METHOD OF DIGITAL PROCESSING OF OPTICAL SPECTRA OF MAGNETRON DISCHARGE PLASM[A](#page-0-1)

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Received May 25, 2024; revised July 10, 2024; accepted August 07, 2024

To solve the actual problems associated with the development of the theory of magnetron discharge and the expansion of its practical application, a digital method of recording and processing the discharge plasma luminescence spectra is proposed in this work. To obtain the discharge plasma glow spectra, a photographic technique was used, which allowed simultaneous recording of the entire radiation spectrum in the 390.0÷700.0 nm region. An additional advantage of this technique is the ability to track spatial changes in the composition and properties of the plasma in the discharge in the selected direction. A Canon EOS 80D digital camera with remote control was used to record the optical signal. A graphical application OSA was created to process digital images of the discharge plasma luminescence spectra. The paper describes the functionality of this application: determination of the wavelength of a spectral line and its belonging to a certain chemical element; measurement of the spatial distribution of the intensity of a spectral line along the selected direction of radiation registration. Determining the wavelength of a spectral line in the application is possible in two modes of operation - automatic and manual. In the first mode, the algorithm developed in this paper determines the wavelength for all spectral lines whose intensity exceeds the background value at a height of 10% of the lower spectral limit. The second mode allows you to independently select a single spectral line or several to determine their wavelengths. The first mode is used for quick analysis, while the second mode allows you to determine the length of the spectral line with greater accuracy. To interpret the spectral lines, the methodology of reference lines from the databases of spectral line tables for various elements is used. The possibility of both full automatic verification, where all elements are sequentially searched, and selective verification, where one or more elements are selected, is provided. The paper shows that the spatial distribution of the intensity of tungsten spectral lines, and thus of excited atoms in a magnetron discharge, is a complex function of the distance from the cathode, which depends on the discharge parameters. The proposed digital methodology makes it possible to significantly speed up the process of obtaining physical information and increase the accuracy in determining the spectrum parameters.

Keywords: *optical emission spectrometry, magnetron discharge, plasma emission spectrum, excited particles*

PACS: 32.30, 34.35, 34.50, 34.80.Dp, 52.70.Kz, 52.80.Vp

1. INTRODUCTION

Interest in the study of magnetron discharge physics is due to its traditional application for coating. These can be as metal coatings for a wide range of industrial uses [1, 2], bio-coatings used in healthcare products [3] or coatings with high insulating properties [4, 5]. One of the factors that influence on the obtaining of coatings with specified properties is the control of the magnetron discharge plasma. Information about the composition and parameters of the plasma allows monitoring the deposition conditions of the films and regulating the formation of their properties.

It is convenient to control plasma parameters by optical spectroscopy [6, 7]. The main advantage of spectroscopy, in contrast to the probe technique, is the ability to perform plasma analysis without disturbing the plasma itself. An additional advantage is that this method does not require complex equipment: only diagnostic ports that provide direct visibility through the plasma are required. The spectroscopy method is informative and widely used to obtain various parameters of magnetron discharge plasma. For example, the population of excited states of plasma particles can be determined by the intensity of the corresponding spectral lines, and the intensities of the lines of various plasma components make it possible to determine the ion composition [8, 9].

Most often a photoelectric registration system is used in the spectroscopy to obtain physical information, in which the optical signal is converted into an electrical one with the help of a photomultiplier. At that, the integral intensity of a separate spectral line is obtained, which depends on the radiation intensity of the entire investigated area of luminescence along the selected direction. A feature of this registration system is the need to scan radiation spectra to study the selected spectral range. This, firstly, requires some time, and, secondly, when examining a narrow spectral interval, it is not possible to monitor changes in the intensity of spectral lines in the other part of the spectral range. These problems can be solved if a broadband detector, such as a CCD, is used as an optical signal converter [10]. At that, the dispersive element of the spectral device is fixed in a certain position, in which the studied region of the spectrum is projected onto the focal plane. This allows recording optical radiation simultaneously in a fairly wide spectral range, which increases the reliability of

Cite as: I. Afanasieva, S. Afanasiev, V. Bobkov, V. Gritsyna, A. Skrypnyk, East Eur. J. Phys. 3, [166](#page-0-0) (2024), [https://doi.org/10.26565/](https://doi.org/10.26565/2312-4334-2024-3-16) [2312-4334-2024-3-16](https://doi.org/10.26565/2312-4334-2024-3-16)

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experimental results. An additional advantage of this design is that, in contrast to the photoelectric registration system, it makes it possible to obtain the spatial distribution of the intensity of a separate spectral line, and therefore of the investigated area of fluorescence along the selected direction. In this way, it is possible to monitor the spatial changes in the composition and properties of the discharge plasma in the selected direction.

2. EXPERIMENTAL METHOD

Spectrometers that use CCD as a converter of optical radiation, have high sensitivity and resolution, but are quite expensive, which somewhat limits their wide use in scientific institutions. Also, the software delivering with the device, usually doesn't allow for any modifications or scripts that might be needed while working in a research lab. Therefore, the question arises of creating a high-quality, but affordable CCD-based optical radiation recorder; it can be a digital camera.

The principle scheme of obtaining and digital processing of optical images of radiation spectra was presented in [11, 12]. The researches were carried out on the magnetron sputtering system (MSS) described in [13]. MSS operating conditions were as follows: buffer gas pressure (argon) $p_{Ar} = 10 - 18$ Pa, anode voltage V_a = 300 – 350 V, discharge current $I_d = 10 - 160$ mA, magnetic field induction B = 0.05 T. The optical radiation of the area of bright glow of the discharge was output through the diagnostic window of the vacuum chamber, focused with an achromatic lens on the input slit of the ISP-51 spectrometer, in which the radiation was dispersed using a triple prism system and focused in the focal plane of the output collimator of the spectrometer. With this geometry, a 4-fold reduced image of the optical spectrum of the magnetron discharge emitting region was projected onto the focal plane $(1 = 4h)$, where l is the height of the discharge along the axis, h is the height of the spectral line) in the spectral range of $400.0 \div 600.0$ nm.

At the first stage (work [11]), a comparison of physical data obtained by two methods was carried out: i) by the photographic photometry [14] with the photographing of the optical spectrum on photographic film, ii) with the analysis of the corresponding digitized frame. The frames were scanned on a specialized high-resolution slide scanner (size – 5040×3360 pixels) getting black-and-white digital images with the extension *.jpg.

To determine the qualitative and quantitative characteristics of magnetron discharge plasma, the creation of a multifunctional dialog GUI application of Optical Spectrum Analysis (OSA) was started. The OSA application was created in the Python programming language based on the Tkinter graphic library using a set of additional modules: PIL, Numpy, Scipy, Pandas, and Matplotlib [15]. With the the PIL module, the selected digital image of the discharge glow spectrum was converted into a numerical matrix, each element of which has an integer value proportional to the intensity I[x,y] at a given point of the image plane (x and y are integers describing the column number or rows of the matrix, in which this element is placed). The intensity range is from 0 to 255. Mathematical algorithms and procedures implemented in OSA allow to process this matrix and present the results of the processing on the image in the form of graphic objects and text. The Matplotlib library was used as a tool for data visualization with two-dimensional graphics. The graphical application was created within the framework of object-oriented programming (OOP), with the ability to perform a new calculation when a number of parameters were changed and immediately present the obtained data on the image and graphs. In parallel, these results were recorded in an external file.

At the second stage (work [12]), photography of the working area was carried out using a user digital camera with the aim of directly obtaining digital images. Digital images were of better quality than digitized photographic film, and this made it possible to obtain the main characteristics of the magnetron discharge plasma radiation spectrum (wavelength, intensity of spectral lines) with better resolution.

At this stage of research, spectrum registration was carried out using a Canon EOS 80D professional digital camera with a resolution of 7000×5000 pixels, which was controlled remotely via Wi-Fi. Also, along with the improvement of the recording technique, some blocks were improved and new ones were added in the OSA application. The paper will provide a detailed description of the functional capabilities of the OSA application for digital processing of the optical emission spectra of magnetron discharge plasma glow and provide some experimental results.

3. BASIC POSSIBILITIES OF DIGITAL PROCESSING OF OPTICAL SPECTRA

3.1. The zone of the optical spectrum in the image and the spectrogram

The part of the digital image of the radiation spectrum of excited particles of a magnetron discharge in an argon atmosphere with a copper cathode is shown in fig.1. The MSS operating mode was as follows: buffer gas pressure p_{Ar} = 10 Pa, anode voltage V_a = 320 V, discharge current I_d = 25 mA, magnetic field induction B = 0.05 T, exposure time t = 90_s

At the first, preliminary stage, the spectrum zone is automatically determined and the primary spectrogram is taken. The spectral lines do not occupy the entire area of the digital photograph, as Fig. 1 shows. It is obvious that the lines along which the pixels corresponding to the spectrum lines are located have a higher intensity compared to other lines. To determine the horizontal boundaries of the spectrum zone of each row, $I^{sum} = \sum_{i=1}^{n} I_i/n$, was determined, where n is the number of pixels along the row, I_i is the intensity of the ith pixel. Histogram the distribution of I^{sum} depending on the row number is shown in Fig. 2a. The dashed curve shows the results of fitting with a linear function. The coordinates of the intersection of the linear function with the histogram correspond to the lower and upper limits of the spectrum zone and are shown in Fig. 1 with solid horizontal lines. The values of the spectrum boundary coordinates have been used to

Figure 1. An example of an optical emission spectrum.

construct a spectrogram – dependence of the intensity of each pixel for a conventional line located across the spectrum at a height (difference between the upper and lower boundaries) of 10% from the lower boundary.

Figure 2. Preliminary estimation of spectrum parameters: a) determination of geometric boundaries, b) determination the coordinates of the most intense lines.

The histogram for the one shown in Fig. 1 spectrum is presented in Fig. 2b. As can be seen from the figure, the most intense spectral lines appear in the form of strong discrete maxima. The background layer is determined by fitting with a Gaussian function (dashed line in Fig. 2b). To automatically determine the position of these maxima, the groupby() function from the Pandas module have been used, which performs grouping by one or more parameters and determines inflection points (extrema). The position of the maxima of the most intense spectral lines in Fig. 2b are indicated by dots.

Thus, a coordinate in pixels along the horizontal axis is automatically determined for each of the intense spectral lines. It is for these lines that the wavelength is determined in the future, that is, the spectrum is deciphered.

3.2. Determination of the wavelength of an arbitrary spectral line and its interpretation

To obtain qualitative and quantitative parameters of the spectrum, it is necessary to bind the digital coordinate system (pixels) to the experimental one. A reference spectrum with known lengths of spectral lines (neon, mercury or hydrogen lamp) is used to obtain a dependence that connects the coordinates of a single pixel along the horizontal direction and the wavelength of a known spectral line.

For the ISP-51 spectrograph, when the radiation is decomposed into a spectrum, nonlinear dispersion [14] is

characteristic, which implies the presence of a nonlinear calibration scale (Fig. 3a), which relates the value of the line position to the wavelength λ in nm. The scale of the values of the digital matrix in pixels is placed along the ordinate axis to the right. In the available range of wavelengths for the reference lines on the abscissa scale, the corresponding values on the ordinate scale (left) in mm are found by interpolation. This allows you to enter a pixel-mm scale factor and automatically determine the wavelength λ for an arbitrary line on a digital image in the pixel coordinate system using reverse interpolation.

Figure 3. a) calibration function, b) intensity distribution of spectral lines along their height.

In the OSA application, it is possible to use two modes of operation - automatic and manual. In the first mode, for all spectral lines whose intensity at a height of 10% from the lower limit of the spectrum exceeds the background value, the wavelength is determined by the algorithm described above. The second mode allows you to independently choose a separate spectral line or several of the most interesting for determining their wavelengths. The first mode is used for quick analysis, the second allows to determine the length of the spectral line with greater accuracy, thanks to the possibility of using the digital optical zoom function (ZOOM). The value of the wavelength of the spectral lines in nm is displayed on the spectrum and is also recorded in a separate file.

As an example of the manual mode of operation in Fig. 4 shows a fragment of the spectrum, where vertically arranged numbers indicate the wavelength λ for several lines: λ_{λ}^{exp} λ_1^{exp} =522.4 nm, λ_2^{exp} $\frac{exp}{2}$ =498.1 nm, λ_3^{exp} $^{exp}_{3}$ =488.5 nm. The wavelengths of a set of spectral lines have been repeatedly measured and the statistical error has been obtained $\delta\lambda$ when determining the wavelength using the OSA application; on average, $\delta \lambda$ is in the range from 0.1 to 0.3 nm.

The most difficult stage in optical spectrometry is the interpretation of the decoded spectrum (that is, determining whether the spectral lines observed in the spectrum belong to certain chemical elements). At the initial stage, it is best to use the method of interpretation based on reference lines - the lines of the studied element, which are the last to disappear from the spectrum of the sample when the concentration of the given element decreases in it. The reference lines of all elements are well known and their parameters (wavelength, excitation energy, intensity, etc.) are given in atlases of spectral lines. For the reliability of element identification, a set of reference lines is always used, with which the lengths of the spectral lines present in the luminescence spectrum of the material under study are compared. In this paper, spectral line databases for various elements were used for the interpretation of spectral lines [16]. In the OSA application, in a separate block, the possibility of both a full automatic check, where a sequential review of all elements takes place, and a selective one (one or several elements) is created.

A simple comparative search fixes the range of values of wavelengths in the table, in which one of the experimental values falls. Of the two limiting values, the one with the lower value of the excitation energy is chosen. In case of equality on this parameter, the third element is used - intensity. Preference is given to the option with the maximum intensity value. Yes, shown in Fig. 4 spectral lines were interpreted as tungsten lines W I – λ_1^{tabl} = 522.5 nm, λ_2^{tabl} = 498.3 nm, λ_3^{tabl} = 488.7 nm.

3.3. Distribution of the intensity of a spectral line along its height

One of the significant advantages of using the photographic method of recording optical spectra is the possibility of obtaining information about the spatial distribution of excited particles along the chosen direction. Since the intensity of the spectral line (I) is an energy quantity and is related to the number of excited particles (n^{*}) and the quantum energy (hv) by the ratio I=n^{*} · $h\nu$, the change in the intensity of the spectral line along the registration direction reflects the change in the number of excited particles, emitting photons at the wavelength of the investigated line. In this work, the registration system was located so that the height of the h lines in the spectrum corresponded to the direction of the ionization zone along the magnetron axis.

In Fig. 4 circles indicate the coordinates of the points where the intensity of the spectral line along its height was fixed. The method of determining the coordinates of points along a line with some curvature was described in [10]. In this work, the optimization of the method is carried out, thanks to which it is possible to determine the distribution for low-intensity lines and a unified form of data output - with the same step for any line. It was also possible to determine the integral intensity of a spectral line by summing the intensity value (I) of all pixels forming this line, taking into account the line width.

Figure 4. Part of the spectrum with certain values of the wavelengths (vertical inscriptions) of some lines and the distribution of points along these lines.

The distribution of the intensity of three lines belonging to the W I spectrum along their height shows in Fig. 3b as an example. It can be seen from the figure that the spatial distribution of the intensity of the spectral lines, and therefore of the excited tungsten atoms in the magnetron discharge, is a complex function of the distance from the cathode. Moreover, it has been established that depending on the mode of operation of the magnetron, the relative intensity of the studied lines changes significantly. Moreover, this change is different for particles excited into states characterized by different excitation energies. This is probably related to the different efficiency of excitation of the upper state of the studied transition in the tungsten atom by electrons of the ionization zone of the discharge plasma, because excited particles in the magnetron discharge are formed not only by sputtering atoms of the cathode material under the action of incident gas ions, but also by collision particles with a large number of free electrons knocked out of the surface of the cathode in the magnetic field in the ionization (and excitation) zone of the magnetron plasma.

4. CONCLUSIONS

To solve the current problems related to both the development of the theory of the magnetron discharge and the extension of the field of its practical application, a digital method of recording and processing the discharge plasma glow spectra is proposed in the paper. The spectrum was recorded using a Canon EOS 80D digital camera with a resolution of 7000*5000 pixels, which was controlled remotely via Wi-Fi.

For the digital processing of the spectra, a graphic OSA application was created, which made it possible to obtain qualitative and quantitative characteristics (wavelength, interpretation and intensity) of the spectral line of the magnetron discharge plasma radiation. In addition, the use of digital techniques made it possible to obtain an information on the spatial distribution of excited particles along the chosen direction of radiation registration. The OSA application was created in the Python programming language based on the Tkinter graphics library. With the help of the PIL module, access to the matrix of the selected digital image of the glow spectrum of the discharge was obtained. Mathematical algorithms and procedures were developed that allow you to process this digital matrix, visualize the results of the processing on the image, and present the results of the processing in the form of two-dimensional graphics. The graphical application was created within the framework of object-oriented programming, with the ability to make a new calculation when changing a number of parameters and immediately present the output data on images and graphs.

The proposed digital technique made it possible to significantly speed up the process of obtaining physical information and increase the accuracy in determining the parameters of the spectrum. Digitally obtained snapshots of the luminescence spectra of reference objects, supplemented with the data of their processing by the OSA graphic application, made it possible to create a database containing both electronic atlases of the luminescence spectra of various elements and quantitative parameters of these spectra. a data bank containing both atlases of the luminescence spectra of various elements in electronic form, as well as the quantitative parameters of these spectra.

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МЕТОДИКА ЦИФРОВОЇ ОБРОБКИ ОПТИЧНИХ СПЕКТРIВ ПЛАЗМИ МАГНЕТРОННОГО РОЗРЯДУ

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Нацiональний Науковий Центр "Харкiвський Фiзико-Технiчний Iнститут", вул. Академiчна, 1, 61108, Харкiв, Україна Для вирiшення актуальних задач, пов'язаних з розробкою теорiї магнетронного розряду та розширенням областi його практичного застосування, в роботi запропонована цифрова методика реєстрацiї та обробки спектрiв свiтiння плазми розряду. Для отримання спектрiв свiтiння плазми розряду використовувалась фотографiчна методика, яка дозволяла одночасно реєструвати весь спектр випромiнювання в областi 390.0÷700.0 нм. Додатковою перевагою даної методики є можливiсть вiдслiдковувати просторовi змiни складу та властивостей плазми в розрядi в обраному напрямку. Для реєстрацiї оптичного сигналу в роботi використовувалась цифрова камера Canon EOS 80D з вiддаленим керуванням. Для обробки цифрових знiмкiв спектрiв свiтiння плазми розряду створено графiчний застосунок OSA. В роботi наведено опис функцiональних можливостей даного застосунку: визначення довжини хвилi спектральної лiнiї та її приналежностi певному хiмiчному елементу; вимiрювання просторового розподiлу iнтенсивностi спектральної лiнiї вздовж обраного напрямку реєстрацiї випромiнювання. Визначення довжини хвилi спектральної лiнiї в застосунку можливо в двох режимах роботи – автоматичному та ручному. В першому режимi за розробленим в роботі алгоритмом визначається довжина хвилі для усіх спектральних ліній, інтенсивність яких на висоті 10% від нижньої межi спектру перевищує фонове значення. Другий режим дозволяє самостiйно обрати окрему спектральну лiнiю або декiлька для визначення їх довжин хвиль. Перший режим використовується для швидкого аналiзу, другий дозволяє провести визначення довжини спектральної лiнiї з бiльшою точнiстю. Для iнтерпретацiї спектральних лiнiй в роботi використано методику реперних лiнiй з баз табличних даних спектральних лiнiй для рiзних елементiв. Забезпечена можливiсть як повної автоматичної перевiрки, де вiдбувається послiдовний перебiр всiх елементiв, так i вибiркової – за одним або декiлькома елементами. В роботi показано, що просторовий розподiл iнтенсивностi спектральних лiнiй вольфраму, а, отже, й збуджених атомiв в магнетронному розрядi, є складною функцiєю вiдстанi вiд катоду, яка залежить вiд параметрiв розряду. Запропонована цифрова методика дає можливiсть iстотно прискорити процес отримання фiзичної iнформацiї та пiдвищити точнiсть у визначеннi параметрiв спектра. **Ключовi слова:** *оптична емiсiйна спектрометрiя, магнетронний розряд, спектр випромiнювання плазми, збудженi частинки*