Analysis of deviations in wavelength measurements with a diffraction grating monochromator with respect to a certified reference spectral lamp

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Abstract. This paper shows the analysis of the deviations in the wavelength measurements made with a DK-480 monochromator of diffraction grating respect to the values reported for a certified calibration spectral lamp. The radiation emitted by the calibration lamp was dispersed using diffraction gratings of 300, 1200 and 2400 grooves/mm provided in the monochromator. The emitted spectrum contains neutral Mercury and neutral Argon lines, which was registered with a photomultiplier tube coupled to an amplifier circuit. In this study it was applied the method of least squares to the results of the spectral measurements, and it was obtained for each diffraction grating, the linear model or linear fitting of the comparison with respect to the values of the wavelengths of the reference lamp. With the general model of the propagation of the uncertainty, the uncertainty function was obtained for each diffraction grating, in order to estimate the uncertainty of wavelengths interpolated in each spectral range, which are useful for measuring wavelengths of any other spectral source.

1. Introduction

The study of spectral sources or luminous plasmas, it is fundamentally required a dispersive equipment such as a monochromator, which makes possible the analysis of the light radiation emitted by the plasma [1,2]. A monochromator has an optical configuration that allows focusing in the plane of the narrow output slit, the radiation dispersed by the diffraction grating. In modern monochromators, diffraction gratings are mounted on a mechanical or turret system, controlled by a stepper motor for the selection of wavelengths and scanning of the spectra in the spectral range. The precision in the position of the wavelengths of the spectra depends on several factors, among them: structure and quality of the mechanical system [3], resolving power of the diffraction gratings [4], type of the optical configuration (Littrow, Czerny-Turner, etc.), quality of entrance and exit slits, and detection systems [5]. These factors, as well as others, must be taken into account when making an adjustment or calibration of the system; procedure that must be carried out by an operator with expertise and experience in the management of spectral equipment; in order to obtain spectra of optimum quality for a good measurement of the lines or spectral bands.

Hence, for the use of the monochromator in investigative purposes, it is necessary to make precise measurements of the wavelengths of the spectra; so, to carry out periodic adjustments of some components of the equipment in order to have it spectrally calibrated. These adjustments for spectral calibration commonly include the careful manual repositioning of some of the optical components: mirrors, lenses or diffraction gratings [4,6]. For modern monochromators that come equipped with
management software, once the manual repositioning has been performed, the adjustment can be validated by making a calibration of the system through the appropriate selection of some parameters required by the software.

In this paper, we report the statistical analysis of the differences in measurements made with wavelengths DK-480 monochromator. The method consisted of comparing the measured values of the wavelengths (for each diffraction grating) with those respective values of wavelengths reported by the manufacturer of the certified calibration lamp. The experimental results obtained were used to apply statistical methods and then to find the parameters and statistical functions of correlation between the wavelengths measured with the equipment and the reference wavelength. In the spectral adjustment of the monochromator, atomic lines of Hg I and Ar I were used from the calibrated lamp of Hg/Ar. Around ten spectral lines were included in the application of the statistical method of least squares and the general model of the propagation of uncertainty [7]. This last result allowed estimate the parameters of linear adjustment and the functions of uncertainty, which are useful to estimate values of wavelengths interpolated or measured with the diffraction gratings of 300, 1200 and 2400 grooves/mm provided in the monochromator.

2. Description and experimental assembly

In this section, we reveal the spectral equipment used in this work, an optical monochromator (Model DK 480, Spectral Products, USA), dispersive assembly type Czerny-Turner whose scheme is shown in Figure 1. The monochromator is equipped with diffraction gratings of 300 grooves/mm, 1200 grooves/mm, and 2400 grooves/mm and with detection system by photomultiplier [8]. The radiation coming from the light source (L) penetrates through the narrow entrance slit S$_1$, it is reflected by the plane mirror R$_1$ towards the concave spherical mirror M$_1$ which reflects it and illuminates the diffraction grating G. The grating disperses the radiation in its different wavelengths at different angles towards a second concave spherical mirror M$_2$ reflecting the wavelengths to the plane mirror R$_2$. This mirror reflects the wavelengths to the plane of the exit slit S$_2$ where the detector P is placed. When the diffraction gratings mounted on the turret are rotated by a stepper motor, the spectrum is scanned on the plane of the narrow exit slit and registered by the photomultiplier connected to the computer through an interface.

Furthermore, the photomultiplier tube is coupled to a data acquisition system, constituted by a controller-amplifier circuit (Model AD111, Spectral Products, USA), which allows the control of the operating parameters, both of the photomultiplier and the monochromator. The control software installed on the computer runs on the LabVIEW platform (National Instruments NI visual programming language), functioning as an interface between the monochromator and the photomultiplier, allowing communication between them through the DKDemoLabVIEW2012 program. The default main panel of the AD111/CM/DK executable program displays a window to select the different operating parameters of the monochromator (diffraction grating selection, spectral range, width of the input and output slits, grating scanning speed, etc.); and, the operating parameters of the detector (high voltage values, amplification factor, exposure time, etc.) [9].

Figure 2 it shows the experimental assembly used to obtain spectra of the spectral calibration lamp. The reference spectral source (Model HG-1, Ocean Optics, the USA), is a low-pressure lamp that emits spectral lines of excited neutral mercury (Hg I) and spectral lines of excited neutral argon (Ar I). The radiation emitted by the lamp was focused on the entrance slit with a quartz lens of 20 cm focal length. The radiation inside the monochromator follows the trajectory according to the Czerny-Turner assembly indicated in Figure 1. The scattered radiation reaches the exit slit of the monochromator where the photomultiplier is coupled. The AD 111 unit receives the signal from the photomultiplier whose data is processed through the computer to obtain the intensity spectra as a function of the wavelength.

Figure 3(a) and Figure 3(b) shows the spectra obtained with the diffraction gratings: a) grating of 300 grooves/mm and b) 2400 grooves/mm. The spectral lines observed with the grating of 2400 grooves/mm have better resolution and their measurement is closer to the reference value.
Figure 1. The Czerny-Turner optical assembly diagram of the DK 480 monochromator.

Figure 2. The experimental assembly diagram for the acquisition of spectra of the Hg-Ar calibration lamp, together with the DK 480 monochromator, the AD111 Module and the photomultiplier.

Figure 3. Spectra of the calibration lamp Hg-Ar. (a) With a grating of 300 grooves/mm and (b) With a grating of 2400 grooves/mm.

3. Statistical processing data
On the other hand, the spectra for statistical analysis measured with the DK 480 monochromator cover a range of 250-900 nm with narrow profile lines. The lines measured with the three diffraction gratings, selected for their intensity and well-defined profiles, they are shown in Table 1. The Table 1 compares the spectral lines measured with each diffraction grating and those reported by the lamp manufacturer [10].

In other words, applying the statistical method of least squares calculations of the reference values of the wavelengths compared with the values of the wavelengths, measured with each diffraction grating, the linear adjustment was obtained for each diffraction grating [11]. Equation (1), Equation (2) and Equation (3) correspond to the linear adjustment functions for the diffraction gratings of 300 grooves/mm, 1200 grooves/mm, and 2400 grooves/mm respectively.

$$\lambda_{\text{est}}(\lambda_m) = (1.0027 \pm 0.0022) \cdot \lambda_m + (0.2969 \pm 0.9959) \, [\text{nm}]$$

(1)
\[
\lambda_{\text{est}}(\lambda_m) = (1.0029 \pm 0.0013) \cdot \lambda_m + (-0.6720 \pm 0.6130) \text{ [nm]} \tag{2}
\]
\[
\lambda_{\text{est}}(\lambda_m) = (0.99970 \pm 0.00026) \cdot \lambda_m + (0.38389 \pm 0.11014) \text{ [nm]} \tag{3}
\]

Table 1. Wavelength reference and measures with the diffraction gratings of 300 grooves/mm, 1200 grooves/mm, and 2400 grooves/mm.

| Wavelength reference lamp | Grating 300 grooves/mm | Grating 1200 grooves/mm | Grating 2400 grooves/mm |
|---------------------------|-------------------------|-------------------------|-------------------------|
| Hg I                      |                         |                         |                         |
| 253.652                   | 252.71                  | 252.91                  | 253.51                  |
| 296.728                   | 295.31                  | 296.52                  | 296.30                  |
| 302.150                   | -                       | 301.70                  | 301.82                  |
| 313.155                   | -                       | 312.51                  | 312.90                  |
| 334.148                   | -                       | -                       | -                       |
| 365.015                   | 363.01                  | 364.51                  | 364.74                  |
| 404.656                   | 403.32                  | 404.51                  | 404.25                  |
| 407.783                   | 406.61                  | 407.64                  | 407.52                  |
| 435.833                   | 435.15                  | 435.43                  | 435.66                  |
| 546.074                   | 544.32                  | 545.61                  | 545.79                  |
| 576.960                   | 577.14                  | 576.73                  | 576.80                  |
| 579.066                   | 759.73                  | 578.83                  | 578.90                  |
| Ar I                      |                         |                         |                         |
| 696.543                   | -                       | -                       | -                       |
| 738.393                   | -                       | -                       | -                       |
| 750.387                   | -                       | -                       | -                       |
| 763.511                   | 759.73                  | 760.54                  | -                       |
| 772.376                   | -                       | -                       | -                       |
| 800.616                   | -                       | -                       | -                       |
| 811.531                   | -                       | -                       | -                       |
| 842.465                   | -                       | -                       | -                       |
| 912.297                   | -                       | -                       | -                       |

3.1 Uncertainty for interpolated wavelengths

The general model of the propagation of uncertainty is given by the following Equation (4),

\[
u^2(y) = \sum \left( \frac{\partial y}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum \sum \left( \frac{\partial y}{\partial x_i} \right) \left( \frac{\partial y}{\partial x_j} \right) u(x_i, x_j) \tag{4}\]

This expression allows estimating the uncertainty \(u(y)\) associated with the parameters \(b_0\) and \(b_1\) for a given value of \(x\) in the linear equation \(y = b_1x + b_0\) [12]. By developing this mathematical procedure to the linear models obtained for each diffraction grating, we obtain the functions of uncertainty and the derivative of the uncertainty functions with respect to \(x\); which allow us to determine the wavelength with minimum uncertainty for each of the diffraction gratings. Equation (5), Equation (6) and Equation (7) express the uncertainty functions for the diffraction gratings of 300, 1200 and 2400 grooves/mm respectively.

\[
u^2(y) = 0.99175 \text{ nm}^2 - 4.1107 \cdot 10^{-3} x \text{ nm} + 4.7143 \cdot 10^{-6} x^2 \tag{5}\]
\[ u^2(y) = 0.37575 \text{ nm}^2 - 1.5517 \times 10^{-3} x \text{ nm} + 1.7776 \times 10^{-6} x^2 \]  \hspace{1cm} (6)

\[ u^2(y) = 1.2132 \times 10^{-2} \text{ nm}^2 - 5.5462 \times 10^{-5} x \text{ nm} + 6.8117 \times 10^{-8} x^2 \]  \hspace{1cm} (7)

Figure 4(a), Figure 4(b) and Figure 4(c) shows the graphs of the uncertainty functions for each diffraction grating. Each graph was obtained with the measurements of the wavelengths of the spectrum of the calibration lamp in correlation with their respective uncertainty calculated by the uncertainty function. In the graphs, the wavelength is indicated, with minimum uncertainty.

4. Conclusion
This work describes the statistical analysis of a wavelength shift in measurements with a DK480 monochromator, counting with three diffraction grids, using a certified Hg/Ar calibration lamp as a wavelength’s values reference. Linear fitting and the uncertainty functions were performed for interpolated wavelengths. The uncertainty functions were useful to obtain the uncertainty associated with each diffraction grid.
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