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Spectra registration with a multichannel detector on the 6.65-meter VUV-UV spectrometer

© P.S. Antsiferov[1,2], L.V. Stepanov[1,2], N.D. Matiukhin[1,3]

[1] Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow, Russia
[2] National Research University Higher School of Economics, Moscow, Russia
[3] Moscow Institute of Physics and Technology (National Research University), Moscow Oblast, Dolgoprudny, Russia
e-mail: lvstepanov@edu.hse.ru

Received October 14, 2025
Revised October 14, 2025
Accepted December 28, 2025

A system for obtaining spectra using a CCD linear array has been elaborated for a unique VUV spectrometer based on a spherical diffraction grating with a radius of 6.65 m. A HAMAMATSU S11156-2048-02 linear array was used. It was installed tangentially to the Rowland circle with the possibility of mechanical displacement for spectral scanning. Spectrograms were obtained in the wavelength range 2130−2270 Å. A method for matching the recorded spectral segments to obtain an overview spectrogram is described. A technique for analyzing the wings of spectral lines in order to extract the Lorentzian contribution is proposed.

Keywords: electrical discharges, multicharged ions, CCD, UV-spectroscopy.

DOI: 10.61011/EOS.2026.02.63474.8633-25

Introduction

The Institute of Spectroscopy of the Russian Academy of Sciences possesses a unique spectrometer for the 50−250 nm range, built on a spherical grating with a radius of 6.65 m in normal incidence and having a theoretical spectral resolution $\lambda/\delta\lambda \cong 10^5$. With its help, a number of important results have been obtained on the identification of energy levels of ions that have applications in various fields of physics, such as astrophysics [1], VUV range lasers [2], lithography [3] etc. Designed to work with photographic materials, the spectrometer currently needs to be upgraded to a spectrum registration system based on other principles. This paper reports on the creation of a spectrum registration system based on a CCD linear array. In addition to describing the method of operating such a system, the article also discusses new capabilities for spectrum processing. Results obtained using an arc discharge with iron electrodes in the region of 200 nm are presented.

Registration of spectra using a CCD-linear array

The spectrometer uses a concave diffraction grating (radius of curvature $R = 6.65$ m) with a gold coating, with a total working size of 175 mm, having a groove density of 1200 gr/mm, providing an inverse linear dispersion of 1.25 Å/mm (Fig. 1). In the present measurements, the spectrometer is tuned to the range from 1900 to 2500 Å, which made it possible to operate without evacuating the spectrometer volume. Radiation falls on the grating at an angle $\varphi = 3.7°$, the short-wavelength and long-wavelength boundaries of the range correspond to angles 9.4° and 13.62° respectively (Fig. 1).

In this paper the CCD-linear array HAMAMATSU S11156-2048-02 is used, which contains 2048 elements with height of 1 mm and pixel size in direction of dispersion 14 μm. The total size of the linear array in dispersion direction is 28 mm. The linear array is installed in the cassette assembly of the spectrometer tangential to the Rowland circle (Fig. 1). The relatively small size of the array, on the one hand, ensures focusing over its entire length, but, on the other hand, makes it necessary to scan the registered spectrum to obtain a sufficient spectral overview. In the presented version of the registration system, the carriage with the CCD-linear array moves along existing guides in the Rowland circle using a lead screw with a spring-loaded mechanism (Fig. 2). For test experiments, an arc discharge with iron electrodes and an operating current

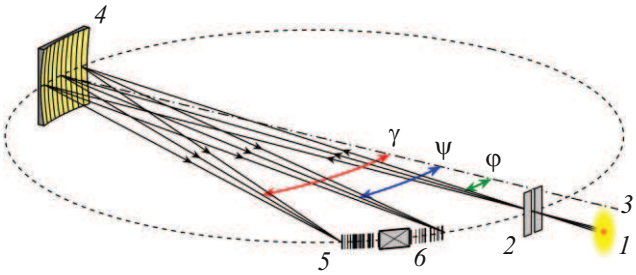


Figure 1. Spectrometer scheme. *1* — source of radiation (electric arc), *2* — entrance slit of the spectrometer, *3* — normal line to diffraction grating, *4* — concave diffraction grating, *5* — focusing surface of spectral lines, *6* — CCD-linear array; $\varphi = 3.7°$, $\psi = 9.4°$, $\gamma = 13.62°$.

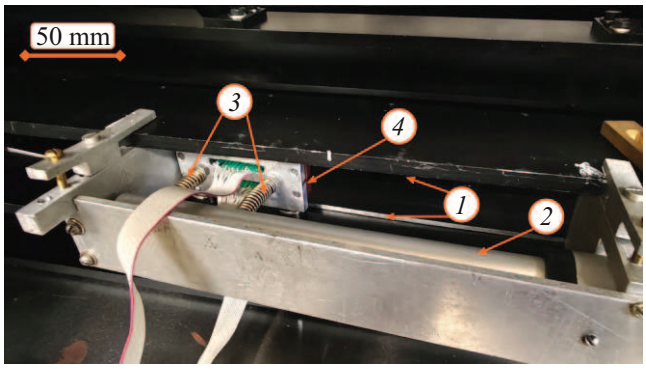


Figure 2. Assembly of CCD-linear array. *1* — guides long Rowland circle, *2* — linear actuator, *3* — clamping springs, *4* — carriage with a CCD-matrix (not seen in the figure). The figure scale is indicated in the left top corner.

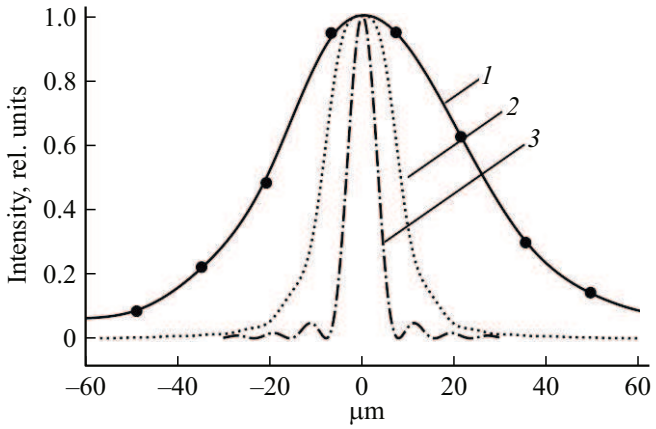


Figure 3. *1* — experimental profile of the spectral line Fe II $3d^64s^5D_{3/2} - 3d^64p^4F_{3/2}$, $\lambda = 2250.175$ Å, *2* — numerical model of instrumental function, *3* — contribution to instrumental function from diffraction at grating aperture.

of 6 A was used as a radiation source. The electrodes were water-cooled and purged with an argon flow at a pressure of 1 bar. The exposure time of the CCD-linear array was 3 s.

Fig. 3 presents a profile of the spectral line Fe II $3d^64s^5D_{3/2}-3d^64p^4F_{3/2}$, $\lambda = 2250.175$ Å [4] together with the contribution from diffraction on the grating aperture [5] and the result of spectrometer instrumental function modeling using Zemax software. You can see that the spectrometer resolution enables to study the spectral profile of the lines of the applied arc, and the main contribution to its width is made by pressure broadening [6,7].

The dependence of the average width of spectral lines $FWHM$ on the value of the entrance slit width was obtained. The results are shown in Fig. 4, *a*. Each experimental point on the graph is averaged over 10 spectral lines selected uniformly over the entire obtained spectrum. The results of calculating the instrumental width of spectral lines obtained using the Zemax software, which characterize the real capabilities of the spectrometer, are also given here.

The second series of test measurements was the study of the dependence of the recorded line widths on the grating aperture size. The results are shown in Fig. 4, *b*. Here you can see the increase in the width of the lines, when the working size of the grating is limited below 100 mm. It is related to the increase in the diffraction contribution, which is illustrated by the calculation using Zemax software. Some non-monotonicity of the experimental points can be attributed to the instability of the arc discharge conditions.

Cross-linking of adjacent spectral segments

As a rule, CCD-matrices and linear arrays are small in size. For example, the linear array used in this case is capable of covering a spectral segment of 28 mm. The actual size of spectrograms obtained in spectral systems similar to the one described is several tens of cm. Consequently, as already noted, it becomes necessary to scan the spectrum by moving the CCD-linear array tangentially to the Rowland

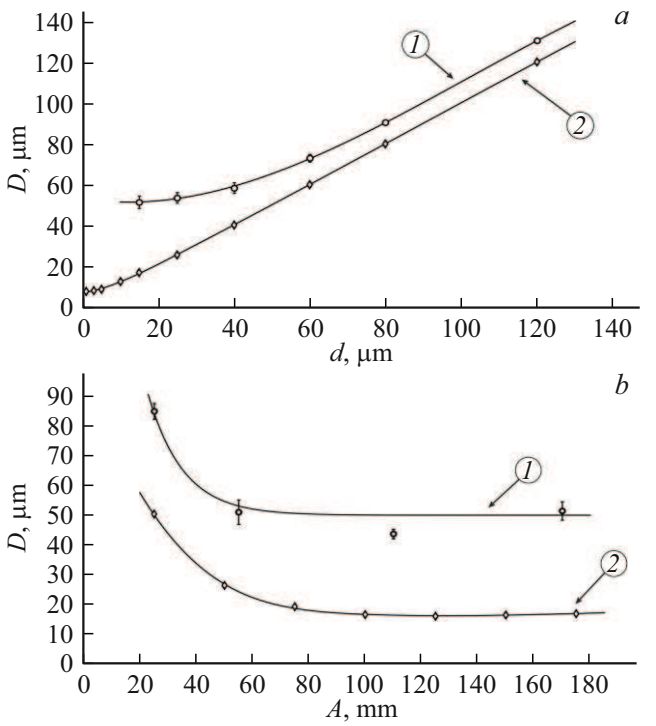


Figure 4. (*a*) Dependence of the widths of spectral lines on the entrance slit width. *1* — experimental data (error at the level of 3σ), *2* — result of computer modeling using Zemax software. D — width of observed spectral lines (μm), d — width of spectrometer entrance slit (μm). (*b*) Dependence of width of spectral lines on width of working area of concave diffraction grating. *1* — experimental data. Each point is averaged by 12 measurements, error at the level 3σ, *2* is the result of computer modeling using Zemax software. D — width of observed spectral lines (μm), A — width of working area of diffraction grating (mm). The width of the spectrometer entrance slit in this series of experiments is $d = 15\,\mu$m.

circle. In this case, the complete spectrogram is composed of individual fragments that must be „cross-linked“ together in wavelengths. In principle, such a problem can be solved using a precision positioning system for the carriage with the CCD-linear array. This paper uses a method for cross-linking individual spectral segments based on the analysis of the correlation function of overlapping parts. The experimental spectrogram is interpolated with splines, and then the correlation function Γ for the overlap of spectrograms $S_i(x)$ and $S_{i+1}(x)$ is numerically constructed:

$$\Gamma_{i,i+1}(\Delta x) = \int S_i(x) S_{i+1}(x + \Delta x) dx. \qquad (1)$$

The procedure of cross-linking 5 spectrograms was conducted: Fig. 5 shows the overlapping area of the first and second spectrograms, and Fig. 6 provides the corresponding correlation function normalized to maximum.

The position $\Delta x_{\max}$ determines the value of relative shift of neighboring spectrograms, which makes it possible to establish the single coordinate scale for all received spectrograms. To evaluate the accuracy of the proposed cross-linking procedure, six independent spectrograms were obtained, each cross-linked of five parts. Mean-square

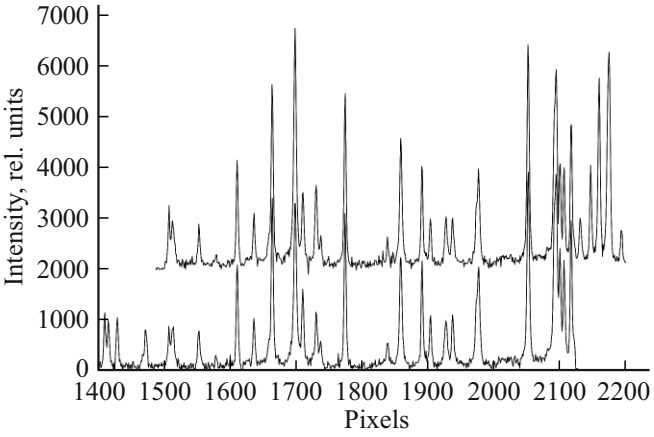


Figure 5. Overlapping area of cross-linked spectrograms.

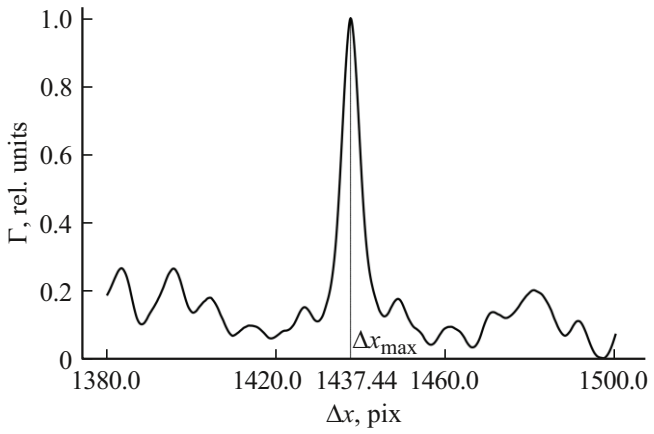


Figure 6. Correlation function of spectrograms cross-linked in Fig. 5.

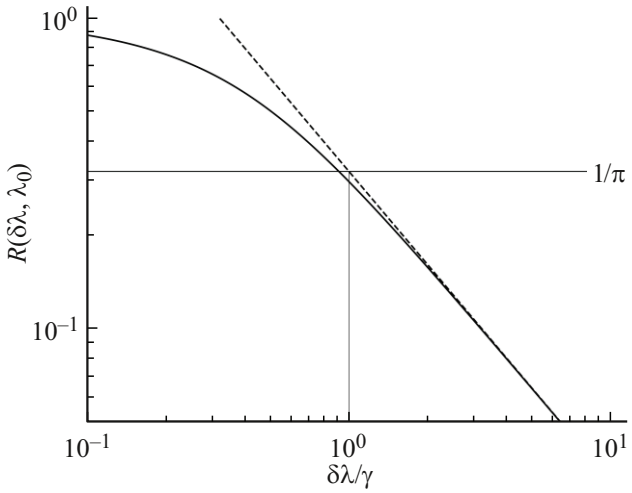


Figure 7. Relative integral intensity in wings of Lorentzian profile.

error of the difference in the positions of the shortest and longest wavelength lines, the distance between which was 120.1 mm, turned out to be equal to 1.2 μm. The full spectrogram was calibrated by wavelengths according to data [4], the calibration accuracy was 0.01 Å in the range of 2130–2270 Å.

Extraction of the Lorentzian contribution to the spectral profile of an individual line

The profile of a spectral line registered by any spectral system is determined by several contributions. In addition to the contribution of the instrumental function, for systems with high spectral resolution, contributions related to broadening in the plasma, as well as the natural width, become significant. All contributions to the broadening of a spectral line can be divided into two groups — contributions with rapidly decaying wings (Doppler, slit instrumental) and contributions with Lorentzian wings (natural, pressure broadening). The paper [8] proposed the idea of extracting the Lorentzian contribution based on measuring the integrated relative intensity of the wings of a spectral line. If the shape of the spectral line $S(\lambda, \lambda_0)$ is Lorentzian with $FWHM = \gamma$ (λ — current wavelength, λ_0 — center of spectral line), the dependence of the relative integral intensity of the wings $R(\delta\lambda)$, defined as

$$R(\delta\lambda, \lambda_0) = \frac{\int_{-\infty}^{\lambda_0 - \delta\lambda} S(\lambda, \lambda_0) d\lambda + \int_{\lambda_0 + \delta\lambda}^{\infty} S(\lambda, \lambda_0) d\lambda}{\int_{-\infty}^{\infty} S(\lambda, \lambda_0) d\lambda}, \qquad (2)$$

has asymptotics

$$R(\delta\lambda, \lambda_0)_{\delta\lambda \to \infty} \to \frac{\gamma}{\pi \delta\lambda},$$

which is easily confirmed by direct calculations, results of which are demonstrated in Fig. 7.

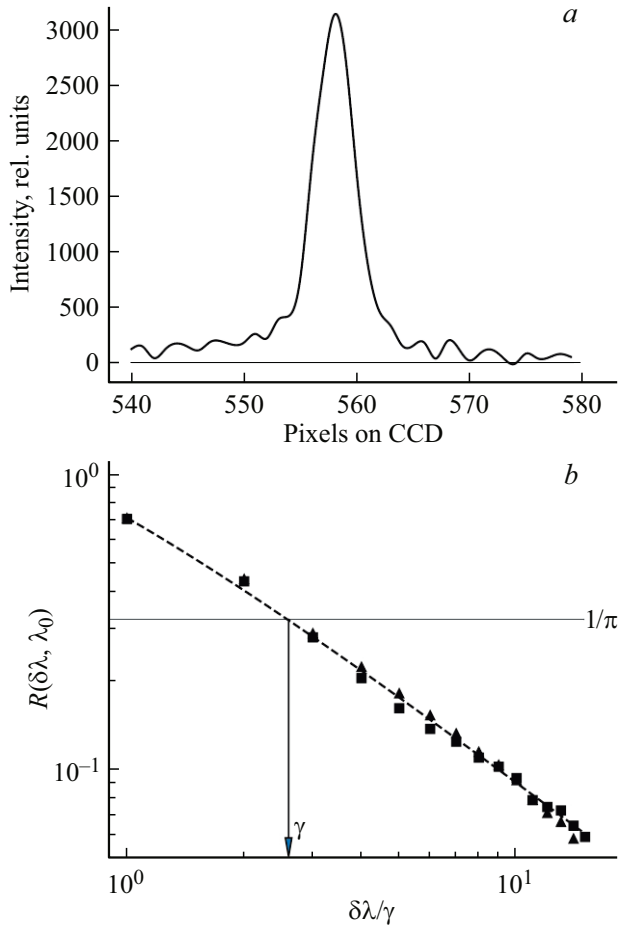


Figure 8. (*a*) Spectral line Fe I $3d^64s^2\,{}^5D-3d^64s4p\,{}^3F^o$ $\lambda = 2132.017$ Å. (*b*) Asymptotics of integral intensity of wings, triangles — right wing, squares — left wing.

In paper [8], it is argued that the asymptotics of the integrated intensity of the wings in a spectral line does not change, if the Lorentzian contour is convolved with any other contour having rapidly decaying wings. This property was applied to analyze the profile of spectral lines obtained using CCD-registration of spectra on the 6.65 meter spectrometer. Fig. 8 shows an example of processing the spectral line Fe I $3d^64s^2\,{}^5D-3d^64s4p\,{}^3F^o$, $\lambda = 2132.017$ Å. The processing algorithm includes taking into account real integration over finite limits, as well as background fitting.

The full width at half maximum of this line is 3.77 pixels ($53\,\mu$m), the measured Lorentzian contribution is 2.63 pixels ($37\,\mu$m). For different lines, the Lorentzian contribution varies within 2–3 pixels. Since the applied arc operates at atmospheric pressure, the main mechanism giving the Lorentzian contribution is pressure broadening [6]. The Doppler contribution is about one pixel. Thus, the contribution of the instrumental function to the observed profile is small compared to the line width, which corresponds to the result shown in Fig. 3.

Conclusion

This paper describes a variant of using a CCD-linear array for recording spectra obtained using the unique 6.65 meter spectrometer. The proposed technique makes it possible to continue studying the spectra of multicharged ions in the VUV range using this spectrometer. One of the problems solved within the framework of this technique is the formation of an overview spectrum using a CCD-linear array, which has a relatively small size (28 mm). In general, to solve this problem, it is necessary to scan the spectrum by mechanically moving the linear array tangentially to the Rowland circle with precision control of its position (with an accuracy of about $1\,\mu$m). In the case of a dense spectrum, it is possible to cross-link the individual spectral segments by analyzing the correlation function of their overlapping regions.

The paper also reports on the possibility of extracting the Lorentzian contribution to the observed profile of a single line by analyzing the intensity distribution in its wings, which makes it possible to study the pressure broadening of spectral lines.

In papers on the study of the energy structure of multicharged ions, an important moment is the use of adequate radiation sources. For example, an arc at atmospheric pressure gives relatively wide lines, which limits the measurement accuracy. A possible radiation source that gives narrow spectral lines in the VUV range could be a plasma-beam discharge [9]. Its use is included in the plans for further works on the unique spectrometer.

Acknowledgments

The authors are deeply grateful to A.N. Ryabtsev and E.Ya. Kononov, whose efforts created the unique complex of 6.65 meter spectrometer, for their support and help in this work.

Funding

This study was carried out under State assignment FFUU-2025-0005.

Conflict of interest

The authors declare that they have no conflict of interest.

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Translated by M.Verenikina