

METHODS OF VIRTUAL STANDARDS IMPLEMENTATION IN MEASURING AND TESTING TASK

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Abstract: This paper investigates the factors that influence to accuracy of recording spectra using virtual standards during atomic emission spectral analysis. A device and a data processing unit that increase the stability and reproducibility of the instrument calibration curve. The paper describes a mathematical model that compensates of influencing factors to the measurement results, and the possibility of its application in software of automated measuring systems. Result calibration characteristics, built on the proposed model remain stable when external conditions change, or can be transferred to the devices of the same type without loss of accuracy due to individual calibration parameters.

Key words: atomic emission spectral analysis, sensors, virtual standards, stable calibration curves, influencing factors.

Introduction

In modern conditions prevalent in the theory and practice of measurements are used virtual instruments. Under virtual instruments (VI) understand the class of measuring devices that use a personal computer (PC) as part of the instrument. PC in this case, processes and displays the measurement results. Virtual devices can not perform measurements without the use of external software, installed on a PC.

Various examples of virtual instruments using in different areas of measuring technology and engineering testings. In the laboratories of electrical and radio measurements received widespread virtual instruments to implement the functions of the oscilloscope, generator, multimeter and other instruments. The measurement signals of remote modules and further processing of signals by means of a microcontroller or computer have improved the accuracy of the final result [1, 2].

In papers [3, 4] proposed the idea to the implementation of virtual standards of electrical quantities. Technology of virtual standard (VS) is used in the calibration of working measuring instruments. Virtual standards include measuring unit for measuring, and the software performs the functions of conversion of physical units.

The measuring unit may have a lower accuracy class compared with calibrated measuring instruments. After a series of measurements and processing of data receive individual correction values to compensate of measurement errors and to determine a more accurate value of the physical quantity.

To monitor the status of rolling bearings in paper

[5] proposed a new class of test vibration signals virtual standards defects of bearing assemblies are described possible ways to implement such signals. It was justified by receiving vibration test signal by reduction of the time signal of the three kinds of spectra measured signal.

When implementing virtual standards may solution two types of problems, the first of which is associated with the stabilization of measurement conditions, finding the most significant factors by regression analysis. Another approach involves finding additional information in the measured signal in order to build mathematical relationship transformation, invariant to changes in the conditions of the experiment.

Consider the both approaches when building virtual standards in the spectral analysis of materials. The real standards or reference materials used in spectral analysis for the construction of calibration characteristics conversion of the measured value the emission intensity of the spectral lines in the output value quantitative content of components in the test sample.

1. Implementation of virtual standards by improving the stability of the calibration characteristics of devices

To monitor the change in the factors affecting the spectral analysis have been proposed an apparatus and a data processing unit that increase the stability and reproducibility of the final results. In carrying

out atomic emission spectral analysis measured influencing factors for the intensities is corrected and, as a consequence increase the stability of the calibration dependence instrument.

To spectral device are connected seven sensors for transmit data to the processing unit. The functions of connected sensors are as follows: S1 – sensor measures the pressure of argon in the optical unit of spectrometer; S2 – control the flow of argon during the analysis; S3 – measures the temperature of the room air during the analysis; S4 – measures the air pressure in the room during the analysis; S5 – measures current, frequency and shape of the pulses from the electrical generator, transmits the data on digital storage oscilloscope; S6 – monitors the position of the electrode relative to the sample and form an electric arc; S7 – controls the position of the sample and the presence surface defects at the proposed site of analysis [6 – 8].

Fig. 1 is a block diagram of design apparatus consisting of atomic emission spectrometer and additionally introduced seven sensors and two microcontroller units for data processing and constructs a stable calibration characteristic, when changing influencing factors.

The device operates as follows. After installing the analyzed sample sensor S7 transferred its image to PC screen. In the case of incorrect installation or presence of surface defects (stains from previous firings, etc.) Will be issued a warning, obtained from the sensor S7 by analyzing the image. When the electrical discharge appears, detector S6 measures the distance

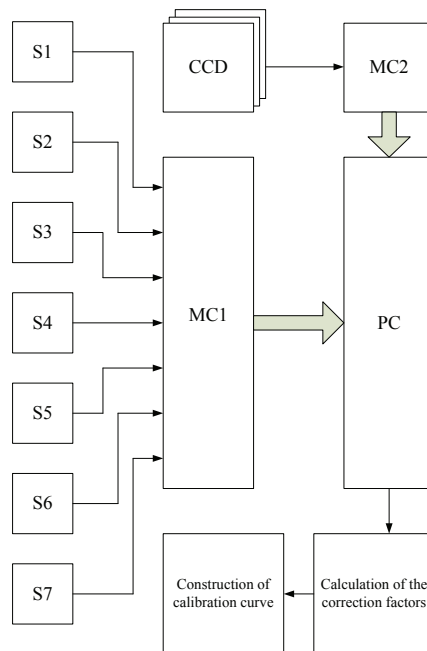


Fig. 1. Wiring physical quantity sensors to the control unit atomic emission spectrometer: MC1 and MC2 – microcontrollers for sensors and spectral radiation detectors (CCD) readings.

between the analyzed sample and the electrode and consequently recorded size of the cloud discharge.

Function scheme of sensors in the unit of the spectrometer shown in Fig. 2.

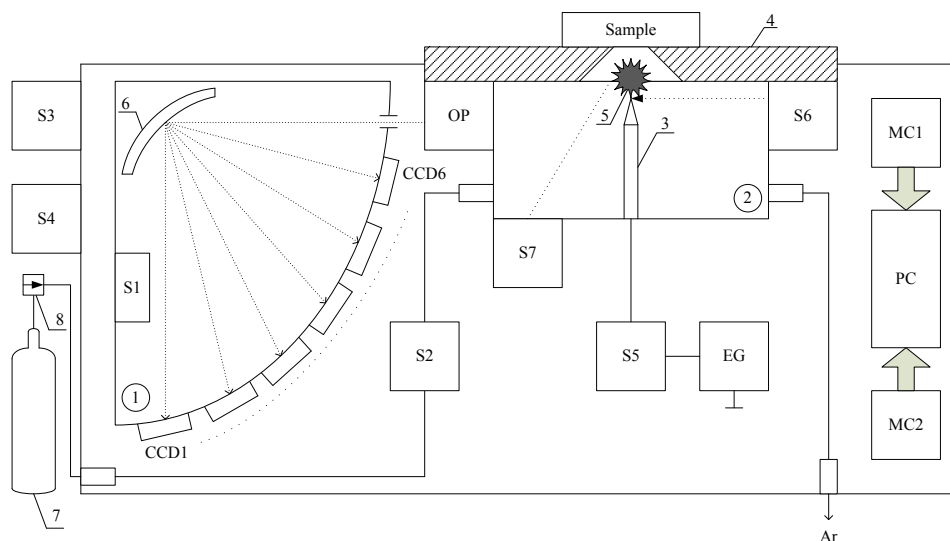


Fig. 2. The sensors position scheme in the unit of the spectrometer

The pressure sensor S1 is located within sealed optical block 1 in which there are also situated the diffraction grating 6 and the radiation detectors CCD1 CCD6. The emission from the sample falls into the unit through the optical transmitter – OP. The flow sensor S2 is set to supply argon pipe of discharge chamber 2 of spectrometer. The temperature and humidity sensors S3 and S4 mounted on the outside of the spectrometer. Sensor electrical discharge parameters S5 located in a chain of current circuit from the electrical generator EG to the tungsten electrode 3. Sensors S6 and S7 are technical endoscopes, they are arranged so as to provide the desired surface review test sample mounted on the table 4, and the discharge cloud 5.

In the case where all measured parameters are normal, the end result of the measurement is considered reliable. If the values of some parameters are outside the acceptable limits, it is necessary to make adjustments to the calibration, depending on the standard models.

2. Implementation of standards through the creation of virtual software automatic measuring system

Another way to create virtual standards is using a set of real standard samples to create a mathematical model, compensating factors influence the measurement result and its application in the software of the automated measuring systems.

With the purpose of obtaining an invariant models measure the intensity of the spectral lines under various experimental conditions. For a positive result it is necessary to get the most divergence of the measured parameters. To build the model selected spectral lines with different power characteristics (different response to influence factors) [9, 10].

To account for the different energy characteristics of spectral lines proposed the use of generalized functions of the form:

$$F_j = \frac{\sum_{i=1}^N a_i I_{anij}}{\sum_{i=1}^M b_i I_{cpij}} = \frac{a_0 I_{an0j} + a_1 I_{anS1j} + \dots + a_N I_{anNj}}{b_0 I_{cp0j} + b_1 I_{cp1j} + \dots + b_M I_{cpMj}} \quad (1),$$

where I_{an} the intensity of the spectral lines of the analyte; I_{cp} comparing the intensity of the lines having different energy performance; a_i, b_i stable calibration weights; N number of analyte lines; M the number of comparison lines.

Calibration curves built by the proposed model

are stable when external conditions changes, or can be transferred to the devices of the same type without loss of accuracy due to individual calibration parameters[1117].

Afterword

Thus, the virtual standards can be considered as real standard samples in conjunction with software that processes the output signal from these samples using the additional information from the recorded spectrum to compensate components error due to changes of external conditions of the experiment.

References

- [1] **I.A. Shumskij** Virtualnaya USB laboratoriya – proryv v budushchee/ *I.A.Shumskij Kontrolnoizmeritelnye pribory i sistemy*.2003.№ 4.S.1921.
- [2] **A.A. Afonskij** Vozможnosti rasshirenojj sinhronizatsii v virtualnykh ostsillografakh. Ak-takom/ A.A. Afonskij, E.V. Sukhanov // *Kontrolnoizmeritelnye pribory i sistemy*. 2010. № 3. S. 8 – 13.
- [3] **S.M. Ermishin** Vozможnosti sozdaniya virtualnykh ehtalonov / S.M. Ermishin // *Izmeritelnaya tekhnika*. 2002. № 10. S. 10 – 13.
- [4] **S.M. Ermishin** Virtualnye ehtalony – novyy klass virtualnykh priborov / S.M. Ermishin, P.G. Shabanov // *Avtomatizatsiya v promyshlennosti*. 2004. № 10. S. 26 – 30.
- [5] **V. Y. Tetter** Modeling of virtual standards of vibration of defective bearing units / V. Y. Tetter, O. N. Sidorov, E. A. Sidorova// *Measurement Techniques*. USA. 2013. June. Volume 56. Issue 3. P. 278 – 282.
- [6] **A. A. Kuznetsov** Issledovanie faktorov, vliyayushchikh na rezultaty izmereniya intensivnostej pri spektralnom analize materialov / A. A.Kuznetsov, O.B. Meshkova, V.A. Sleperev // *Omskij nauchnyj vestnik*. 2011. № 3. S. 242 – 245.
- [7] **Z. V. Semenov** Programma videokontrolya protsessa atomnoehmissionogo spektralnogo spektralnogo analiza / Z. V. Semenov, O.A. Neklyudov i dr.// *Materialy XI mezhdunar. simpoziuma «Primenenie analizatorov MAEHS v promyshlennosti»*. *Imt neorganicheskoy khimii SO RAN. Novosibirsk*, 2011. S. 70 – 73.
- [8] **P. Martinsen** Temporal Sensitivity of the Wavelength Calibration of a Photodiode Array Spectrometer/ P. Martinsen, V. A. McGlone et al. // *Applied Spectroscopy*. Vol. 64. № 12. 2010. P. 1325 – 1329.
- [9] **A. A. Kuznetsov** Realizatsiya mobilnykh graduirovocnykh kharakteristik priborov spektral-

nogo analiza materialov s ispolzovaniem virtualnykh ehtalonov / A. A. Kuznetsov , V.A. Slepterev, A.V. Peleznev // *Omskij nauchnyj vestnik*. 2013. № 3(125). S. 241 – 246.

[10] **A. A. Kuznetsov** Razrabotka algoritma i programmnoho obespecheniya ustojchivogo graduirovaniya priborov atomnoehmissionnoj spektroskopii / A. A. Kuznetsov ,V.A. Slepterev // *Sb. nauch. tr. SWorld po materialam mezhdunar. nauch. prakt. konf. «Nauchye issledovaniya i ikh prakticheskoe primenenie. Sovremennoe sostoyanie i puti razvitiya»*. Odessa: Chernomore, 2011. S. 23 – 26.

[11] **E. Vasilyeva** Calibration model of simultaneous multielement atomicemission analysis using analytical line groups of each determined element / E. Vasilyeva, E. V. Shabanova // *Fresenius J. Anal. Chem.* – 1998. – V. 361. – №3. – P.280282.

[12] **A. V. Maiorova, O. V. Evdokimova, N. V. Pechishcheva, K. Yu Shunyaev., A. A. Shchepetkin, P. V.Zaitseva, A. A. Pupyshv** Selection of internal standard for icpaes analysis of ores, concentrates and slags by thermodynamic modeling / *The optimization of the composition, structure and properties of metals, oxides, composites, nano and amorphous materials. Proceedings of the twelfth BiNational Workshop Russian Israeli.*" Editors: M.Zinigrad, L.Leontiev. 2013. C. 314326.

[13] **J. A. Broekaert , F. Leis , H. Laqua** Some aspects of matrix effects caused by sodiumtetraborate in the analysis of rare earth minerals with the aid of inductively coupled plasma atomic emission spectroscopy // *Spectrochimica acta. Part B*. 1979. V.34, №4. P. 167175.

[14] **Jorge Trincavelli, Silvina Limandri, Rita Bonetto** Standardless quantification methods in electron probe microanalysis. *Spectrochimica Acta Part B*: Volume 102 (2014). Pages 7685.

[15] **Staci Brown, Charlemagne C. Alan Ford, Akpovo, Jorge Martinez, Lewis Johnson** Matrix effects in laser ablation molecular isotopic spec-

troscopy./ *Spectrochimica Acta Part B: Volume 101* (2014) Pages 204212

[16] **Veerle Devulder, Lara Lobo, Karen Van Hoecke, Patrick Degryse, Frank Vanhaecke.** Common analyte internal standardization as a tool for correction for mass discrimination in multicollector inductively coupled plasmamass spectrometry. *Spectrochimica Acta Part B: Atomic Spectroscopy* Volume 89, (2013) Pages 2029.

[17] **Xiongwei Li, Zhe Wang, SiuLung Lui, Yangting Fu, Zheng Li, Jianming Liu, Weidou Ni.** A partial least squares based spectrum normalization method for uncertainty reduction for laserinduced breakdown spectroscopy measurements. *Spectrochimica Acta Part B: Atomic Spectroscopy*. Volume 88 (2013), Pages 180185.

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СПОСОБЫ РЕАЛИЗАЦИИ ВИРТУАЛЬНЫХ ЭТАЛОНОВ В ЗАДАЧАХ ИЗМЕРЕНИЙ И КОНТРОЛЯ

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Резюме: В работе исследуются факторы, влияющие на точность регистрации спектров с использованием виртуальных приборов и эталонов при проведении атомноэмиссионного спектрального анализа. Предложено устройство и блок обработки данных, повышающих стабильность и воспроизводимость градуировочной зависимости прибора. Приведено описание математической модели, компенсирующей влияние влияющих факторов на результаты измерений, и возможность ее применения в программном обеспечении автоматизированной системы измерений. После анализа полученных результатов установлено, что градуировочные характеристики, построенные по предложенной модели, сохраняют стабильность при изменении внешних условий или могут переноситься на приборы одного типа без потери точности, обусловленной индивидуальными параметрами калибровки.

Ключевые слова: атомноэмиссионный спектральный анализ, датчики, виртуальные приборы, виртуальные эталоны, градуировочные графики, влияющие факторы, стандартные образцы, калибровка.

НАЧИНИ ЗА РЕАЛИЗАЦИЯ НА ВИРТУАЛНИ ЕТАЛОНИ В ЗАДАЧИТЕ ЗА ИЗМЕРВАНЕ И КОНТРОЛ

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Резюме: В доклада се изследват факторите, които влияят на точността на регистрация на спектри с помощта на виртуални инструменти и еталони при провеждане на атомноемисионен спектрален анализ. Предложено е устройство и блок за обработка на данни, повишаващи стабилността и възпроизвеждането на градуираната зависимост на уреда. Дава се описание на математическия модел, който компенсира влиянието на влияещите фактори върху резултатите от измерването, както и възможността за неговото прилагане в софтуера на автоматизирана измервателна система. След анализ на получените резултатите е установено, че градуираните характеристики, изградени по предложението модел остават стабилни при изменение на външните условия, или могат да бъдат прехвърлени към изделия от същия тип, без загуба на точност, определена от индивидуалните параметри на калибриране.

Ключови думи: атоменемисионен спектрален анализ, датчици, виртуални инструменти, виртуални еталони, градуирани криви, влияещи фактори, стандартните образци, калибриране.