-Popova.docx) [↑](#footnote-ref-1)