The possibility of direct registration of the optical spectrum derivatives using the acousto-optic spectroscopy methods

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Abstract. Using the example of the spectrometer based on acousto-optical (AO) cell with jump phase manipulation developed at the Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences, the possibility of creating a new class of instruments, i.e. differential AO spectrometers with arbitrary addressing working in real time, is shown. In the paper it is calculated how the error value determining the maximum position changes when the position of the combined peaks changes, as well as the dependence of this error on the peak width and height.

1. Introduction

The main task of spectrometry is to determine the components of the spectrum, in particular the exact position of all spectral lines. The most common case introducing an error in the registration is the situation when a narrower low intensity peak (LIP) is located in the spectrum against the background of wider high intensity peak (HIP). In this case, as shown in figure 1, measuring the spectral position of the maximum LIP occurs with a significant error.

Figure 1. Overlapping LIP (2) and HIP (1).
2. Methods

Let us estimate the value of the possible error $\Delta \lambda$ when measuring the position of the LIP in different situations. When the maximum peaks coincide or when the location of the maximum LIP is on the edge of a large peak, there is no measurement error. However, between these situations, as shown in figure 1, there is an error in measuring the maximum position.

Figure 2 (a) shows measurement errors when recording the spectrum. Figure 2 (b) presents a graph of the dependence of the error in measuring the position of the LIP $\Delta \lambda$ (in relative units) depending on the adjustment of the position of the maximum LIP relative to the maximum HIP $\Delta \lambda_{\text{LIP-HIP}}$ (0 is where the maximums coincide, 1 is where the smaller maximum is going beyond the width of the larger).

**Figure 2.** Dependence of the error in position measuring of the LIP $\Delta \lambda$ (in relative units) on the shift of the maximum LIP position relative to the maximum HIP position.

Also of interest is the dependence of error $\Delta \lambda$ on the width of the LIP. If a smaller peak represents a delta function, there is no error in measuring its position. If the width of a smaller peak coincides with
the width of a larger one, it simply does not stand out as the second maximum and it is senseless to speak about the error of its measurement. Figure 3 (a) shows pictures of three situations where the LIP has a different width and the graph of the error dependence of $\Delta \lambda$ on the ratio of the LIP FWHM $Q_{\text{LIP}}$ to the HIP FWHM $Q_{\text{HIP}}$ at the point of the LIP position corresponding to the maximum error (figure 3 (b)).

To estimate the value of the maximum error $\Delta \lambda$ we will take experimental data. In the visible wavelength range, in the area of green light (532 nm), let's take the HIP with FWHM of about 20 nm. In this case the error reaches 2 nm. Is it big or small?

Figure 4 shows the hardware function of a double acousto-optic monochromator. We can see that when suppressed outside the monochromator’s bandwidth of 50 dB, the FWHM of the main maximum is 2 angstroms, i.e. 0.2 nm. For a reliable distinction between the two peaks close to each other it is necessary that they fall successively into the adjacent main peaks of the monochromator's transmittance function during scanning in the spectrum, when they overlap at $\sqrt{2}$ height. This corresponds to a resolution of 0.2 nm, which is 10 times less than the possible error $\Delta \lambda$. Thus, the study of the possibility to improve the accuracy of determining the actual position of spectral lines in the overlapping spectra is quite relevant.

![Figure 4. Dual acousto-optic monochromator hardware function.](image)

![Figure 5. Result of the overlapping spectral lines differentiation.](image)

Such a problem is solved by differentiation of spectral dependence and LIP position is determined with sufficient accuracy (figure 5). This method is used in molecular spectroscopy and analytical
chemistry to study turbid liquids and complex solutions [1-3]. The procedure consists in measuring the frequency dependence of the spectral density of the sample, then removing the noise component (smoothing) and the subsequent differentiation of the result.

For example, challenges now arise in chemistry, biology and environmental monitoring where real time data on object change is needed to be able to influence the process. In [4, 5] it was shown theoretically that it is possible to record the spectrum of optical radiation and its derivatives during the measurement process. The work is based on acousto-optical (AO) diffraction on the phase lattice created by an acoustic wave with a sharp periodic phase shift.

3. Results and discussion
In the Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences on the basis of collinear AO cell was created a model of the spectrometer, which allows registering derivative optical spectra. As a test experiment, the radiation of a neon lamp with a well-known linear spectrum was recorded. Figure 6 shows one registered line of the spectrum, as well as its first derivative. It can be seen from the graph that the created layout quite effectively registers both the spectrum of the optical signal and its derivative.

![Figure 6. Part of the neon lamp spectrum recorded by the differential AO spectrometer.](image)

![Figure 7. Results of the neon lamp registered spectrum differentiation by the two methods.](image)

It remains to be determined to what extent the derivative measured by the differential AO spectrometer coincides with the mathematical one calculated from the frequency dependence of the
spectral density. Two neon lamp emission peaks were selected; their spectra and derivatives were recorded by the differential AO spectrometer. For the mathematical method, the spectrum was smoothed out and differentiated. Both results of differentiation are shown in figure 7. The differences between the two methods are noticeable: the derivative obtained by the spectrometer is narrowed and additional extrema appear due to the hardware function of the AO monochromator. Consequently, the technique cannot be fully called differential and is not suitable for many spectroscopy tasks. However, at the spectral peaks, i.e. at the intersection areas of zero line derivatives, the results coincide, which allows the use of AO spectroscopy methods to find a derivative of the optical spectrum to reveal their fine structure.

4. Conclusion
Due to the development of digital high-frequency technology the possibilities of synthesis of electrical signals of complex shape and, consequently, the possibility of excitation of acoustic waves of “extraordinary” structure are expanding. The justification of the use of differential spectrometers presented in the article and in the articles [6–7] allows speaking about their application in scientific and practical purposes for the analysis of multicomponent spectra. In this connection prospects of creation of new acousto-optical devices with extended characteristics and new properties are opened.

References
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