Study on the wavelength calibration of type III concave grating spectrometry system

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We discuss and calibrate the spectrometry system based on concave reflection grating. The working principle, structure and parameters of the spectrometry system are introduced. For the wavelength calibration problem, three methods are put forward and discussed in detail with formulation calculation method, circular iteration method and interpolation. Interpolation is used to calibrate the concave reflection grating spectrometry system and the error is less than 1 nm. Four spectrum images that the system collected are given in this paper. The experimental results indicate that a spectrometry system can be based on concave reflection grating and be calibrated by interpolation.

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Spectrometry instrument is important in optical research. Its function is to measure the colors and analyze the spectrum of objects. Because the spectrometry instruments have many advantages, such as high analytical accuracy, large measuring range and high measuring speed, it is applied broadly in many different fields. In recent years, spectrometry instrument becomes more miniature and more intelligent than before. Obviously, these developments make it more convenient.

Traditional spectrometry instruments often use flat gratings as light splitter. When using flat grating, the optical system needs a collimated lens and an imaging lens. In order to form a proper optical path, these two lenses should be separated from the grating in some distance. Therefore, it is difficult in miniaturization. Concave reflection grating is superior to flat grating in that it can not only split the light but also image. So using concave reflection grating simplifies the optical system of the spectrometry instrument[1].

In this paper, the aim is to introduce the working principle of concave reflection grating spectrometry system and give corresponding data of the experiment. A concave reflection grating consists of a flat reflection grating and a concave mirror. Therefore, it has the function of flat reflection grating and the function of concave mirror. Using concave reflection grating can simplify the structure of optical system, so the first important work is to choose a proper concave grating. According to the difference in working condition and record parameters, holographic concave grating can be divided into 4 types. We choose type III concave grating as the light splitter in the spectrometry system because that it has flat spectrum while type I and type II concave gratings have spectra in their Rowland circles. A flat spectrum is easy to be received by a charge coupled device (CCD) or a photodiode array detector, so flat field concave grating will contribute to realize the rapid analyses of spectrum[2].

Optical fiber is used to transfer the light from light source to the object that is to be measured and transfer the reflected light signal to optical system. When receiving the light, the concave reflection grating splits it and produces an image. The flat spectrum image is detected by linear CCD and transformed to electric signal. After being collected and disposed, the electric signal is transferred to the computer by USB line. Working with corresponding software, the result will be obtained. The course is showed in Fig. 1.

The light source is a tungsten bromide lamp, which is a standard light source in color measurement.

An optical fiber is used as the light picker. The advantage of using optical fiber as picker is that there is no demand of measured object. No matter how thick or asymmetric it is, optical fiber picker can measure it easily.

The light splitter is a type III concave reflection grating (Tsinghua University).

We use TOSHIBA TCD1304AP as the detector. This is a 2048-pixel linear CCD, and its response between 400 and 700 nm is no less than 80%, so using TCD1304AP as detector meets the request of visible light measurement.

We use USB communication interface because it has many advantages: the characteristics of plug-and-play and hot attach & detach make it convenient to use; the transport speed already reaches to 480 Mb/s in USB 2.0 edition; a computer can expand to 127 peripheral equipments from its USB port[3].

This spectrometry can be used to measure luminophor's emission spectrometry and the reflectance or the transmittance of noluminophor. The spectrum range is from 380 to 760 nm, the measuring precision is ±1 nm, and the resolution can be chose as 5 or 1 nm.

There are some technical difficulties. First, we must insure that the system can receive enough light energy, especially in measuring the reflectance and transmittance.

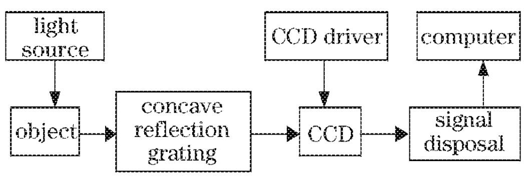

Fig. 1. Working principle of the experimental system of concave reflection grating spectrometry.

Therefore, lens is used to enhance the brightness of light source and the diameter of optical fiber is increased. Second, the design of the light picker is very important. Because we use optical fiber as light picker, its structure should guarantee the incidence angle of reflected light unchangeable. Third, the spectrum response of the system is not uniform. This depends on the spectrum characteristic of each part of the system, such as light source, concave grating and CCD detector. Combining all these effects in system, the response of short wave is below the demand. In order to solve this problem we use light color filter to enhance the blue light's intensity and restrain the response of red light.

The system can be used after calibration. The choice of calibration method is a very important task, because the wavelength calibration accuracy affects the experimental result greatly. The received data are the electrical signal from CCD when light illuminates it. Each electrical signal relates to one pixel of CCD. To calculate the colorimetric parameters, we must know the relationship between the CCD pixel and the wavelength, which is named wavelength calibration.

In flat grating, angular dispersion rate formula can be deduced from grating equation

$$\frac{\mathrm{d}\theta}{\mathrm{d}\lambda} = \frac{m}{\mathrm{d}\cos\theta}. \quad (1)$$

In the range near the normal line of the grating, the diffraction angle θ is small. The value of $\cos\theta$ hardly changes when θ alters. That is to say, θ and λ can be considered to be with a linear relationship. Accordingly, the location of the spectrum is easy to calculate through their linear relation. Of course this method is very simple, and it is not enough in precise measurement.

Regarding of the nonlinear and the asymmetric of the linear dispersion distance, circular iteration method also can be used to calculate the wavelength location. From Eq. (1), we may infer that

$$\frac{\mathrm{d}s}{\mathrm{d}\lambda} = f\cdot\frac{\mathrm{d}\theta}{\mathrm{d}\lambda} = \frac{fm}{\mathrm{d}\cos\theta}. \quad (2)$$

When the interval $\Delta\lambda$ between wavelengths is little, the corresponding linear dispersion distance Δs is also very little, thus Eq. (2) can be changed to

$$\frac{\Delta s}{\Delta\lambda} = \frac{fm}{\mathrm{d}\cos\theta}, \quad (3)$$

so,

$$\Delta s = \frac{fm}{\mathrm{d}\cos\theta}\cdot\Delta\lambda. \quad (4)$$

In Eq. (4) the expression of θ is

$$\theta = \arcsin\left(\frac{m\lambda}{d} - \sin i\right). \quad (5)$$

Therefore, when the incident angle i and the focal length f of the imaging lens are known, we can know the location of the CCD pixel corresponding to each wavelength, which is calculated from the formula above by measuring the position s_0 of a standard spectral line λ_0 and choosing proper value of $\Delta\lambda$ that meets the accuracy demand such as 1, 2 or 5 nm[4]. Using this method, the system structure must be very precise, so that even a small change of it will alter the result of the wavelength measurement. Surely, this strict demand is not adapted to use. Except that, because our experiment system of spectrometry uses concave reflection grating as its light splitter, the situation is even more complex than the spectrometry instrument based on the flat grating. Common grating equation is not suitable to evaluate a concave reflection grating.

Interpolation method is often used in calibrating. The process of this method is to measure several given wavelength spectral lines, find their locations in CCD pixels and build the interpolation function to calculate the locations of every wavelength. When using interpolation to calibrate, there is no need to know the relationship between the concave reflection grating and the spectrum that it spited. The demand of the system structure is not very strict. Therefore, interpolation is a good choice to calibrate the concave reflection grating spectrometry system. (λ_i, x_i) (i= $0 - n$) is used as an interpolation point, then the wavelength function $x(\lambda)$ can be built from Lagrange interpolation formula

$$x(\lambda) = \sum_{i=0}^{n} x_i \cdot \frac{(\lambda-\lambda_0)\ldots(\lambda-\lambda_{i-1})(\lambda-\lambda_{i+1})\ldots(\lambda-\lambda_n)}{(\lambda_i-\lambda_0)\ldots(\lambda_i-\lambda_{i-1})(\lambda_i-\lambda_{i+1})\ldots(\lambda_i-\lambda_n)}. \quad (6)$$

Based on Eq. (6), it is easy to locate every wavelength between $\lambda_0 - \lambda_n$ in the CCD pixels[5].

In order to make the measurement result more accurate, we ought to choose aware wavelength spectral lines as many as possible and these spectral lines should be in a broad range[6]. In this paper, standard spectral lines are selected from Hg lamp and semiconductor laser. Hg lamp has many spectral lines in visible light range, six of which are selected to calibrate, they are 365.0, 404.7, 435.8, 546.1, 577.0, and 727.0 nm. Considering that there is no calibration point near 600 nm, the semiconductor laser whose wavelength is known as 650.0 nm is added. The seven spectral lines mentioned above span in a broad range.

The interpolation method is used to calibrate the experiment system of concave reflection grating spectrometry and then check it.

The Hg lamp is tested. Because its 365.0-, 404.7-, 435.8-, 546.1-, 577.0-, and 727.0-nm spectral lines are used to calibrate, we should test the locations of other spectral lines. In this experiment, two of them are selected, one is the spectral line of 579.0 nm, the other is 519.6 nm. The 519.6-nm spectral line is not recorded in Hg lamp spectral lines list, we measure it by spectrometric instrument FMC-9204.

The spectral lines of the Na lamp are suitable to measure. Na lamp has two standard spectral lines 568.3 and 589.3 nm. Photodiode is also used in the experiment to test the spectrometry system. It emits 465.0-nm (blue) light.

Spectral lines images of Hg lamp, semiconductor laser, Na lamp and photodiode are shown in Figs. 2 – 5.

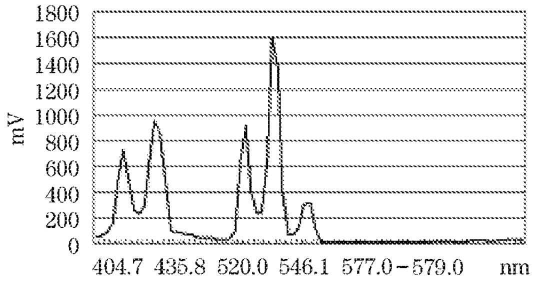

Fig. 2. Hg lamp spectral lines.

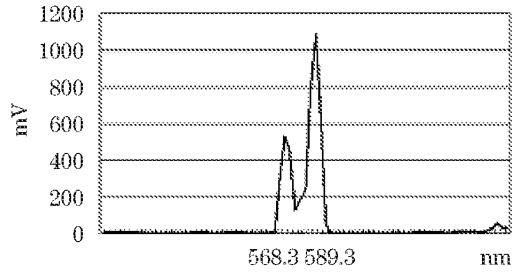

Fig. 4. Na lamp spectral lines.

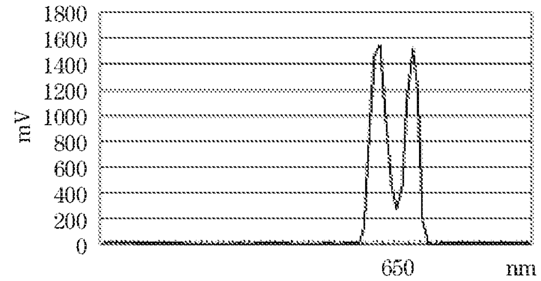

Fig. 3. Semiconductor laser spectral lines.

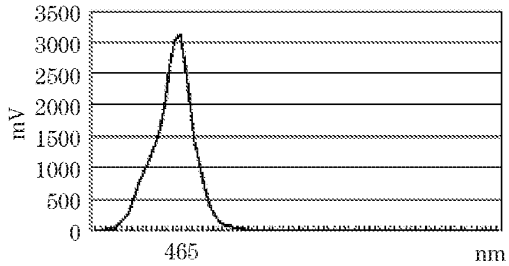

Fig. 5. Photodiode spectral lines.

Table 1. Experimental Wavelength Data (Unit: nm)

Standard	First Measurement	Second Measurement	Third Measurement	Average	Absolute Error
465.0	465.0	465.0	466.0	465.3	0.3
519.6	520.0	520.0	520.0	520.0	0.4
568.3	568.0	567.0	568.0	567.7	0.6
579.0	580.0	580.0	579.0	579.7	0.7
589.3	589.0	590.0	590.0	589.7	0.4

Every peak value in these figures can be found from their X-coordinates except Fig. 3. In Fig. 3, the marker of 650 nm represents the value of the valley that between two peaks because this is a two-line semiconductor laser.

Experimental records are listed in Table 1. Each tested wavelength was measured for three times. The average value and the absolute error of the experiment are also given in Table 1.

Table 1 indicates that the maximum absolute error is 0.7 nm. Considering the fact that the resolution of another spectrometry instrument EPP2000 is 0.5 nm and the calibration error is 1 nm, it is feasible to use concave reflecting grating as light splitter and the interpolation can be used to calibrate concave reflecting grating spectrometry system. In addition, because the accuracy of the signal collection in the software is 1 nm, that is to say, the interval of sampling point is 1 nm, this sampling accuracy affects the accuracy of the system in some degree. Increasing the number of sampling points in the software and selecting more known spectral lines in calibration may improve the accuracy of the concave reflection grating spectrometry system.

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